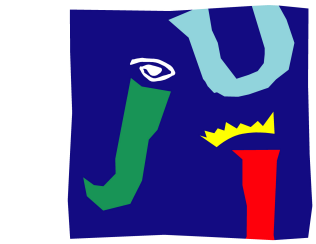

UNIVERSITAT JAUME·I

Programa de doctorado en Ciencias

Escuela de Doctorado de la Universitat Jaume I

Métodos de escisión y composición para ecuaciones diferenciales y aplicaciones

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Memoria presentada por Alejandro Escorihuela-Tomàs para optar al grado de doctor por la Universitat Jaume I.

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A Arnau, a Marçal i a Sara.

Si tens un fill, ensenya'l a ser lliure.
Encara que siga a costa teua.

En realitat, haurà de ser a costa teua...

Joan Fuster i Ortells.

Perquè hi haurà un dia que no podrem més
i llavors ho podrem tot.

Vicent Andrés Estellés.

Tu destino está en los demás
tu futuro es tu propia vida
tu dignidad es la de todos.

Palabras para Julia
José Agustín Goytisolo.

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Estructura y publicaciones

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  Applied Mathematics and Computation, 414 (2022), p. 126700.

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Esta tesis dispone de la aceptación de los coautores de las publicaciones que el doctorando presenta como tesis y su renuncia expresa a presentarlas como parte de otra tesis doctoral (ver apéndice C).

Índice general

Capítulo 1

Introducción

1.1. Tratamiento numérico de ecuaciones diferenciales

Las ecuaciones diferenciales fueron propuestas por primera vez a finales del siglo XVII por Newton y Leibniz, de diferentes formas pero para un mismo propósito: modelar las leyes básicas de la Mecánica. El símbolo de la integral fue escrito por primera vez en 1675 por Leibniz en la ecuación $\int x dx = \frac{1}{2}x^2$ [71]. Pero años antes, aunque publicado en 1736, Newton clasificó las ecuaciones diferenciales en tres tipos:

- Primer tipo: $\dfrac{dy}{dx} = f(x)$, $\dfrac{dy}{dx} = f(y)$,
- Segundo tipo: $\dfrac{dy}{dx} = f(x, y)$,
- Tercer tipo: $x\dfrac{\partial u}{\partial x} + y\dfrac{\partial u}{\partial y} = u$.

No las escribió de esta forma; es más, tampoco las llamó ecuaciones diferenciales, sino que, utilizó las palabras *fluente* y *fluxión*. Un fluente era la cantidad x y fluxión la velocidad de este fluente, $\dot{x}$, es decir, la derivada respecto del tiempo. Así, Newton escribió $\frac{\dot{y}}{\dot{x}} = f(x, y)$ para el segundo tipo.

De estos tres tipos que planteó Newton, los dos primeros corresponden a ecuaciones diferenciales ordinarias (EDOs) y el tercero a un caso particular de ecuación diferencial en derivadas parciales (EDP). Los métodos de integración que abordaremos en este trabajo se restringirán a EDOs, y aunque, en ciertas ocasiones, integremos numéricamente EDPs será siempre discretizando previamente una de las variables para obtener un sistema de EDOs.

Hoy en día, las ecuaciones diferenciales son ampliamente utilizadas en muchos campos científicos, desde la física más elemental hasta las ciencias

sociales, para construir modelos matemáticos que permitan describir adecuadamente los hechos observables. Sucede a menudo que para estas ecuaciones diferenciales no es posible encontrar una solución analítica que pueda expresarse como combinación de funciones elementales, o bien cuando ésta es posible, la solución es costosa de evaluar. Es entonces cuando se hace uso de la integración numérica para encontrar una aproximación a esta solución, y depende del método numérico utilizado lo buena que sea esta aproximación.

Dependiendo del problema a modelizar se utiliza un tipo de tratamiento numérico u otro. Aquí nos centraremos en problemas que se pueden expresar como un *problema de valor inicial*, en el cual se tiene una EDO y un punto de la solución:

$$\dot{x} \equiv \frac{dx}{dt} = f(t, x), \qquad \text{con} \qquad x(t_0) = x_0, \tag{1.1}$$

donde $f : \mathbb{R} \times \mathbb{R}^D \to \mathbb{R}^D$ es una función vectorial que depende de la variable $t \in \mathbb{R}$ y de $x(t) \in \mathbb{R}^D$, siendo $x(t)$ las variables que describen el sistema dinámico en el instante t.

Para utilizar un integrador numérico, primero se fija un tiempo final de integración t_N, luego se discretiza el intervalo $[t_0, t_N]$ en N puntos temporales obteniendo una serie de valores $t_1, t_2, \ldots, t_n, \ldots$ Así, el integrador numérico aproximará la solución en el instante t_n, $x(t_n)$ por el valor x_n. La separación entre dos puntos temporales consecutivos (t_n y t_{n+1}) se llama tamaño de paso, y nosotros nos centraremos en tamaños de paso constantes, así pues:

$$t_{n+1} = t_n + h \qquad\qquad n = 0, 1, \ldots, N-1,$$

siendo h el tamaño de paso. La aproximación x_{n+1} es obtenida usando un integrador χ_h de un paso con la anterior aproximación x_n: $x_{n+1} = \chi_h(x_n)$. Así, el procedimiento para obtener una evolución numérica es: empezar con la solución a tiempo inicial t_0, $x_0 = x(t_0)$; aplicar el integrador para obtener una aproximación al tiempo t_1, $x_1 = \chi_h(x_0)$; aplicar el integrador a x_1 para obtener una aproximación a t_2, $x_2 = \chi_h(x_1)$, etc. Repetiremos este procedimiento hasta el tiempo final t_N, $x_N = \chi_h(x_{N-1}) = \chi_h^N(x_0)$, para así obtener una serie de puntos $x_n, (n = 1, 2, \ldots)$ que aproximan la solución exacta $x(t_n)$. En la mayoría de los casos los métodos numéricos utilizarán diferentes evaluaciones de la función $f(t, x)$ para calcular la aproximación de la solución.

A continuación introduciremos el concepto de flujo, tanto para el caso de la solución exacta como para la aproximación numérica, indicando las propiedades que éste verifica; continuaremos con los integradores numéricos más básicos, y definiremos el adjunto de un método.

El flujo exacto de un sistema en el tiempo t, φ_t, es la función que, al punto x_0 le asocia el valor $x(t)$ de la solución de (1.1)

$$\varphi_t(x_0) = x(t_0 + t) \qquad \text{si} \quad x_0 = x(t_0).$$

Este flujo exacto φ_t constituye un grupo uniparamétrico de transformaciones, cumpliendo las propiedades:

$$\varphi_{t_1} \circ \varphi_{t_2} = \varphi_{t_1+t_2}, \qquad t_1, t_2 \in \mathbb{R} \tag{1.2}$$
$$\varphi_0 = \mathrm{Id}, \tag{1.3}$$

donde Id es el flujo identidad, $\mathrm{Id}(x) = x$ y la propiedad (1.2) se conoce como la composición de flujos. De estas propiedades se puede deducir la siguiente:

$$(\varphi_t)^{-1} = \varphi_{-t}, \tag{1.4}$$

conocida como el inverso de un flujo exacto. En el caso de tener dos sistemas diferentes:

$$\dot{x}^{[A]} = f^{[A]}(t, x),$$
$$\dot{x}^{[B]} = f^{[B]}(t, x),$$

el inverso de una composición cumple:

$$\left(\varphi_{t_1}^{[A]} \circ \varphi_{t_2}^{[B]}\right)^{-1} = \left(\varphi_{t_2}^{[B]}\right)^{-1} \circ \left(\varphi_{t_1}^{[A]}\right)^{-1}. \tag{1.5}$$

Esta propiedad y las anteriores se muestran con más detalle, haciendo uso del formalismo de Lie, en el apéndice A.2.

Un integrador numérico puede expresarse como un flujo, al que llamamos flujo numérico. El flujo numérico asociado a un integrador con tamaño de paso h, χ_h es la función que, al punto x_0 le asocia una aproximación numérica obtenida por el integrador y tiene orden r si verifica:

$$\chi_h(x_0) = \varphi_h(x_0) + \mathcal{O}(h^{r+1}) \qquad \text{si} \quad x_0 = x(t_0),$$

para $h \to 0$. Los flujos numéricos también verifican las propiedades (1.3) y (1.5):

$$\chi_0 = \mathrm{Id},$$
$$(\chi_{h_1} \circ \phi_{h_2})^{-1} = (\phi_{h_2})^{-1} \circ (\chi_{h_1})^{-1}, \tag{1.6}$$

para dos flujos numéricos diferentes χ_h y ϕ_h. El inverso de un flujo $x_{n+1} = \chi_h(x_n)$ corresponde a intercambiar $x_n \leftrightarrow x_{n+1}$.

Una característica de los métodos numéricos es que cuando aproximan la solución de $\dot{x} = f(t, x)$ lo hacen resolviendo exactamente la ecuación diferencial:

$$\dot{\tilde{x}} = f_h(t, \tilde{x}) = f(t, \tilde{x}) + h f_2(t, \tilde{x}) + h^2 f_3(t, \tilde{x}) + \cdots, \tag{1.7}$$

donde f_h es el *campo de vectores modificado* [62]. Al estudio de este campo de vectores modificado se le conoce como *backward error analysis* y al estudio

del error local $(\chi_h(x_0) - \varphi_h(x_0))$ o global $(\chi_h^N(x_0) - \varphi_h^N(x_0))$ de la solucion se le conoce como *forward error analysis*.

El integrador más básico que existe y que suele ser usado a modo de introducción en el tratamiento numérico de las EDO es el método *explícito* de Euler:

$$\chi_h^{\mathrm{EE}}: \quad x_{n+1} = x_n + hf(t_n, x_n). \tag{1.8}$$

A su vez, existe el llamado método *implícito* de Euler:

$$\chi_h^{\mathrm{IE}}: \quad x_{n+1} = x_n + hf(t_{n+1}, x_{n+1}). \tag{1.9}$$

Ambos métodos son de orden uno, es decir aproximan la solución exacta $x(t_1)$ mediante x_1 con un error $\mathcal{O}(h^2)$, y como sólo utilizan una evaluación de la función f se dice que tienen una etapa ($s = 1$). Para la versión implícita necesitaremos resolver un sistema de ecuaciones algebraicas que en general no será lineal, y es que ésta es la característica que define los métodos implícitos. Aunque pueda parecer un inconveniente, en ocasiones esto se contrarresta por el hecho que los métodos implícitos suelen necesitar menos etapas para alcanzar un orden dado y tienen buenas propiedades conservativas. Ahora, a continuación veamos el concepto de adjunto de un método y con él, el de método simétrico–temporal.

Dado un integrador numérico χ_h, el método adjunto, denotado con un asterisco, χ_h^*, es el flujo inverso del método con un tamaño de paso cambiado de signo $-h$:

$$\chi_h^* \equiv \chi_{-h}^{-1}.$$

Se puede visualizar este concepto con el siguiente ejemplo: utilizando el adjunto de un método avanzamos de x_0 a x_1: $x_1 = \chi_h^*(x_0)$, y para volver al punto de partida utilizamos el método con tamaño de paso cambiado de signo: $x_0 = \chi_{-h}(x_1)$. En el caso (b) de la figura 1.1 [62] se observa este comportamiento. Utilizando la propiedad (1.6) para el adjunto de un método se puede obtener:

$$(\chi_{h_1} \circ \phi_{h_2})^* = (\phi_{h_2})^* \circ (\chi_{h_1})^*, \tag{1.10}$$

para dos flujos numéricos diferentes χ_h y ϕ_h. También, es fácil observar que $\chi_h = (\chi_h^*)^*$. A modo de ejemplo podemos ver cómo los métodos de Euler presentados son uno el adjunto del otro, $\chi_h^{\mathrm{IE}} = \left(\chi_h^{\mathrm{EE}}\right)^*$:

$$\begin{aligned}
\chi_h^{\mathrm{EE}}: &\quad x_{n+1} = x_n + hf(t_n, x_n), \\
\left(\chi_h^{\mathrm{EE}}\right)^{-1}: &\quad x_{n+1} = x_n - hf(t_{n+1}, x_{n+1}), \\
\left(\chi_h^{\mathrm{EE}}\right)^* = \left(\chi_{-h}^{\mathrm{EE}}\right)^{-1}: &\quad x_{n+1} = x_n + hf(t_{n+1}, x_{n+1}),
\end{aligned}$$

donde la última expresión corresponde con el método implícito de Euler χ_h^{IE}.

Un flujo numérico χ_h posee simetría temporal (o es simétrico–temporal) si y sólo si verifica:

$$\chi_h = \chi_h^* \qquad \text{o} \qquad \chi_h \circ \chi_{-h} = \text{Id}.$$

En este caso, se puede avanzar desde x_0 a x_1 con $x_1 = \chi_h(x_0)$ y volver a x_0 con el mismo método con el tamaño de paso cambiado de signo $x_0 = \chi_{-h}(x_1)$ tal como se observa en el caso (c) de la figura 1.1. Nótese que, si χ_h es un integrador que posee simetría temporal la propiedad (1.4) también se satisface, $\chi_h^{-1} = (\chi_{-h})^* = \chi_{-h}$, y la propiedad (1.10) se convierte en:

$$(\chi_{h_1} \circ \phi_{h_2})^* = \phi_{h_2} \circ \chi_{h_1}, \tag{1.11}$$

para dos integradores con simetría temporal χ_h y ϕ_h.

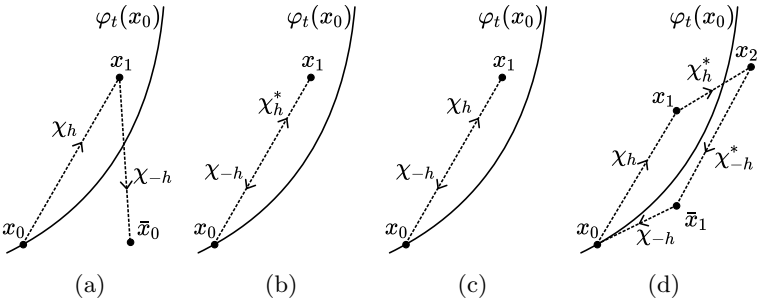

Figura 1.1: Reversibilidad de la evolución numérica. La línea continua representa la solución exacta $\varphi_t(x_0)$. (a) Primer paso con un método χ_h que no tiene simetría temporal, segundo paso con el mismo método con un tamaño de paso $-h$. (b) Primer paso con el adjunto de un método χ_h, segundo paso con el método original con un tamaño de paso $-h$. (c) Primer paso con un método con simetría temporal χ_h, segundo paso con el mismo método con tamaño de paso $-h$. (d) Primer paso con un método sin simetría temporal χ_h, segundo con su adjunto χ_h^*, tercer paso con χ_{h-}^*, y cuarto paso con χ_{-h}.

Obtendremos un integrador simétrico–temporal si intercalamos el uso de un método y su adjunto a cada paso de integración. Podemos visualizar esta evolución en el caso (d) de la figura 1.1. Dicho de otro modo, si componemos un método con su adjunto:

$$\chi_h = \phi_{\frac{h}{2}} \circ \phi^*_{\frac{h}{2}}, \tag{1.12}$$

el resultado será un método simétrico–temporal. Con los métodos de Euler explícito e implícito podemos obtener métodos simétricos temporales con estas dos combinaciones:

$$\chi_h^{\text{T}} = \chi_{\frac{h}{2}}^{\text{IE}} \circ \chi_{\frac{h}{2}}^{\text{EE}}: \qquad x_{n+1} = x_n + \tfrac{h}{2}\left(f(t_{n+1}, x_{n+1}) + f(t_n, x_n)\right),$$
$$\chi_h^{\text{M}} = \chi_{\frac{h}{2}}^{\text{EE}} \circ \chi_{\frac{h}{2}}^{\text{IE}}: \qquad x_{n+1} = x_n + hf\left(t_n + \tfrac{h}{2}, \tfrac{x_{n+1}+x_n}{2}\right).$$

Ambos métodos son de orden 2, al primero se le conoce como la regla del trapecio y al segundo como la regla del punto medio. Obsérvese que, al componer con un método implícito necesariamente se obtiene un esquema implícito.

Una de las familias de métodos más utilizados en la integración numérica de ecuaciones diferenciales es la de los métodos Runge–Kutta (RK) [78] Este tipo de métodos se suelen expresar mediante la siguiente formulación acompañada del tablero de Butcher [30]:

$$\begin{aligned} Y_i &= x_n + h\sum_{j=1}^{s} a_{ij}k_i \\ k_i &= f(t_n + c_i h, Y_i) \\ x_{n+1} &= x_n + h\sum_{i=1}^{s} b_i k_i \end{aligned} \quad , \qquad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

Este corresponde a un método Runge–Kutta de s etapas con coeficientes a_{ij}, b_i y $c_i = \sum_{j=1}^{s} a_{ij}$. Nótese cómo los métodos que posean algún elemento no nulo en la parte triangular superior derecha del tablero de Butcher serán implícitos y aquellos en que estos elementos sean nulos serán explícitos. A modo de ejemplo, mostramos los siguientes tableros de dos métodos RK de orden 4: uno, el famoso método RK4 de 4 etapas (a la izquierda) es explícito, y el otro, el método Gauss–Legendre de 2 etapas (a la derecha) es implícito:

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \qquad \begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

1.2. Integración numérica geométrica

Según McLachlan y Quispel [91], un integrador geométrico sería aquel que preserva alguna propiedad física y/o matemática del sistema que aproxima (hasta error máquina). Es decir, el campo de vectores modificado cumple alguna de las propiedades físicas y/o matemáticas del campo de vectores original. El término fue acuñado por Sanz-Serna en 1997 en su artículo [102].

Los primeros integradores geométricos fueron los integradores simplécticos de sistemas Hamiltonianos [58] y parece correcto establecer su nacimiento en el artículo que no se llegó a publicar de De Vogelaere en 1956 [47, 108]. De Vogelaere diseñó estos integradores especialmente para ser utilizados en la física de los aceleradores de partículas.

Un sistema Hamiltoniano (ver el apéndice A.4) es aquel donde $x = (q, p)^\top \in \mathbb{R}^{2d}$, la dinámica viene definida por la función Hamiltoniana $H(q, p)$

y las ecuaciones del movimiento tienen la forma:

$$\dot{q} = \nabla_p H(q,p), \qquad \dot{p} = -\nabla_q H(q,p). \tag{1.13}$$

La principal característica que diferencia a los integradores simplécticos del resto es que en el caso de un integrador simpléctico el flujo numérico es una transformación simpléctica y por tanto las $f_j(x)$ del campo de vectores modificado (1.7):

$$\dot{\tilde{x}} = f_h(\tilde{x}) = f(\tilde{x}) + hf_2(\tilde{x}) + h^2 f_3(\tilde{x}) + \cdots ,$$

son de la forma $f_j(x) = J\nabla H_j(x)$ [20, 62, 13] siendo J la matriz canónica. Esto no sucede en los integradores que no son simplécticos cuando son aplicados a problemas Hamiltonianos. Entonces, en el caso de un integrador simpléctico existe un Hamiltoniano modificado de la forma:

$$\tilde{H}_h(q,p) = H(q,p) + hH_2(q,p) + h^2 H_3(q,p) + \cdots ,$$

el cual es resuelto de manera exacta por dicho integrador. Esta serie en general no converge, simplemente es asintótica [62].

A los integradores simplécticos se llegó, históricamente, por tres caminos distintos: por un lado a través de las funciones generatrices [50]; por otro, imponiendo a los métodos de Runge-Kutta ciertas condiciones a los coeficientes [79, 103, 111], y por último a través de la idea de escisión y composición [47]. Posteriormente, a principios del siglo XXI Marsden y West [84] propusieron una nueva forma de construir integradores simplécticos a través del principio variacional de Hamilton [58] dando origen a los llamados integradores variacionales.

Los integradores simplécticos basados en funciones generatrices se basan en el formalismo existente en Mecánica Hamiltoniana [58] para construir transformaciones canónicas (simplécticas) mediante unas funciones llamadas funciones generatrices. Éste fue el punto de partida de Feng Kang [50] para construir integradores simplécticos.

En cuanto a los integradores simplécticos basados en métodos RK, fue en el año 1988 cuando, de manera independiente, Lasagni [79], Sanz-Serna [103] y Suris [111] demostraron que todos aquellos métodos RK que cumpliesen:

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0 \quad \forall i,j = 1 \dots s,$$

preservaban invariantes del tipo $I(x) = x^\top C x + d^\top x$, siendo C y d una matriz y un vector, respectivamente. Además, cuando un método RK que cumple esta condición es aplicado a un sistema Hamiltoniano el método en cuestión es simpléctico. Un inconveniente de este tipo de métodos es que necesariamente han de ser implícitos [13]. El método RK de Gauss–Legendre que hemos presentado antes cumple esta condición y tal como hemos visto es implícito.

Para el caso de los métodos de escisión y composición hay que remontarse de nuevo hasta los años 50 del siglo XX, cuando De Vogelaere planteó integradores simplécticos para sistemas Hamiltonianos. Entre otros, propuso el siguiente integrador de primer orden para el sistema (1.13):

$$\begin{aligned} q_{n+1} &= q_n + h\nabla_p H(q_{n+1}, p_n), \\ p_{n+1} &= p_n - h\nabla_q H(q_{n+1}, p_n), \end{aligned}$$

que se trata de una composición de un método de Euler implícito para las q y un Euler explícito para las p. Si el sistema Hamiltoniano es *separable* en dos partes, $H(q,p) = T(p) + V(q)$, siendo T la energía cinética y V la energía potencial, el método se convierte en

$$\begin{aligned} q_{n+1} &= q_n + h\nabla_p T(p_n), \\ p_{n+1} &= p_n - h\nabla_q V(q_{n+1}), \end{aligned}$$

conocido como el método de Euler simpléctico. Este método es explícito para ambas variables. Además, como el sistema es separable, la primera ecuación corresponde con la solución exacta de $\dot{q} = \nabla_p T(p)$ y la segunda a la solución exacta de $\dot{p} = -\nabla_q V(q)$. Así, este método corresponde a resolver primero exactamente una ecuación del sistema separable y luego la otra:

$$\chi_h^{\mathrm{S}} = \varphi_h^{[V]} \circ \varphi_h^{[T]},$$

siendo $\varphi_h^{[V]}$ y $\varphi_h^{[T]}$ las soluciones exactas correspondientes a $H = V$ y $H = T$ respectivamente:

$$\varphi_t^{[V]} : \begin{cases} q(t) = q_0 \\ p(t) = p_0 - t\nabla_q V(q_0) \end{cases}, \qquad \varphi_t^{[T]} : \begin{cases} q(t) = q_0 + t\nabla_p T(p_0) \\ p(t) = p_0 \end{cases}.$$

El método obtenido es el ejemplo más simple de método de escisión, se trata de un método simpléctico de primer orden, pero no simétrico. Podemos utilizar la composición con su adjunto (1.12) y así obtener un método simétrico–temporal:

$$\mathcal{S}_h^{[2]} = \chi_{\frac{h}{2}}^{\mathrm{S}} \circ \chi_{\frac{h}{2}}^{\mathrm{S}*} = \varphi_{\frac{h}{2}}^{[V]} \circ \varphi_h^{[T]} \circ \varphi_{\frac{h}{2}}^{[V]},$$

donde se ha hecho uso de la propiedad (1.2). El método resultante se conoce como método de Störmer-Verlet, método de Strang-Marchuk y *leapfrog* y se trata de un método simétrico–temporal, simpléctico, de orden 2 utilizado ampliamente en diferentes contextos [61, 112, 29]. Nótese cómo hemos utilizado un superíndice entre corchetes para indicar el orden del método. Esta práctica será bastante común en el resto de la tesis para métodos formados por composición de otros métodos.

Casi treinta años después de los integradores planteados por De Vogelaere, en el año 1983 Ruth [101] presenta, entre otros, un método simpléctico de

escisión de orden 3, que para sistemas Hamiltonianos $H(q,p) = T(p) + V(q)$ toma la forma:

$$\begin{aligned}
p^* &= p_n - c_1 h \nabla_q V(q_n),\\
q^* &= q_n + d_1 h \nabla_p T(p^*),\\
p^{**} &= p^* - c_2 h \nabla_q V(q^*),\\
q^{**} &= q^* + d_2 h \nabla_p T(p^{**}),\\
p_{n+1} &= p^{**} - c_3 h \nabla_q V(q^{**}),\\
q_{n+1} &= q^{**} + d_3 h \nabla_p T(p_{n+1}),
\end{aligned}$$

para el paso $(q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$. Aquí hemos utilizado los superíndices con asteriscos para marcar los pasos intermedios. Como cualquier método de escisión, se puede escribir cómo composición de flujos exactos:

$$\mathcal{M}_h^{[3]} = \varphi_{d_3 h}^{[T]} \circ \varphi_{c_3 h}^{[V]} \circ \varphi_{d_2 h}^{[T]} \circ \varphi_{c_2 h}^{[V]} \circ \varphi_{d_1 h}^{[T]} \circ \varphi_{c_1 h}^{[V]}.$$

Ruth muestra este esquema de forma general, planteando las ecuaciones que se deben resolver para que el método sea de orden 3:

$$\begin{aligned}
&c_1 + c_2 + c_3 = 1, && d_1 + d_2 + d_3 = 1,\\
&c_2 d_1 + c_3 (d_1 + d_2) = \tfrac{1}{2}, &&\\
&c_2 d_1^2 + c_3 (d_1 + d_2)^2 = \tfrac{1}{3}, && d_3 + d_2 (c_1 + c_2)^2 + d_1 c_1^2 = \tfrac{1}{3}.
\end{aligned}$$

El sistema está sobredeterminado, pues hay un parámetro libre. Ruth elige $d_3 = 1$ y obtiene los coeficientes:

$$\begin{aligned}
c_1 &= \tfrac{7}{24}, & c_2 &= \tfrac{3}{4}, & c_3 &= -\tfrac{1}{24},\\
d_1 &= \tfrac{2}{3}, & d_2 &= -\tfrac{2}{3}, & d_3 &= 1
\end{aligned}$$

Aunque Ruth no lo hiciese, el valor del parámetro libre (o parámetros) se puede utilizar para optimizar el método, planteando una función objetivo. Por ejemplo, podemos plantear como función objetivo el error en la conservación de la energia, o los términos de error a orden superior, o la 1–norma de los coeficientes, etc.

Si se simetriza el integrador $\mathcal{M}_h^{[3]}$ se obtiene uno de orden 4 simétrico–temporal:

$$\begin{aligned}
\mathcal{M}_h^{[4]} &= \mathcal{M}_{\frac{h}{2}}^{[3]} \circ \mathcal{M}_{\frac{h}{2}}^{[3]*}\\
&= \varphi_{\frac{d_3}{2}h}^{[T]} \circ \varphi_{\frac{c_3}{2}h}^{[V]} \circ \varphi_{\frac{d_2}{2}h}^{[T]} \circ \varphi_{\frac{c_2}{2}h}^{[V]} \circ \varphi_{\frac{d_1}{2}h}^{[T]} \circ \varphi_{c_1 h}^{[V]} \circ \varphi_{\frac{d_1}{2}h}^{[T]} \circ \varphi_{\frac{c_2}{2}h}^{[V]}\\
&\quad \circ \varphi_{\frac{d_2}{2}h}^{[T]} \circ \varphi_{\frac{c_3}{2}h}^{[V]} \circ \varphi_{\frac{d_3}{2}h}^{[T]}.
\end{aligned}$$

Este hecho es explicado por Forest [53], utilizando el formalismo de Lie. En particular, demostró cómo un integrador de orden impar basado en composición al simetrizarlo aumenta un orden. En el mismo artículo, Forest presenta el primer método de orden 6 basado en escisión y muestra cómo no es necesario cumplir todas las condiciones de orden cuando el Hamiltoniano tiene la forma $H = p^2/2 + V(q)$.

Por la misma época, pero de manera separada y en ámbitos distintos Suzuki[113] y Yoshida[121] crean la primera regla para generar métodos de composición de orden arbitrario. Esta famosa técnica para incrementar el orden se suele denominar en la literatura como *triple–jump* o Suzuki–Yoshida y se basa en la composición de esquemas $\mathcal{S}_h^{[2]}$:

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]}, \quad \text{donde } \alpha = \frac{1}{2 - 2^{1/3}} \text{ y } \beta = 1 - 2\alpha, \tag{1.14}$$

para así obtener un método simétrico–temporal de orden cuatro. Se puede volver a aplicar la misma composición para obtener un método de orden seis y, en general, para llegar a un método de orden $2k+2$ partiendo de un método de orden $2k$:

$$\mathcal{S}_h^{[2k+2]} = \mathcal{S}_{\alpha h}^{[2k]} \circ \mathcal{S}_{\beta h}^{[2k]} \circ \mathcal{S}_{\alpha h}^{[2k]}, \quad \text{donde } \alpha = \frac{1}{2 - 2^{1/(2k+1)}} \text{ y } \beta = 1 - 2\alpha.$$

Aunque aumentar el orden implique mayor coste computacional, se espera que éste sea compensado con una mejora en la precisión, pero esto no sucede siempre. Por ejemplo, con la técnica del *triple–jump* un método $\mathcal{S}_h^{[6]}$ puede dar aproximaciones con menor precisión que un método $\mathcal{S}_h^{[4]}$. Esta es la razón por la cual necesitamos técnicas ventajosas si queremos construir métodos de orden alto que presenten mejoras en la precisión.

Aparte del tipo de métodos nombrados anteriormente existen otros que también son integradores geométricos [13], por ejemplo: los integradores en grupos de Lie [72], los métodos variacionales [64, 84], los métodos de preservación de volumen [51], etc.

1.3. Escisión y composición

Los métodos de escisión y composición que hemos presentado tienen la característica básica de que si los métodos base utilizados en la composición son simplécticos el método resultante también lo es. Otra característica es que tanto el método resultante como su adjunto son explícitos si los métodos base involucrados lo son. En general para un método numérico explícito su adjunto es implícito (véase el caso del método de Euler explícito).

Los integradores tratados en esta tesis se utilizarán para problemas autónomos,

$$\dot{x} \equiv \frac{dx}{dt} = f(x), \qquad \text{con} \qquad x(t_0) = x_0. \tag{1.15}$$

Si f depende explícitamente del tiempo, $f = f(t, x)$, será siempre en aquellos problemas donde podamos considerar la variable t cómo una variable más conjuntamente con la ecuación $\dot{t} = 1$ [13]. Para visualizarlo, hagamos $z = (x, t)^\top$ y $f(z) = (f(t, x), 1)^\top$. Entonces, el sistema resultante es:

$$\dot{z} = \begin{pmatrix} \dot{x} \\ \dot{t} \end{pmatrix} = \begin{pmatrix} f(t,x) \\ 1 \end{pmatrix}, \quad \text{con} \quad z(t_0) = \begin{pmatrix} x_0 \\ t_0 \end{pmatrix}.$$

Volvamos al caso autónomo. Para una ecuación diferencial como (1.15) los métodos de escisión se pueden construir cuando la función $f(x)$ se puede descomponer en dos o más partes resolubles exactamente:

$$f(x) = f^{[1]}(x) + f^{[2]}(x) + \cdots + f^{[m]}(x) = \sum_i^m f^{[i]}; \tag{1.16}$$

esto es, a cada parte, $f^{[i]}$, le corresponde una solución exacta obtenida mediante la función $\varphi_t^{[i]}(x_0)$, es decir, el flujo exacto de $f^{[i]}$. Por lo tanto

$$x(t_0 + h) = \varphi_h^{[i]}(x_0),$$

corresponde a la solución a tiempo $t = t_0 + h$ del subproblema

$$\dot{x} = f^{[i]}(x), \quad \text{con} \quad x(t_0) = x_0.$$

Ahora, podemos obtener un integrador para el problema completo mediante la combinación de todos los flujos

$$\chi_h = \varphi_h^{[m]} \circ \cdots \circ \varphi_h^{[2]} \circ \varphi_h^{[1]}. \tag{1.17}$$

Este integrador, conocido como el método de Lie-Trotter, aproxima la solución exacta del problema completo a primer orden y se corresponde con el método simpléctico de Euler χ_h^{S} cuando $m = 2$ en (1.16).

Podemos componer los flujos de forma que el método completo sea palindrómico.

$$\mathcal{S}_h^{[2]} = \varphi_{\frac{h}{2}}^{[1]} \circ \varphi_{\frac{h}{2}}^{[2]} \circ \cdots \circ \varphi_h^{[m]} \circ \cdots \circ \varphi_{\frac{h}{2}}^{[2]} \circ \varphi_{\frac{h}{2}}^{[1]}, \tag{1.18}$$

obteniendo el método de Störmer-Verlet cuando $m = 2$ en (1.16). Este método puede ser escrito como $\mathcal{S}_h = \chi_{\frac{h}{2}}^* \circ \chi_{\frac{h}{2}}$. Nótese, de nuevo, cómo hemos utilizado un superíndice entre corchetes para indicar el orden del método. No debe confundirse con los superíndices de $\varphi_h^{[i]}$ que simplemente indican el flujo exacto correspondiente a la escisión (1.16).

En el caso particular de los métodos construidos por composición, el adjunto del método χ_h tiene la siguiente forma:

$$\chi_h^* \equiv \chi_{-h}^{-1} = \left(\varphi_{-h}^{[m]} \circ \cdots \circ \varphi_{-h}^{[2]} \circ \varphi_{-h}^{[1]}\right)^{-1}$$

$$= \left(\varphi_{-h}^{[1]}\right)^{-1} \circ \left(\varphi_{-h}^{[2]}\right)^{-1} \circ \cdots \circ \left(\varphi_{-h}^{[m]}\right)^{-1}$$
$$= \varphi_h^{[1]} \circ \varphi_h^{[2]} \circ \cdots \circ \varphi_h^{[m]},$$

donde se han usado las propiedades (1.4) y (1.5). También, se puede usar la propiedad (1.11) porque las soluciones exactas poseen simetría temporal.

De ahora en adelante, en esta sección, consideraremos que la función $f(x)$ se puede separar en dos partes exactamente resolubles $f(x) = f^{[A]}(x) + f^{[B]}(x)$. Por tanto el método de Lie-Trotter y su adjunto se reducen a:

$$\chi_h = \varphi_h^{[B]} \circ \varphi_h^{[A]}, \qquad \chi_h^* = \varphi_h^{[A]} \circ \varphi_h^{[B]}, \tag{1.19}$$

y el método de Strang a:

$$\mathcal{S}_h^{[2]} = \varphi_{\frac{h}{2}}^{[A]} \circ \varphi_h^{[B]} \circ \varphi_{\frac{h}{2}}^{[A]}, \tag{1.20}$$

donde el número entre corchetes representa el orden del método. A partir de ahora utilizaremos superíndices con letras mayúsculas para representar los flujos exactos en caso de escisión y dejaremos los superíndices con números solamente para indicar el orden de métodos compuestos

Técnicas ventajosas para incrementar el orden. A continuación enumeramos las tres técnicas que se han utilizado en la presente tesis para construir integradores geométricos eficientes de orden mayor que dos:

- **Métodos de escisión**: Esta técnica está basada en la composición de los flujos $\varphi_h^{[i]}$. En particular, en el caso de escisión en dos partes tenemos:

$$\psi_h = \varphi_{a_{s+1}h}^{[A]} \circ \varphi_{b_{s+1}h}^{[B]} \circ \varphi_{a_s h}^{[A]} \circ \varphi_{b_s h}^{[B]} \circ \cdots \circ \varphi_{a_2 h}^{[A]} \circ \varphi_{b_2 h}^{[B]} \circ \varphi_{a_1 h}^{[A]} \circ \varphi_{b_1 h}^{[B]}.$$

- **Composición de método y su adjunto**: Podemos componer esquemas usando métodos de primer orden χ_h y su adjunto χ_h^*:

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}.$$

- **Composiciones simétricas de métodos simétricos**: Otra técnica muy eficiente es componer métodos de segundo orden con simetría temporal:

$$\mathcal{SS}_h = \mathcal{S}_{\alpha_s h}^{[2]} \circ \mathcal{S}_{\alpha_{s-1}h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_2 h}^{[2]} \circ \mathcal{S}_{\alpha_1 h}^{[2]}.$$

En todos los casos, los coeficientes a_j, b_j y α_j se eligen para que el método completo alcance un cierto orden r.

A lo largo de este trabajo, para obtener nuevos integradores numéricos se ha hecho uso del formalismo de Lie [13, 62]. Empleando este formalismo explicaremos en las siguientes secciones las técnicas de construcción de

integradores. No obstante existen otras técnicas equivalentes, entre ellas destacamos la teoría generalizada de los *rooted trees* utilizada en particular en la teoría de los métodos de Runge–Kutta [97, 62].

Dedicaremos unas secciones a estudiar las tres técnicas nombradas anteriormente y luego, por completitud, comentaremos otras tres importantes técnicas que también son ampliamente utilizadas en la literatura sobre métodos de escisión y composición.

1.3.1. Métodos de escisión

Tal como hemos explicado, los métodos de escisión se pueden construir cuando la función $f(x)$ puede separarse en dos o más partes, de manera que el subproblema asociado a cada parte sea resoluble explícitamente. En este apartado trataremos la construcción de métodos de escisión cuando $f(x) = f^{[A]}(x) + f^{[B]}(x)$. Dichos esquemes tienen la forma:

$$\psi_h = \varphi^{[B]}_{b_{s+1}h} \circ \varphi^{[A]}_{a_s h} \circ \varphi^{[B]}_{b_s h} \circ \cdots \circ \varphi^{[A]}_{a_2 h} \circ \varphi^{[B]}_{b_2 h} \circ \varphi^{[A]}_{a_1 h} \circ \varphi^{[B]}_{b_1 h}. \tag{1.21}$$

Nótese cómo, para construir el esquema se ha utilizado la propiedad FSAL (First Same As Last): el primer y el último flujo corresponden a la misma parte de la escisión. Así, de una aplicación del método a la siguiente ambos flujos se pueden computar al mismo tiempo haciendo uso de la propiedad (1.2), en este caso $\varphi^{[B]}_{b_{s+1}h} \circ \varphi^{[B]}_{b_1 h} = \varphi^{[B]}_{(b_{s+1}+b_1)h}$.

A cada flujo exacto $\varphi^{[i]}_h, (i = A, B)$ se le asocia una transformación de Lie [13] (ver apéndice A.2 para más detalles):

$$\varphi^{[A]}_h \equiv e^{hA}, \qquad\qquad \varphi^{[B]}_h \equiv e^{hB},$$

siendo A y B las derivadas de Lie correspondientes a $f^{[A]}$ y a $f^{[B]}$ respectivamente:

$$A \equiv L_{f^{[A]}} = \sum_{i=1}^{d} f_i^{[A]} \frac{\partial}{\partial x_i}, \qquad\qquad B \equiv L_{f^{[B]}} = \sum_{i=1}^{d} f_i^{[B]} \frac{\partial}{\partial x_i}.$$

Por tanto, un esquema como (1.21) puede asociarse a una composición de transformaciones de Lie:

$$\Psi(h) = e^{Z(h)} = e^{b_1 hB} e^{a_1 hA} e^{b_2 hB} e^{a_2 hA} \cdots e^{b_s hB} e^{a_s hA} e^{b_{s+1} hB}, \tag{1.22}$$

de manera que $\Psi(h)$ es el operador diferencial a ψ_h y $Z(h)$ puede interpretarse como el operador asociado al campo de vectores modificado. Se observa que las transformaciones de Lie aparecen con una ordenación opuesta a los flujos en ψ_h (ver apéndice A.2).

La ventaja de utilizar exponenciales de operadores para representar el método es que se puede aplicar recursivamente la fórmula de Baker–Campbell–Hausdorff (BCH) [119]

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,A,B]-\frac{1}{12}[B,A,B]+\ldots},$$

donde $[A,B] = AB - BA$ es el conmutador y aquellos de más de dos elementos se entienden anidados a la derecha $[A,A,B] \equiv [A,[A,B]]$ (ver apéndice A.1.1). Con la aplicación recursiva de la fórmula BCH se puede obtener una expresión de $Z(h) = \log(\Psi(h))$:

$$\begin{aligned} Z(h) = h\omega_{1,1}A + h\omega_{1,2}B + h^2\omega_{2,1}[A,B] + h^3\omega_{3,1}[A,A,B] \\ + h^3\omega_{3,2}[B,A,B] + \mathcal{O}(h^4), \end{aligned}$$

donde $\omega_{i,j}$ son polinomios de los coeficientes a_i y b_i. Los operadores A y B generan un álgebra de Lie que llamamos $\mathcal{L}(A,B)$ y el operador $Z(h)$ pertenece a ella. La base que utilizamos para esta álgebra tiene los conmutadores anidados a la derecha y sus primeros elementos son:

$$\begin{array}{lll} N_{11} = A; & N_{12} = B; & N_{21} = [A,B]; \\ N_{31} = [A,A,B]; & N_{32} = [B,A,B]; & \\ N_{41} = [A,A,A,B]; & N_{42} = [B,A,A,B]; & N_{43} = [B,B,B,A]. \end{array}$$

Además,

$$\mathcal{L}(A,B) = \bigoplus_{i\geq 1}^{\infty} \mathcal{L}^i(A,B),$$

siendo $\mathcal{L}^i(A,B)$ la componente homogénea de grado i, compuesta por todas las combinaciones lineales de conmutadores formados por i operadores A, B. La dimensión de $\mathcal{L}^i(A,B)$ viene determinada por la formula de Witt [90]:

$$n(i) = \frac{1}{i}\sum_{d|i} \mu(d)\nu^{\frac{i}{d}}, \tag{1.23}$$

donde el sumatorio es sobre todos los enteros d que dividen a i, ν es el número de elementos generadores del álgebra, en este caso 2, y la función μ es la función de Möbius, donde $\mu(1) = 1$, $\mu(d) = (-1)^q$ si d es el producto de q factores primos distintos y $\mu(d) = 0$ en cualquier otro caso. Para esta álgebra los primeros valores de las dimensiones de las subálgebras son $n(i) = 2, 1, 2, 3, 6, 9, 18, \ldots$.

El operador $Z(h)$ puede ser expresado mediante combinación lineal de los elementos de la base:

$$Z(h) = \sum_{i\geq 1} h^i \sum_{j=1}^{n(i)} \omega_{i,j} N_{i,j}.$$

Si logramos que el operador $Z(h)$ sea igual hasta cierto orden, digamos r, al operador asociado al campo de vectores de la solución exacta, $X(h) = hA + hB$, es decir que $Z(h)$ sea

$$Z(h) = hA + hB + \mathcal{O}(h^{r+1}),$$

entonces, el operador $\Psi(h) = e^{Z(h)}$ será el asociado a un integrador de orden r. Para realizar esta tarea deberemos resolver las ecuaciones:

$$\omega_{1,1} = \omega_{1,2} = 1, \qquad \omega_{i,j} = 0 \qquad \text{siendo } 1 < i \leq r,\ j \leq n(i),$$

conocidas como condiciones de orden, cuya forma a primeros órdenes es [20, 13]:

$$\omega_{1,1} = \sum_{i=1}^{s} a_i, \qquad \omega_{1,2} = \sum_{i=1}^{s+1} b_i, \qquad \omega_{2,1} = \sum_{i=1}^{s+1} b_i \left(\sum_{j=1}^{i} a_j \right) - \frac{1}{2}, \tag{1.24}$$

$$\omega_{3,1} = \sum_{i=1}^{s+1} b_i \left(\sum_{j=1}^{i} a_j \right)^2 - \frac{1}{3}, \qquad \omega_{3,2} = \sum_{i=1}^{s} a_i \left(\sum_{j=1}^{s+1} b_j \right)^2 - \frac{1}{3},$$

donde se considera $a_{s+1} = 0$.

En la literatura se pueden encontrar métodos de escisión muy eficientes: los métodos de cuarto orden de McLachlan [86] y los métodos de cuarto y sexto orden de Blanes y Moan [28] son buenos ejemplos.

Una característica a remarcar de este tipo de integradores es que los flujos $\varphi_h^{[A]}$ y $\varphi_h^{[B]}$ son intercambiables. A continuación explicaremos un caso donde esto no es cierto.

Un caso particular: Escisión de tipo Runge-Kutta-Nyström Un método Runge–Kutta–Nyström es aquel método tipo Runge–Kutta especialmente diseñado para ecuaciones diferenciales que se pueden escribir en la forma:

$$\ddot{y} = \frac{d^2 y}{dt^2} = g(y), \qquad y \in \mathbb{R}^D. \tag{1.25}$$

En el caso de métodos de escisión, este tipo de ecuaciones diferenciales, mediante la escisión que veremos a continuación provoca que varios elementos del álgebra generada por A y por B se anulen automáticamente. Este hecho hace posible el diseño de métodos de escisión especialmente adaptados. Este tipo de métodos de escisión se conocen en la literatura como métodos de escisión tipo Runge–Kutta–Nyström, de ahora en adelante RKN. A su vez, este hecho comporta que los flujos $\varphi_h^{[A]}$ y $\varphi_h^{[B]}$ no sean intercambiables, teniendo que distinguir entre dos tipos de esquemas: por un lado, los esquemas ABA

$$\mathcal{A}_h = \varphi_{a_{s+1}h}^{[A]} \circ \varphi_{b_s h}^{[B]} \circ \varphi_{a_s h}^{[A]} \circ \cdots \circ \varphi_{b_1 h}^{[B]} \circ \varphi_{a_1 h}^{[A]};$$

y por el otro, los esquemas BAB

$$\mathcal{B}_h = \varphi^{[B]}_{b_{s+1}h} \circ \varphi^{[A]}_{a_s h} \circ \varphi^{[B]}_{b_s h} \circ \cdots \circ \varphi^{[A]}_{a_1 h} \circ \varphi^{[B]}_{b_1 h}.$$

Para aplicar la técnica de escisión a este tipo de problemas deberemos convertir previamente la ecuación de segundo orden $\ddot{y} = g(y)$ en un problema de primer orden. Esto, lo haremos definiendo $v = \dot{y}$ y planteando la siguiente escisión:

$$\dot{x} = \begin{pmatrix} \dot{y} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} v \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ g(y) \end{pmatrix} = f^{[A]}(y, v) + f^{[B]}(y, v).$$

Los sistemas $\dot{x} = f^{[i]}(y, v), (i = A, B)$ tienen como solución exacta:

$$\varphi^{[A]}_h(y, v) = (y + hv, v), \qquad \varphi^{[B]}_h(y, v) = (y, v + hg(y)), \tag{1.26}$$

respectivamente, y las derivadas de Lie correspondientes son:

$$A \equiv L_{f^{[A]}} = \sum_{i=1}^{d} v_i \frac{\partial}{\partial y_i}, \qquad B \equiv L_{f^{[B]}} = \sum_{i=1}^{d} g_i(y) \frac{\partial}{\partial v_i}.$$

El corchete de Lie $[A, B]$ es:

$$[A, B] = -\sum_{i=1}^{d} g_i(y) \frac{\partial}{\partial y_i} + \sum_{i,j=1}^{d} v_i \frac{\partial g_j}{\partial y_i} \frac{\partial}{\partial v_j},$$

y el corchete de Lie $[B, A, B]$ es:

$$[B, A, B] = 2 \sum_{i,j=1}^{d} g_i(y) \frac{\partial g_j}{\partial y_i} \frac{\partial}{\partial v_j}.$$

Nótese que, este último operador sólo depende de y y por tanto $[B, B, A, B] = 0$. La anulación de este operador provoca que para orden mayor que 3 el número de condiciones de orden necesarias se reduzca. Así, el número de condiciones de orden independientes pasa a ser $l(r) = 2, 1, 2, 2, 4, 5, 10, \ldots$ [92].

Un ejemplo relevante es el de los sistemas mecánicos donde el Hamiltoniano asociado es de la forma $H(q, p) = \frac{1}{2} p^\top M^{-1} p + V(q)$ y en consecuencia las ecuaciones del movimiento son $\ddot{q} = -M^{-1} \nabla_q V(q)$. Para este caso los flujos exactos (1.26) toman la forma

$$\varphi^{[A]}_h(q, p) = (q + hM^{-1}p, p), \qquad \varphi^{[B]}_h(q, p) = (q, p - h\nabla_q V(q)),$$

y el corchete de Lie $[B, A, B]$ es la transformación de Lie asociada a la función Hamiltoniana $-(\nabla_q V)^\top M^{-1} \nabla_q V$, que sólo depende de las q.

Otro caso interesante donde se pueden aplicar este tipo de integradores es en sistemas Hamiltonianos que se pueden separar en la forma $H(q,p) = H_0(q,p) + V(q)$ siendo H_0 una función cuadrática en momentos [13].

Hay otro tipo de ecuaciones diferenciales de segundo orden donde también son aplicables este tipo de métodos [20, 13]. Si la ecuación diferencial se puede escribir como

$$\ddot{y} = \frac{d^2y}{dt^2} = M\dot{y} + g_1(y) + g_2(y), \qquad y \in \mathbb{R}^D, \tag{1.27}$$

el problema se puede transformar en una ecuación diferencial de primer orden definiendo $v = \dot{y}$ con la siguiente separación:

$$\dot{x} = \begin{pmatrix} \dot{y} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} v \\ Mv + g_1(y) \end{pmatrix} + \begin{pmatrix} 0 \\ g_2(y) \end{pmatrix} = f^{[A]}(y,v) + f^{[B]}(y,v).$$

La solución exacta de los sistemas asociados a estas funciones es, respectivamente

$$\varphi_h^{[A]}(y,v) = (y + hv, v + hMv + hg_1(y)), \qquad \varphi_h^{[B]}(y,v) = (y, v + hg_2(y)),$$

y podemos aplicar los métodos de escisión tipo RKN.

Los métodos de escisión RKN más eficientes que se pueden encontrar en la literatura son los de orden 4 y 6 presentados por Blanes y Moan en [28] y nuestros métodos de orden ocho presentados en esta tesis (ver capítulo 4) y en [17].

1.3.2. Composición de método y su adjunto

Esta técnica está basada en la composición de un método de primer orden, χ_h, y su adjunto, χ_h^*, de forma intercalada con diferentes coeficientes:

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}. \tag{1.28}$$

Al método base χ_h se le puede asociar el operador $e^{Y(h)}$ y a su adjunto el operador $e^{-Y(-h)}$ (ver apéndice A.3), donde $Y(h)$ tiene la forma:

$$Y(h) = hY_1 + h^2Y_2 + h^3Y_3 + \cdots = \sum_{i\geq 1} h^i Y_i$$

siendo, por consistencia, $Y_1 = F \equiv L_f$ la derivada de Lie asociada a $f(x)$:

$$L_f = \sum_{i=1}^{n} f_i(x) \frac{\partial}{\partial x_i}.$$

Así, el integrador numérico ψ_h tiene asociado el operador $\Psi(h)$, el cual puede ser expresado como producto de estos operadores:

$$\Psi(h) = e^{Z(h)} = e^{-Y(-\alpha_1 h)} e^{Y(\alpha_2 h)} \cdots e^{-Y(-b_{2s-1}h)} e^{Y(\alpha_{2s}h)}.$$

De nuevo, $Z(h)$ se puede obtener aplicando recursivamente la formula BCH:

$$\begin{aligned} Z(h) = h\omega_{1,1}F + h^2\omega_{2,1}Y_2 + h^3\omega_{3,1}Y_3 + h^3\omega_{3,2}[F,Y_2] \\ + h^4\omega_{4,1}Y_4 + h^4\omega_{4,2}[F,Y_3] + h^4\omega_{4,3}[F,[F,Y_2]] + \mathcal{O}(h^5), \end{aligned}$$

donde $\omega_{i,j}$ son polinomios que sólo dependen de los coeficientes α y los conmutadores se entienden anidados a la derecha. Si renombramos los conmutadores como:

$$\begin{aligned} &C_{11} = F; \quad C_{21} = Y_2; \quad C_{31} = Y_3; \quad C_{32} = [F,Y_2]; \\ &C_{41} = Y_4; \quad C_{42} = [F,Y_3]; \quad C_{43} = [F,F,Y_2], \end{aligned}$$

podemos escribir de forma más compacta $Z(h)$ como:

$$Z(h) = \sum_{i\geq 1} h^i \sum_{j=1}^{c(i)} \omega_{i,j} C_{i,j}.$$

Así, los operadores diferenciales Y_i generan un álgebra de Lie que llamamos $\mathcal{L}(Y_1, Y_2, Y_3, \dots)$. Además, este álgebra está graduada:

$$x\mathcal{L}(Y_1, Y_2, Y_3, \dots) = \bigoplus_{i\geq 1}^{\infty} \mathcal{L}^i(Y_1, Y_2, Y_3, \dots),$$

siendo $\mathcal{L}^i(Y_1, Y_2, Y_3, \dots)$ la componente homogénea de grado i compuesta por todos los operadores de grado i (ver apéndice A.1) pertenecientes a $\mathcal{L}(Y_1, Y_2, Y_3, \dots)$ de forma que

$$C_{i,j} \in \mathcal{L}^i(Y_1, Y_2, Y_3, \dots).$$

Las dimensiones de estas subálgebras vienen determinadas por la fórmula de Witt (1.23) [90] aplicada a este caso: $c(r) = 1, 1, 2, 3, 6, 9, 18, \dots$

Ahora, si se consigue que $Z(h)$ sea igual hasta orden r al operador asociado al campo de vectores de la solución exacta, $X(h) = hF$, es decir:

$$Z(h) = hF + \mathcal{O}(h^{r+1}),$$

esto es $\omega_{1,1} = 1$ y $\omega_{i,j} = 0$ para $1 < i \leq r$ y $j \leq c(i)$, el integrador construido será de orden r. Las primeras $\omega_{i,j}$ son explícitamente [20, 13]:

$$\omega_{1,1} = \sum_{i=1}^{2s} \alpha_i, \qquad \omega_{2,1} = \sum_{i=1}^{2s} (-1)^i \alpha_i^2, \qquad \omega_{3,1} = \sum_{i=1}^{2s} \alpha_i^3,$$

$$\omega_{3,2} = \frac{1}{2}\left(\sum_{i=1}^{2s-1} (-1)^{i+1} \alpha_i^2 \sum_{j=i+1}^{2s} \alpha_j + \sum_{i=1}^{2s-1} \alpha_i \sum_{j=i+1}^{2s} (-1)^j \alpha_j^2 \right).$$

Una característica importante de este tipo de composiciones, demostrada por McLachlan en [86], es que cualquier método de escisión en dos partes que al menos sea consistente ($\sum_i a_i = \sum_i b_i = 1$):

$$\psi_h = \varphi^{[B]}_{b_{s+1}h} \circ \varphi^{[A]}_{a_s h} \circ \varphi^{[B]}_{b_s h} \circ \cdots \circ \varphi^{[A]}_{a_1 h} \circ \varphi^{[B]}_{b_1 h},$$

puede ser expresado como una composición de método y adjunto al tomar $\chi_h = \varphi^{[B]}_h \circ \varphi^{[A]}_h$:

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h},$$

donde

$$b_1 = \alpha_1,\ a_i = \alpha_{2i-1} + \alpha_{2i} \text{ y } b_{i+1} = \alpha_{2i} + \alpha_{2i+1}.$$

Así pues, los métodos de escisión en dos partes (1.21) y los de composición (1.28) son equivalentes cuando $\chi_h = \varphi^{[B]}_h \circ \varphi^{[A]}_h$ (o intercambiando A y B), y en consecuencia los métodos más eficientes de escisión en dos partes presentes en la literatura [86, 28] son unos buenos candidatos para utilizar como métodos de composición.

Coeficientes negativos para órdenes mayores que dos. Todos los métodos de escisión (1.21) necesitan al menos un a_i y un b_i negativos si el orden del método es mayor o igual que tres y en el caso de métodos de composición (1.28) uno de los α_i necesariamente ha de ser negativo [11]. Esta característica es inherente a los métodos de escisión y composición.

La existencia de tamaños de paso negativos para métodos de escisión y composición de orden mayor que tres no supone ningún inconveniente en un gran número de problemas, por ejemplo, en la dinámica Hamiltoniana. Pero, por ejemplo, en el caso de ecuaciones en derivadas parciales que involucren al operador Laplaciano esto es una limitación, como veremos más adelante. La prueba de la necesidad de tamaños de paso negativos para orden mayor que 2 fue obtenida originalmente en [107, 106, 115, 57]. A continuación reproducimos la prueba de Blanes y Casas de [11, 13].

Cualquier método de composición de método de primer orden y su adjunto (1.28) para orden mayor que tres debe verificar la condición $\omega_{3,1} = 0$. Por tanto, debe existir al menos un $\alpha_i < 0$. Para esquemas basados en la técnica de escisión tenemos la misma restricción. La condición $\omega_{3,1}$ puede expresarse como:

$$\omega_{3,1} = \sum_{i=1}^{2s} \alpha_i^3 = \sum_{i=1}^{s} (\alpha_{2i-1}^3 + \alpha_{2i}^3) = 0.$$

Entonces debe existir algún i en esta suma que verifique:

$$\alpha_{2i-1}^3 + \alpha_{2i}^3 < 0,$$

y como $x^3 + y^3 < 0$, para todo $x, y \in \mathbb{R}$, implica que $x + y < 0$, tenemos

$$\alpha_{2i-1} + \alpha_{2i} < 0,$$

y esta última ecuación puede ser usada en la conversión de métodos de composición a métodos de escisión tal como hemos visto anteriormente. Por tanto, uno puede escribir:

$$\alpha_{2i-1} + \alpha_{2i} = a_i < 0.$$

El mismo razonamiento se puede usar para coeficientes b_i pero con:

$$\omega_{3,1} = \sum_{i=1}^{2s} \alpha_i^3 = \sum_{i=0}^{s-1} (\alpha_{2i}^3 + \alpha_{2i+1}^3) = 0,$$

en vez de la anterior. En consecuencia, cualquier esquema construido con estas técnicas y que haga uso solamente de coeficientes reales necesariamente requerirá un $a_i < 0$ y un $b_i < 0$ si el esquema en cuestión tiene un orden mayor que dos. Nótese que el razonamiento está ligado a la suposición de que los coeficientes son reales. Si los coeficientes son complejos se pueden construir métodos de escisión y composición manteniendo las partes reales de los coeficientes positivas hasta cierto orden [15]. Volveremos a esto más adelante.

1.3.3. Composiciones simétricas de métodos simétricos de orden 2

Una técnica muy ventajosa a la hora de construir métodos de composición de orden alto es componer métodos simétrico–temporales de orden $2n$ ($n = 1, 2, \dots$) de manera simétrica. Aquí nos centraremos en el caso $n = 1$, pero se pueden construir métodos con una técnica similar a la que vamos a explicar para cualquier n [12].

Denotaremos al método base como $\mathcal{S}_h^{[2]}$, pero esto no significa que sea el método de Störmer-Verlet necesariamente, simplemente un método de segundo orden con simetría temporal. Con esta técnica el esquema resultante tendrá la forma:

$$\mathcal{SS}_h = \mathcal{S}_{\alpha_s h}^{[2]} \circ \mathcal{S}_{\alpha_{s-1} h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_2 h}^{[2]} \circ \mathcal{S}_{\alpha_1 h}^{[2]}, \tag{1.29}$$

y al igual que en el caso previo, al método base $\mathcal{S}_h^{[2]}$ se le puede asociar un operador exponencial $e^{S(h)}$. En este caso, como el método asociado es simétrico–temporal $S(h)$ sólo contiene potencias impares de h (ver apéndice A.3):

$$S(h) = hS_1 + h^3 S_3 + h^5 S_5 \cdots = \sum_{i \geq 1} h^{2i-1} S_{2i-1}$$

donde por consistencia $S_1 = F \equiv L_f$, siendo L_f la derivada de Lie asociada a $f(x)$ de (1.15). Así, el esquema $\mathcal{SS}_h$ tiene asociado un operador diferencial de la forma:

$$\Psi(h) = e^{Z(h)} = e^{S(\alpha_1 h)} e^{S(\alpha_2 h)} \cdots e^{S(b_{s-1} h)} e^{S(\alpha_s h)},$$

siendo $Z(h)$ el operador asociado al campo de vectores modificado. Aplicando recursivamente la fórmula BCH obtenemos:

$$Z(h) = h\omega_{1,1} F + h^3 \omega_{3,1} S_3 + h^4 \omega_{4,1} [F, S_3] + \mathcal{O}(h^5),$$

siendo $\omega_{i,j}$ polinomios que sólo dependen de los coeficientes α. En este caso los elementos generadores del álgebra son los operadores S_i y llamamos a este álgebra $\mathcal{L}(S_1, S_3, S_5, \dots)$, cuyos primeros elementos de la base son:

$$\begin{array}{llll} M_{11} = F; & M_{31} = S_3; & M_{41} = [F, S_3]; & \\ M_{51} = S_5; & M_{52} = [F, F, S_3]; & M_{61} = [F, S_5]; & M_{62} = [F, F, F, S_3], \end{array}$$

donde aquellos con más de dos operadores se entienden anidados a la derecha.

Al igual que en los casos anteriores, este álgebra de Lie está graduada:

$$\mathcal{L}(S_1, S_3, S_5, \dots) = \bigoplus_{i \geq 1}^{\infty} \mathcal{L}^i(S_1, S_3, S_5, \dots),$$

siendo $\mathcal{L}^i(S_1, S_3, S_5, \dots)$ la componente homogénea de grado i compuesta por todos los operadores de grado i (ver apéndice A.1) pertenecientes a $\mathcal{L}(S_1, S_3, S_5, \dots)$ de forma que

$$M_{i,j} \in \mathcal{L}^i(S_1, S_3, S_5, \dots).$$

Las dimensiones de estas subálgebras vienen determinadas por la fórmula de Witt (1.23) [90] aplicada a este caso: $m(r) = 1, 0, 1, 1, 2, 2, 4, \dots$. Utilizando los elementos de la base se puede expresar $Z(h)$ de un forma más compacta:

$$Z(h) = \sum_{i \geq 1} h^i \sum_{j}^{m(i)} \omega_{i,j} M_{i,j}.$$

Si conseguimos que el campo de vectores modificado $Z(h)$ sea igual, hasta cierto orden r, que el campo de vectores asociado a la solución exacta $X(h) = hF$:

$$Z(h) = hF + \mathcal{O}(h^{r+1}),$$

es decir $\omega_{1,1} = 1$ y $\omega_{i,j} = 0$ para $1 < i \leq r, j \leq m(i)$, obtendremos un integrador numérico de orden r y si el método base es un integrador geométrico,

la composición también lo será. En este caso las primeras $\omega_{i,j}$ son explícitamente:

$$\omega_{1,1} = \sum_{i=1}^{s} \alpha_i, \qquad \omega_{3,1} = \sum_{i=1}^{s} \alpha_i^3, \tag{1.30}$$
$$\omega_{4,1} = \frac{1}{2} \sum_{j=1}^{s-1} \left(\alpha_j^3 \left(\sum_{k=j+1}^{s} \alpha_k \right) - \alpha_j \left(\sum_{k=j+1}^{s} \alpha_k^3 \right) \right).$$

Hay muchos integradores numéricos construidos con esta técnica en la literatura. Nosotros destacamos los esquemas de orden 4, 6, 8 y 10 que se pueden encontrar en los artículos [86, 74, 110].

1.3.4. Sobre el patrón de los coeficientes y las etapas

En la tabla 1.1 se muestra el número de condiciones de orden necesarias para alcanzar un orden dado con las diferentes técnicas que se han presentado.

Orden r	1	2	3	4	5	6	7	8	9	10
$n(r)$	2(1)	1	2	3	6	9	18	30	56	99
$l(r)$	2	1	2	2	4	5	10	14	25	39
$m(r)$	1	0	1	1	2	2	4	5	8	11

Tabla 1.1: Número de condiciones independientes a resolver para diferentes casos: $n(r)$ en escisión general, $l(r)$ en escisión RKN, y $m(r)$ para composiciones simétricas de métodos simétricos de segundo orden. El caso de de las composiciones de primer orden utilizando método y adjunto, $c(r)$, se corresponde con $n(r)$ salvo a primer orden.

Si se quiere obtener un integrador de orden r se deberán cumplir, por ejemplo en el caso de escisión, $\sum_{i=1}^{r} n(i)$ condiciones. Pero existe una forma para reducir el número de condiciones necesarias a resolver, y ésta consiste en componer esquemas que sean simétricos temporales por construcción, es decir $\psi_h = \psi_h^*$. Esta forma de construcción hará que el operador asociado $Z(h)$ sólo tenga términos impares en su desarrollo en serie (para más detalles ver el apéndice A.3) y por tanto las $\omega_{2i,j}$ se anulen automáticamente. Así, si componemos esquemas que cumplan esta condición por construcción, las columnas con r par de la tabla 1.1 no se tendrán en cuenta en el cómputo total de condiciones de orden a resolver. Utilizando la propiedad (1.10) de los flujos numéricos es sencillo ver cómo para que los métodos de escisión y composición sean simétricos temporales por construcción, sus coeficientes deben seguir el patrón palindrómico. Así, en el caso de escisión (1.21)

$$\psi_h = \varphi^{[B]}_{b_{s+1}h} \circ \varphi^{[A]}_{a_s h} \circ \varphi^{[B]}_{b_s h} \circ \cdots \circ \varphi^{[A]}_{a_2 h} \circ \varphi^{[B]}_{b_2 h} \circ \varphi^{[A]}_{a_1 h} \circ \varphi^{[B]}_{b_1 h},$$

el método será simétrico–temporal si sus coeficientes cumplen $a_i = a_{s+2-i}$ y $b_i = b_{s+1-i}$; en el caso de composición de método y adjunto (1.28)

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h},$$

el método será simétrico–temporal si $\alpha_i = \alpha_{2s+1-i}$, y, por último, en el caso de composiciones simétricas de métodos simétricos de segundo orden (1.29)

$$\mathcal{SS}_h = \mathcal{S}^{[2]}_{\alpha_s h} \circ \mathcal{S}^{[2]}_{\alpha_{s-1}h} \circ \cdots \circ \mathcal{S}^{[2]}_{\alpha_2 h} \circ \mathcal{S}^{[2]}_{\alpha_1 h},$$

esto se cumplirá cuando $\alpha_i = \alpha_{s+1-i}$.

Utilizando este tipo de patrón en los coeficientes y considerando una etapa como una evaluación de la función $f(x)$ de (1.15), en la tabla 1.2 se muestran el número de etapas mínimas para alcanzar un orden dado utilizando las técnicas descritas en este trabajo para la construcción de integradores.

Orden r	4	6	8	10
S	3	9	27	83
RKN S	3	7	17	42
SS	3	7	15	31

Tabla 1.2: Mínimo número de etapas necesarias para obtener un orden r en métodos de escisión simétricos temporales (o composición) en la primera fila, para escisión RKN simétricos temporales en la segunda fila y para composiciones de $\mathcal{S}^{[2]}_h$ en la tercera fila.

Expliquemos en detalle los resultados de la tabla 1.2 para cada una de las técnicas:

- Escisión. En el caso de escisión, una etapa corresponde a una evaluación del flujo $\varphi^{[A]}_h$ y a una del flujo $\varphi^{[B]}_h$ y si se hace uso de la propiedad FSAL un método como (1.21) tiene un total de s etapas. Con esta técnica el número de etapas es $s = n_c - 1$ siendo n_c el número de condiciones a resolver, por tanto el mínimo número de etapas para un integrador de orden r se puede expresar como $s = \left(\sum_{i=1}^{r/2} n(2i-1)\right) - 1$ y en el caso RKN como $s = \left(\sum_{i=1}^{r/2} l(2i-1)\right) - 1$. Estos valores corresponden con los valores de la segunda y tercera fila de la tabla 1.2 respectivamente.

- Composición de método y su adjunto. En el caso de este tipo de composiciones básicamente es como el caso de escisión: una etapa corresponde a una evaluación de un método y a una de su adjunto. Por ejemplo, un método como (1.28) tiene s etapas.

- Composición simétrica de métodos simétricos de segundo orden. Consideramos una etapa como una evaluación completa del método $\mathcal{S}_h^{[2]}$.

  Con esta técnica el número de etapas necesarias para resolver n_c condiciones de orden corresponde a $s = 2n_c - 1$. Si se sigue el patrón de coeficientes palíndromos para obtener un integrador simétrico–temporal el número de etapas mínimas para un orden r es $s = \left(\sum_{i=1}^{r/2} 2m(2i-1)\right) - 1$, coincidiendo con la última fila de la tabla 1.2.

1.3.5. Otras técnicas ventajosas

En este apartado se presentan otras técnicas apropiadas para construir métodos de escisión y composición.

Sistemas casi–integrables Hay un cierto tipo de sistemas dinámicos en los cuales la ecuación diferencial (1.15) se puede escribir como $\dot{x} = f^{[A]}(x) + \epsilon f^{[B]}(x)$ donde ϵ es un parámetro pequeño, $|\epsilon| \ll 1$, y cada una de las dos partes es exactamente integrable. Se trata de un sistema que permite una escisión en la cual una de las dos partes contribuye más que la otra, de aquí el nombre de casi–integrables. Para este tipo de sistemas el desarrollo en serie del operador $Z(h)$ asociado al método de escisión, $\psi_h = e^{Z(h)}$ se escribe como:

$$\begin{aligned} Z(h) = h(\omega_{1,1}A + \epsilon\omega_{1,2}B) + \epsilon(h^2\omega_{2,1}N_{2,1} + h^3\omega_{3,1}N_{3,1} + h^4\omega_{4,1}N_{4,1}) \\ + \epsilon^2(h^3\omega_{3,2}N_{3,2} + h^4\omega_{4,2}N_{4,2}) + \epsilon^3h^4\omega_{3,4}N_{3,4} + \mathcal{O}(\epsilon h^5). \end{aligned}$$

Entonces, si por ejemplo, se consigue que esta expresión se convierta en:

$$Z(h) = hF + \mathcal{O}(\epsilon h^5 + \epsilon^2 h^4),$$

anulando las condiciones correspondientes, obtendremos un método de escisión de orden generalizado [85] $(4, 3)$, es decir, de orden 4 para ϵ y de orden 3 para ϵ^2. De manera más general, decimos que un método es de orden generalizado $(r_1, r_2, \ldots, r_m)$ si el desarrollo del operador $Z(h)$ es de la forma:

$$Z(h) = hF + \mathcal{O}(\epsilon h^{r_1+1} + \epsilon^2 h^{r_2+1} + \cdots + \epsilon^m h^{r_m+1}).$$

Como ejemplo de este tipo de sistemas, podemos citar los siguientes sistemas Hamiltonianos: el problema de Kepler perturbado [18, 49]; el problema gravitatorio de N cuerpos [18, 49], y el movimiento de una partícula cargada en el seno de un campo magnético perturbado por ondas planas electrostáticas [32]. En todos estos casos los métodos construidos teniendo en cuenta esta característica presentan una mejora significativa frente a la escisión en energía cinética y energía potencial, $H = T + V$.

Los métodos de orden generalizados $(2n, 2)$ se pueden obtener mediante cuadraturas [85, 80]. Para métodos de orden más alto, los presentados en

[18, 49] de orden $(8, 6, 4)$ y $(10, 6, 4)$ ofrecen una mejora de varios órdenes de magnitud para el problema gravitatorio de N cuerpos frente a los métodos de escisión generales.

Uso de potenciales modificados Los métodos de escisión que hemos presentado se han construido mediante los flujos asociados a las transformaciones de Lie e^{hA} y e^{hB}, pero se pueden construir esquemas de integración haciendo uso de otros flujos asociados a otras transformacions de Lie. En [42, 76] encontramos un método de orden 4:

$$\psi_h = \varphi_{\frac{h}{6}}^{[B]} \circ \varphi_{\frac{h}{2}}^{[A]} \circ \varphi_{\frac{h}{3}}^{[B]} \circ \varphi_{\frac{h}{72}}^{[BAB]} \circ \varphi_{\frac{h}{3}}^{[B]} \circ \varphi_{\frac{h}{2}}^{[A]} \circ \varphi_{\frac{h}{6}}^{[B]},$$

donde el flujo $\varphi_h^{[BAB]}$ corresponde a la transformación de Lie $e^{h[B,A,B]}$. En general los flujos $\varphi_h^{[A]}$ y $\varphi_h^{[B]}$ son sencillos de programar, pero el caso de $\varphi_h^{[BAB]}$ no tiene por qué serlo. No obstante, si nos ceñimos al caso del hamiltoniano $H(q,p) = \frac{1}{2}p^\top M^{-1}p + V(q)$, el flujo $\varphi_h^{[BAB]}$ es de la forma:

$$\varphi_h^{[BAB]}(q,p) = \left(q, p + h^3\nabla_q\left(\nabla_q V(q)^\top M^{-1}\nabla_q V(q)\right)\right),$$

y como se trata de un caso RKN, $\varphi_h^{[B]}$ conmuta con $\varphi_h^{[BAB]}$, pudiéndose calcular ambos de manera simultánea:

$$\varphi_{h_1,h_2}^{[B,BAB]}(q,p) = \left(q, p - h_1\nabla_q V(q) + h_2^3\nabla_q\left(\nabla_q V(q)^\top M^{-1}\nabla_q V(q)\right)\right),$$

y así reexpresar el método como

$$\psi_h = \varphi_{\frac{h}{6}}^{[B]} \circ \varphi_{\frac{h}{2}}^{[A]} \circ \varphi_{\frac{2h}{3},\frac{h}{72}}^{[B,BAB]} \circ \varphi_{\frac{h}{2}}^{[A]} \circ \varphi_{\frac{h}{6}}^{[B]}. \tag{1.31}$$

Nótese cómo el flujo $\varphi_{2h/3,h/72}^{[B,BAB]}$ se puede interpretar como el flujo

$$\varphi_h^{[\hat{V}]}(q,p) = (q, p - h\nabla_q\hat{V}(q,h)),$$

asociado a un potencial modificado:

$$\hat{V}(q,h) = \frac{2}{3}V(q) - \frac{1}{72}h^2\nabla_q V(q)^\top M^{-1}\nabla_q V(q).$$

Es importante señalar cómo con el uso de esta técnica el requisito de coeficientes negativos a partir de cierto orden pasa de tres a cinco, tal como se muestra en [43].

Técnica del procesado Al contrario que en los casos anteriores, la técnica del procesado [23] es aplicable conjuntamente con cualquier técnica de las vistas con anterioridad.

Los métodos de procesado se separan en dos partes, por un lado el núcleo ψ_h y por el otro lado el procesador, π_h. De tal forma que, la aplicación del método completo consiste en:

$$\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1}. \tag{1.32}$$

La aplicación de n pasos del integrador $\hat{\psi}_h$ será:

$$\hat{\psi}_h^n = \pi_h \circ \psi_h^n \circ \pi_h^{-1}.$$

Así pues, la ventaja de esta clase de métodos consiste en aplicar el preprocesado al principio π_h^{-1}, realizar la integración numérica con el núcleo ψ_h y solamente al final (o cuando necesitemos obtener datos) aplicar el postprocesado π_h. De esta forma el procesador π_h puede verse como un cambio de coordenadas en el espacio de fases que mejora la precisión del método ψ_h.

Además, para integradores de esta clase, sólo los términos de error en el núcleo que no pueden ser eliminados por un procesador son relevantes a largo término [13].

En la literatura se encuentran diferentes métodos de procesado altamente eficientes para métodos de escisión en dos partes [23], para métodos de escisión tipo RKN [26] y para métodos casi–integrables [87, 24].

1.4. Composiciones con coeficientes complejos

Como hemos dicho anteriormente, una de las características de los métodos de escisión y composición con coeficientes reales es que algunos de esos coeficientes han de ser necesariamente negativos cuando el orden es mayor que dos. Esta característica tiene algunos inconvenientes. Primero, la evolución a cada paso de integración presenta el típico zigzag (o estructura 'fractal') [114, 62] debido a los retrocesos temporales que implican los coeficientes negativos. Segundo, por consistencia deben haber coeficientes positivos grandes, que como consecuencia conducen a errores de truncamiento y errores globales grandes. De hecho, normalmente es necesario considerar más términos de los estrictamente requeridos por las condiciones de orden para conseguir integradores eficientes. Tercero, hay problemas donde utilizar tiempos de paso negativos no es posible. Este es el caso, por ejemplo, cuando se trata de integrar en el tiempo una ecuación diferencial en derivadas parciales que involucra al operador laplaciano: el uso de métodos de escisión con coeficientes negativos conduce a inestabilidades severas en la solución numérica. En estos casos es una buena opción utilizar métodos con coeficientes complejos que tengan la parte real positiva [21].

Además hay otro caso donde el uso de coeficientes complejos también puede resultar beneficioso: problemas donde $\dot{x} = f(x), x \in \mathbb{C}^D$, y por tanto utilizar coeficientes complejos a la hora de aplicar un método de integración no supone una pérdida de rendimiento.

A continuación, a modo ilustrativo, veremos dos ejemplos donde es útil la utilización de métodos con coeficientes complejos. Primero comentaremos el caso de la ecuación semi–lineal de Fisher, que se trata de una EDP de evolución, y el segundo ejemplo que veremos será el de la ecuación de Schrödinger dependiente del tiempo, que además de ser una EDP de evolución, incorpora los complejos en su formulación. Por último daremos algunos métodos básicos de composición con coeficientes complejos existentes en la literatura.

Ecuación semi–lineal de Fisher La ecuación semi–lineal de Fisher tiene la forma:

$$\frac{\partial}{\partial t}u(x,t) = \Delta u(x,t) + F(u(x,t)),$$

donde $u : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$, Δ denota el operador laplaciano y $F(u(x,t))$ es el potencial de Fisher [105]:

$$F(u) = u(1-u).$$

Para aplicar un método de escisión (o composición) discretizaremos el espacio para obtener un sistema de N EDOs. Concretamente en el caso unidimensional tendremos $x \in [x_0, x_N]$, la función $u_n(t) = u(x_n, t)$, y el potencial de Fisher discretizado $F_n(t) = F(u_n(t))$. Definimos

$$U = (u_1, u_2, \ldots, u_n).$$

Así la EDO asociada a la discretización de la EDP es

$$\dot{U} = AU + \tilde{F},$$

donde A es la matriz de diferenciación asociada al operador laplaciano que surge de discretizar y cuyos valores propios son negativos, y $\tilde{F} = (F_1, F_2, \ldots, F_n)$. Ahora ya podemos aplicar el método de escisión (o composición): por un lado resolvemos el sistema $\dot{U} = AU$ y por el otro $\dot{U} = \tilde{F}$. En el primer sistema es donde no es aconsejable utilizar tamaños de paso negativos. Teniendo en cuenta que los valores propios de A son negativos y la solución a $\dot{U} = AU$ es

$$U(t) = e^{tA}U(t_0),$$

el hecho de usar un tamaño de paso negativo, a menos que sea muy pequeño, puede ser contraproducente. Este problema se agrava al considerar el tamaño de paso en el espacio x cada vez más pequeño debido a que los valores propios de A (en módulo) son cada vez más grandes. Esta característica

deriva del hecho matemático que el operador laplaciano no está acotado y por tanto genera que la evolución del sistema continuo ocurra en un semigrupo analítico[36, 66].

Ecuación de Schrödinger dependiente del tiempo En Mecánica Cuántica la ecuación de Schrödinger dependiente del tiempo, salvo constantes, tiene la forma:

$$i\frac{\partial}{\partial t}\Psi(x,t) = -\Delta\Psi(x,t) + V(x)\Psi(x,t),$$

donde $\Psi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$ se conoce como función de onda. En este caso como estamos en el dominio de los complejos no supone ningún coste extra utilizar métodos de integración con coeficientes complejos.

Al igual que en el caso anterior, debemos discretizar el espacio previamente para poder aplicar métodos de escisión (o composición). En el caso unidimensional obtendríamos $x \in [x_0, x_N]$, la función de onda $u_n(t) = \Psi(x_n, t)$, el potencial $V_n = V(x_n)$. A continuación definimos el vector

$$U = (u_1, u_2, \ldots, u_n),$$

y la matriz $V = \mathrm{diag}(V_1, V_2, \ldots, V_n)$. Así la EDO asociada a la discretización de la ecuación de Schrödinger dependiente del tiempo es

$$i\dot{U} = -AU + VU,$$

donde A es la matriz de diferenciación asociada al operador Δ. Al igual que en el caso anterior, en esta EDO es donde aplicaríamos el método de escisión (o composición), resolviendo por un lado la parte cinética y por el otro la parte potencial.

En este caso para el sistema asociado a la energía cinética, $i\dot{U} = -AU$, cuya solución es

$$U(t) = e^{itA}U(t_0),$$

puede no ser buena idea usar tiempos $t \in \mathbb{C}$ porque entonces podríamos recuperar la problemática del caso anterior. Así pues, una buena opción sería utilizar coeficientes reales para la parte de $i\dot{U} = -AU$ y coeficientes complejos para la parte asociada a $i\dot{U} = VU$

Algunos métodos básicos con coeficientes complejos Uno de los esquemas con coeficientes complejos más sencillos encontrado en la literatura [8, 113, 36, 37, 66] es la composición *double–jump*:

$$\mathcal{S}_h^{[3]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]}. \tag{1.33}$$

Aquí los coeficientes α y β deben satisfacer la condición $\omega_{11} = 1$ y $\omega_{31} = 0$ de (1.30) para que el método resultante sea de orden 3:

$$\left.\begin{array}{r} \alpha+\beta=1 \\ \alpha^3+\beta^3=0 \end{array}\right\} \rightarrow \alpha=\bar{\beta}=\frac{1}{2}\pm i\frac{\sqrt{3}}{6},$$

donde, $\Re(\alpha), \Re(\beta) > 0$ y $\alpha = \bar{\beta}$. Fijémonos cómo el primer coeficiente es el complejo conjugado del último. Más adelante trataremos en detalle este tipo de patrón en los coeficientes.

Podemos obtener el famoso método de Suzuki-Yoshida (composición *triple–jump*) [44, 113, 121] añadiendo una etapa de forma que el método sea simétrico:

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]}; \tag{1.34}$$

de nuevo, los coeficientes α y β deben satisfacer $\omega_{11} = 1$ y $\omega_{31} = 0$ de (1.30) para que el método resultante sea de orden 4. La solución a las condiciones de orden en el plano complejo es:

$$\left.\begin{array}{r} 2\alpha+\beta=1 \\ 2\alpha^3+\beta^3=0 \end{array}\right\} \rightarrow \alpha=\left(2-2^{1/3}e^{2i\pi k/3}\right)^{-1}, \quad \beta=1-2\alpha,$$

con $k = 0, 1, 2$. Cuando $k = 0$ recuperamos el método (1.14) con coeficientes reales y con $k = 1, 2$ tenemos un método con coeficientes complejos donde $\Re(\alpha), \Re(\beta) > 0$. Los esquemas (1.33) y (1.34) se pueden generalizar a órdenes mayores [21], en el primer caso:

$$\mathcal{S}_h^{[n+1]} = \mathcal{S}_{\alpha h}^{[n]} \circ \mathcal{S}_{\beta h}^{[n]},$$

con

$$\left.\begin{array}{r} \alpha+\beta=1 \\ \alpha^{n+1}+\beta^{n+1}=0 \end{array}\right\} \rightarrow \alpha=\bar{\beta}=\frac{1}{2}\left(1\pm i\frac{\sin\left(\frac{\pi}{n+1}\right)}{1+\cos\left(\frac{\pi}{n+1}\right)}\right),$$

y en el segundo caso:

$$\mathcal{S}_h^{[n+2]} = \mathcal{S}_{\alpha h}^{[n]} \circ \mathcal{S}_{\beta h}^{[n]} \circ \mathcal{S}_{\alpha h}^{[n]},$$

con

$$\left.\begin{array}{r} 2\alpha+\beta=1 \\ 2\alpha^{n+1}+\beta^{n+1}=0 \end{array}\right\} \rightarrow \alpha=\frac{e^{i\pi/(n+1)}}{2^{1/(n+1)}-2e^{i\pi/(n+1)}} \text{ y } \beta=1-2\alpha,$$

siendo estos coeficientes resultado de la solución a las condiciones de orden con la fase más pequeña. En ambos casos los integradores son de orden $r \geq 3$ y $\Re(\alpha), \Re(\beta) > 0$.

Capítulo 2

Objetivos y principales resultados

A continuación enumeraremos los principales objetivos abordados en esta tesis. Esencialmente, nos hemos enfocado en el diseño y análisis de nuevas familias de métodos de escisión y composición como ejemplos canónicos de integradores numéricos geométricos.

Este trabajo puede dividirse en dos partes. En la primera hemos tratado de contribuir, en la medida de nuestras posibilidades, a la tarea de completar algunos huecos detectados en los estudios sobre este campo. Más concretamente:

1.- En primer lugar, hemos diseñado nuevos métodos de composición especialmente orientados a la integración numérica del problema de valor inicial $\dot{x} = f(x)$, $x(t_0) = x_0$, cuando el campo vectorial $f(x)$ es separable en tres o más partes y cada una de estas partes se puede resolver exactamente. Como es bien sabido, para esta clase de problemas, uno puede usar un método de escisión válido cuando $f(x)$ es separable en *dos* partes, debido a la relación existente entre métodos de escisión y métodos de composición [90] que hemos comentado en la sección 1.3.2. Sin embargo, resulta que un método de escisión en dos partes optimizado no conduce necesariamente a un método de composición eficiente para el problema donde $f(x)$ es separable en tres o más partes, por lo que el problema que analizamos en detalle es cómo construir métodos de composición especialmente diseñados para el problema original. Este es el contenido del capítulo 3, publicado como [34]:

   - F. Casas, A. Escorihuela-Tomàs. *Composition methods for dynamical systems separable into three parts.* Mathematics, 2020, 8, 533.

2.- En segundo lugar, hemos construido métodos de escisión de orden alto para ecuaciones diferenciales de segundo orden de la forma $\ddot{y} = g(y)$,

$y \in \mathbb{R}^D$. Este tipo de métodos, tal como hemos visto en la sección 1.3.1, reciben el nombre de métodos de escisión RKN, y las ecuaciones $\ddot{y} = g(y)$ aparecen frecuentemente en las aplicaciones. Aunque la forma más sencilla de conseguir un orden alto (por ejemplo 8 o 10) en este caso es usar una composición simétrica de métodos simétricos, hay que tener en cuenta que la estructura especial del problema conlleva una reducción significativa del número de condiciones de orden a cumplir. Así que en principio parece posible conseguir métodos muy competitivos de orden 8 haciendo uso de esta técnica aunque plantear y resolver las condiciones de orden no sea un problema trivial. Este problema es tratado en el capítulo 4, y corresponde al artículo [17]:

- S. Blanes, F. Casas, A. Escorihuela-Tomàs. *Runge–Kutta–Nyström symplectic splitting methods of order 8*. Aceptado para su publicación en Applied Numerical Mathematics.

Como se ha comentado en el capítulo anterior, varios autores han propuesto el uso de métodos de escisión con coeficientes *complejos* con la parte real positiva [21]. Los primeros esquemas dentro de esta familia estaban destinados principalmente a fines teóricos más que a realizar integraciones prácticas, teniendo en cuenta el coste computacional adicional debido a la aritmética compleja. Sin embargo, durante la primera década del siglo XXI se han llevado a cabo más estudios dando lugar a diferentes esquemas que han sido probados en varios escenarios: los sistemas Hamiltonianos en mecánica celeste [37], la ecuación de Schrödinger dependiente del tiempo en la mecánica cuántica [7, 100] y también en el contexto más abstracto de las ecuaciones de evolución con operadores no acotados que generan semigrupos analíticos [36, 66]. Durante el desarrollo de estos métodos, se han evidenciado la existencia de varias propiedades interesantes, aunque todavía falta un análisis teórico y sistemático de esta clase de esquemas, en particular con respecto a sus propiedades de conservación.

La segunda parte de la tesis puede considerarse como un paso preliminar en este análisis sistemático. Durante nuestro estudio hemos constatado la existencia de algunas propiedades notables que poseen estos métodos, y se han diseñado nuevas familias de integradores obtenidos por composición de esquemas básicos con excelentes propiedades de conservación incluso para integraciones a tiempos largos. Más concretamente, nuestras principales contribuciones en este ámbito se pueden resumir de la siguiente manera:

3.- Hemos propuesto una nueva estrategia para la construcción de métodos de orden alto basada en composiciones de *double–jump* con coeficientes complejos pensada para ser proyectada en el eje real. Los esquemas resultantes son simétricos temporales y simplécticos hasta órdenes altos si el integrador básico es simétrico–temporal y simpléctico. Además,

requieren menos etapas que las composiciones estándar del mismo orden. El análisis se realiza en el capítulo 5, que corresponde al artículo publicado [33]

- F. Casas, P. Chartier, A. Escorihuela-Tomàs, Y. Zhang. *Compositions of pseudo–symmetric integrators with complex coefficients for the numerical integration of differential equations*. Journal of Computational and Applied Mathematics, 381 (2020), p. 113006.

4.- Cuando proyectamos sobre el eje real esquemas como los anteriores, estamos efectuando una combinación lineal muy concreta de los métodos involucrados. Además, algunos de los métodos involucrados en los esquemas del punto anterior siguen un patrón de coeficientes particular al que hemos denominado *simétrico–conjugado*:

$$\psi_h = \mathcal{S}^{[2n]}_{\alpha_1 h} \circ \mathcal{S}^{[2n]}_{\alpha_2 h} \circ \cdots \circ \mathcal{S}^{[2n]}_{\alpha_{s-1} h} \circ \mathcal{S}^{[2n]}_{\alpha_s h} \tag{2.1}$$

donde $\alpha_j \in \mathbb{C}$ y $\bar{\alpha}_{s+1-j} = \alpha_j$.

Resulta natural analizar lo que sucede cuando se considera una combinación lineal más general de composiciones simétrico–conjugadas y sus complejas conjugadas. Tal como vemos en el capítulo 6 y en el artículo publicado [35]:

- F. Casas, A. Escorihuela-Tomàs. *High order integrators obtained by linear combinations of symmetric–conjugate compositions*. Applied Mathematics and Computation, 414 (2022), p. 126700,

es posible construir nuevos métodos de orden superior conservando la simetría temporal (y la simplecticidad). Además, la familia de métodos construida está muy bien adaptada para su implementación en entornos paralelos, y por tanto requiere menos esfuerzo computacional que los métodos construidos en el punto anterior.

5.- Las composiciones simétrico–conjugadas juegan un papel importante en los dos ítems anteriores y sus propiedades de conservación nos motivaron a analizar sistemáticamente este tipo de composiciones cuando el esquema básico es un integrador simétrico–temporal de segundo orden. Cuando el campo vectorial que define la ecuación diferencial es real, la aplicación directa de un método de composición con coeficientes complejos conduce en general a una aproximación compleja en cada paso, de modo que hay dos formas de proceder: o bien proyectamos la solución al final de cada paso de integración, o bien solamente se proyecta al final de la evolución temporal (o de forma más general, sólo cuando se necesitan datos de salida). En el capítulo 7, que corresponde al artículo [14]:

- S. Blanes, F. Casas, P. Chartier, A. Escorihuela-Tomàs. *On symmetric–conjugate composition methods in the numerical integration of differential equations*. Mathematics of Computation, 91 (331) (2022), p. 1739-1761.

nos limitamos únicamente a la primera posibilidad (proyectar a cada paso) y analizamos las preservación de propiedades del integrador. Se muestra, en general, que la proyección a cada paso preserva las propiedades cualitativas del sistema a un orden superior al orden del propio método. Además, se demuestra que es posible obtener esquemas de orden superior que involucran un número menor de integradores básicos en comparación a cuando se utilizan composiciones palindrómicas.

6.- En la sección 1.4 hemos mencionado cómo la aplicación de métodos de escisión y composición con coeficientes complejos a ecuaciones diferenciales cuyo campo vectorial es complejo no supone ningún incremento en el coste computacional, y hemos mencionado el caso concreto de la ecuación de Schrödinger dependiente del tiempo. En este caso, al utilizar métodos con coeficientes complejos perdemos la unitariedad de la solución. Este problema es abordado en el capítulo 8, que corresponde al artículo [16]:

- S. Blanes, F. Casas, A. Escorihuela-Tomàs. *Applying splitting methods with complex coefficients to the numerical integration of unitary problems*. Journal of Computational Dynamics, 9(2) (2022), p. 85-101.

Aunque esto constituye sólo un estudio preliminar, se muestra que los métodos de escisión simétrico–conjugados aplicados a la integración numérica de la ecuación de Schrödinger en el grupo SU(2) son conjugados a un método unitario para valores suficientemente pequeños del tamaño de paso. Además, los experimentos numéricos muestran que una cierta clase de métodos de escisión simétrico–conjugados se pueden aplicar con seguridad a este problema, al igual que otros métodos que sólo involucran coeficientes reales.

A continuación proporcionamos un breve resumen de las principales contribuciones mencionadas, tal como se presentan en los capítulos 3 a 8.

Capítulo 3: Composition methods for dynamical systems separable into three parts

Hay problemas relevantes donde la $f(x)$ del problema de valor inicial $\dot{x} = f(x)$ con $x(0) = x_0$ debe descomponerse en tres o más partes para garantizar que cada subproblema se pueda resolver explícitamente. Algunos

ejemplos son el flujo de Arnold–Beltrami–Childress (ABC) [3], la ecuación de Schrödinger discreta no lineal y desordenada (DDNLS de sus siglas en inglés) [109], el movimiento de una partícula cargada en un campo electromagnético sometida a la fuerza de Lorentz [68, 69], y las ecuaciones de Vlasov-Maxwell en la física de plasmas [9]. El objetivo principal del artículo es presentar un tipo de métodos de integración eficientes para este tipo de problemas y comparar su rendimiento en algunos ejemplos físicos de esta clase.

Para simplificar, se analiza en detalle el caso en que $f(x)$ se divide en tres partes. De esta manera se tiene

$$f(x) = f^{[A]}(x) + f^{[B]}(x) + f^{[C]}(x), \tag{2.2}$$

donde cada subproblema $\dot{x} = f^{[i]}(x)$ $(i = A, B, C)$ puede resolverse explícitamente con $x(t) = \varphi_t^{[i]}(x_0)$. Por supuesto, también se puede considerar un método de escisión de la forma

$$\Psi_h = \varphi_{a_1 h}^{[A]} \circ \varphi_{b_1 h}^{[B]} \circ \varphi_{c_1 h}^{[C]} \circ \varphi_{b_2 h}^{[B]} \circ \varphi_{a_2 h}^{[A]} \circ \cdots \circ \varphi_{c_s h}^{[C]} \circ \varphi_{b_{2s} h}^{[B]} \circ \varphi_{a_{s+1} h}^{[A]}, \tag{2.3}$$

y determinar los coeficientes a_j, b_j, c_j para que (2.3) sea un método de integración de, digamos, orden r. El principal inconveniente de este enfoque es el gran número de condiciones de orden (y, por tanto, el número de etapas) que intervienen en la composición, tal como se observa en la tabla 2.1. Así, un método de escisión simétrico–temporal de cuarto orden requeriría resolver 11 condiciones de orden, mientras que uno de orden 6 requiere 56.

Un segundo enfoque consiste en considerar métodos de composición formados con el esquema básico de primer orden

$$\chi_h = \varphi_h^{[A]} \circ \varphi_h^{[B]} \circ \varphi_h^{[C]} \tag{2.4}$$

(o cualquier permutación de sus flujos) y su adjunto

$$\chi_h^* = \varphi_h^{[C]} \circ \varphi_h^{[B]} \circ \varphi_h^{[A]}.$$

En este caso el esquema será

$$\Psi_h = \chi_{\alpha_1 h} \circ \chi_{\alpha_2 h}^* \circ \cdots \circ \chi_{\alpha_{2s-1} h} \circ \chi_{\alpha_{2s} h}^*, \tag{2.5}$$

donde los coeficientes α_j son elegidos para conseguir el orden deseado. En este caso, el número de condiciones de orden a resolver es mucho menor (ver tabla 2.1). Obsérvese que el esquema general sigue siendo de la forma (2.3).

Se puede, de hecho, construir una clase particular de métodos (2.5) tomando en consideración la relación existente entre los métodos de composición y escisión cuando $f(x)$ se separa en *dos partes*, tal como se ha visto en la sección 1.3.2. En otras palabras, cualquier método de escisión existente diseñado para sistemas separables en dos partes se puede adaptar a esta

Orden r	1	2	3	4	5	6	7	8
Escisión ABC	3	3	8	18	45	116	312	810
Composición	1	1	2	3	6	9	18	30

Tabla 2.1: Número de condiciones requeridas para alcanzar orden p con escisión y composición cuando la $f(x)$ se debe separar en tres partes.

situación tomando (2.4) como esquema básico. Sin embargo, se puede hacer mejor y diseñar un método de la forma (2.5) desde cero, es decir, resolviendo las condiciones de orden y aplicando criterios de optimización especialmente orientados. En el presente artículo, procediendo de esta manera buscamos integradores numéricos de orden 4 que minimizan la 1-norma del vector formado por los coeficientes, el principal término de error del campo vectorial modificado de orden 5, y también el error en la conservación de energía para sistemas Hamiltonianos.

Hemos construido nuevas familias de métodos de composición de cuarto orden más eficientes que los mejores métodos de escisión diseñados para sistemas separables en dos partes [28] cuando son aplicados a problemas de este tipo.

Capítulo 4: Runge–Kutta–Nyström symplectic splitting methods of order 8

Como se ha dicho antes, hay un amplio abanico de problemas que pueden escribirse como una ecuación diferencial de segundo orden de la forma $\ddot{y} = g(y), y \in \mathbb{R}^D$. Entre ellos podemos destacar todos aquellos sistemas Hamiltonianos donde la función Hamiltoniana es $H(q,p) = \frac{1}{2}p^\top M^{-1}p + V(q)$. Para este tipo de problemas las composiciones simétricas de métodos simétricos nos valen como integradores simplécticos si los integradores básicos lo son. Pero podemos hacer uso de la anulación del operador $[B,B,A,B]$ para poder reducir las condiciones de orden necesarias y así obtener lo que en la literatura se denomina un método de escisión RKN (ver sección 1.3.1). De esta forma se pueden construir esquemas más eficientes para este tipo de problemas.

Las condiciones que se han de resolver para alcanzar un orden dado se dan en la tabla 2.2. Se puede observar cómo para orden 8 los métodos de escisión RKN pueden llegar a ser competitivos.

En este área estábamos interesados en la construcción de este tipo de métodos de orden 8 que como mínimo fueran más eficientes que las composiciones simétricas de métodos simétricos ($\mathcal{SS}_h^{[8]}$) cuando se aplican a problemas del tipo $\ddot{y} = g(y)$.

Podemos encontrar en la literatura otros métodos de escisión RKN de or-

Orden r	2	4	6	8	10
Escisión	1	2	6	18	56
Escisión RKN	1	2	4	10	25
$\mathcal{SS}$ composiciones	1	2	4	8	16

Tabla 2.2: Número de condiciones requeridas para alcanzar orden r para métodos simétricos temporalmente con la técnica de escisión, con escisión RKN y con composiciones simétricas de métodos simétricos.

den ocho, pero utilizan algunas modificaciones en el esquema, especialmente dos: por un lado usando la técnica del procesado [25, 26] y por el otro utilizando potenciales modificados [25, 99] (ver sección 1.3.5). Nosotros estamos interesados en esquemas de escisión RKN sin ningún tipo de modificación, es decir, sin procesador y solamente usando evaluaciones de la función $g(y)$ en cada paso. En este caso, sólo existe en la literatura un método de escisión RKN de orden ocho, un esquema ABA de 17 etapas [98], pero no tiene un buen rendimiento.

Nuestra contribución en este artículo ha sido obtener, implementar y resolver las condiciones de orden de métodos de escisión RKN para así construir métodos eficientes de 17, 18 y 19 etapas. Realizamos esta búsqueda para esquemas ABA y BAB, y obtuvimos más de 2000 posibles integradores de estos seis posibles tipos, seleccionando los más eficientes para cada posibilidad.

Para obtener las condiciones de orden hemos utilizado las técnicas especificadas en el apéndice B. Dada la complejidad del problema, no es posible resolver las ecuaciones no lineales con un CAS (Computer Algebra System), y por ello nos vimos obligados a utilizar técnicas numéricas. Concretamente, las hemos resuelto utilizando la función `fsolve` de Python [117] de la librería SciPy [120], un *wrapper* de las subrutinas HYBRD y HYBRJ de MINPACK [95]. El algoritmo está basado en una modificación del método híbrido de Powell. Cuando el sistema de ecuaciones no lineales asociado presentaba parámetros libres hemos utilizado las siguientes estrategias:

- $s = 18$ etapas. El problema en este caso involucra resolver un sistema polinómico de 18 ecuaciones con 19 variables. Cogemos el primer coeficiente del esquema como parámetro libre y exploramos el intervalo $[0, 1]$ fijando cada vez el valor del coeficiente. La solución luego es utilizada como punto de partida de un método de continuación numérica (concretamente *arc-length continuation*) para seguir la solución a través de la curva implícita buscando un mínimo de la 1-norma de los coeficientes.

- $s = 19$ etapas. Añadiendo un nuevo parámetro al sistema, tenemos 18 ecuaciones con 20 variables y por tanto la estrategia varía un poco.

En esquemas ABA cogemos a_1 y a_2 como parámetros libres y en los esquemas BAB b_1 y b_2, y exploramos el intervalo $[0.05, 0.15]$. Luego, utilizamos una solución como punto de partida para un método de continuación, denotando por $\mathbf{u}_0$ el vector de coeficientes de la solución; generamos un hiperplano mediante el vector aleatorio $\boldsymbol{\alpha}$ que verifica $\boldsymbol{\alpha} \cdot (\mathbf{u} - \mathbf{u}_0) = 0$, y aplicamos continuación a lo largo de la curva que resulta de la intersección del espacio de soluciones con el hiperplano generado aleatoriamente para buscar un mínimo de la 1-norma del vector de coeficientes.

Comparamos los nuevos métodos, 6 en total, con los mejores integradores de composición tipo $\mathcal{SS}$ [74, 110] para ilustrar cómo nuestros métodos son más eficientes para problemas RKN. También, comparamos con otros integradores simplécticos RKN de orden 4 y 6 [28] y con métodos de extrapolación [63] (no simplécticos) para concluir que los nuevos métodos presentados son buenos candidatos para integrar un problema tipo RKN cuando se busca a la vez una precisión alta y preservar el comportamiento cualitativo de las soluciones.

Capítulo 5: Compositions of pseudo–symmetric integrators with complex coefficients for the numerical integration of differential equations

A partir de este capítulo es cuando empieza la parte de la tesis que se ha centrado en la construcción de métodos con coeficientes complejos. Como se ha comentado anteriormente, numerosos autores han propuesto el uso de coeficientes complejos en los métodos de integración, primero con fines teóricos, pero más tarde llevados a la práctica.

Nuestro estudio sobre el uso de coeficientes complejos en métodos de escisión y composición empieza con composiciones simétricas de métodos simétricos, concretamente con la composición *double–jump* introducida en la sección 1.4:

$$\mathcal{S}_h^{[3]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]}, \tag{2.6}$$

donde $\Re(\alpha), \Re(\beta) > 0$ y $\alpha = \bar{\beta}$. Si este método (de orden 3) se utiliza para integrar numéricamente un ecuación diferencial $\dot{x} = f(x)$ donde $f(x) \in \mathbb{R}^D$ y se proyecta sobre el eje real en cada paso de integración, entonces el método resultante es de orden 4:

$$R_h^{[4]} = \Re\left(\mathcal{S}_h^{[3]}\right) = \frac{1}{2}\left(\mathcal{S}_h^{[3]} + \bar{\mathcal{S}}_h^{[3]}\right) = \frac{1}{2}\left(\mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} + \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]}\right).$$

Esto ocurre porque en el desarrollo en serie de potencias de h, los términos que van con h^4 son imaginarios puros y al proyectar desaparecen. Este hecho ya fue observado por Chambers [37] y por Bandrauk y Shen [8]. A su vez

$R_h^{[4]}$ preserva la simetría temporal y la simplecticidad hasta orden 7 si el método base $\mathcal{S}_h^{[2]}$ es simétrico–temporal y simpléctico. Así, a partir de ahora hablaremos [40, 5] de integradores ψ_τ pseudo–simétricos de orden q cuando cumplan:

$$\psi_\tau^* = \psi_\tau + \mathcal{O}(\tau^{q+1}),$$

y hablamos de integradores ψ_τ pseudo–simplécticos de orden r cuando cumplan:

$$(\psi_\tau')^\top J \psi_\tau' = J + \mathcal{O}(\tau^{r+1}).$$

En este primer artículo sobre métodos con coeficientes complejos presentamos una nueva secuencia para construir métodos de orden más alto haciendo uso de la proyección sobre el eje real a cada paso de integración, al igual que se ha hecho para obtener $R_h^{[4]}$. La secuencia que planteamos empieza de la siguiente manera:

- Componer $\mathcal{S}_h^{[2]}$ mediante la técnica del *double–jump* para obtener $\mathcal{S}_h^{[3]}$.
- Proyectar $\mathcal{S}_h^{[3]}$ para obtener $R_h^{[4]}$.
- Componer mediante la técnica del *double–jump* $R_h^{[4]}$ y así obtener $R_h^{[5]}$:

$$R_h^{[5]} = R_{\mu h}^{[4]} \circ R_{\nu h}^{[4]}, \qquad \text{con } \mu = \bar{\nu} = \frac{1}{2}\left(1 + \sqrt{1 - \frac{2}{\sqrt{5}}}\right),$$

- Proyectar $R_h^{[5]}$ y conseguir $R_h^{[6]}$:

$$R_h^{[6]} = \Re\left(R_h^{[5]}\right) = \frac{1}{2}\left(R_h^{[5]} + \bar{R}_h^{[5]}\right) = \frac{1}{2}\left(R_{\mu h}^{[4]} \circ R_{\nu h}^{[4]} + R_{\nu h}^{[4]} \circ R_{\mu h}^{[4]}\right).$$

El hecho que el método $R_h^{[4]}$ preserve el comportamiento cualitativo de la solución hasta orden 7 condiciona que esta secuencia no pueda extenderse más allá del orden 7.

Este procedimiento puede ser generalizado partiendo de un método base $\mathcal{S}_h^{[2n]}$ de orden $2n$ y pseudo–simétrico de orden q, primero obteniendo la composición:

$$\psi_h^{[2n+1]} = \mathcal{S}_{\gamma^{[2n]}h}^{[2n]} \circ \mathcal{S}_{\bar{\gamma}^{[2n]}h}^{[2n]},$$

donde los coeficientes $\gamma^{[2n]}$ tienen el valor

$$\gamma^{[2n]} = \frac{1}{2}\left(1 + i\tan\left(\frac{\pi}{2(2n+1)}\right)\right),$$

para después proyectar sobre el eje real y obtener

$$R_h = \Re\left(\psi_h^{[2n+1]}\right) = \frac{1}{2}\left(\psi_h^{[2n+1]} + \bar{\psi}_h^{[2n+1]}\right). \tag{2.7}$$

Nótese cómo, para cada n se tiene $\Re(\gamma^{[2n]}) > 0$. El orden del método y el orden de pseudo–simetría de éste dependenderán del valor de q. Si $q \geq 2n+2$, el método R_h será de orden $2n+2$ y pseudo–simétrico de orden $\min(q, 4n+3)$. En caso contrario, si $q = 2n+1$, el método R_h tendrá el valor de q como orden y como orden de pseudo–simetría.

Utilizando esta técnica, podemos construir una familia de métodos pseudo–simétricos empezando por un método simétrico de orden $2n$, $\mathcal{S}_h^{[2n]}$:

$$\mathcal{S}_h^{[2n]} \to R_h^{[2n+2]} \to R_h^{[2n+4]} \to \cdots \to R_h^{[2(n+m)]},$$

siempre y cuando $2(n+m) < 4n+3$. Para esta familia, se puede escribir una regla recursiva de la forma:

$$R_h^{[2m+2]} = \frac{1}{2}\left(R^{[2m]}_{\gamma^{[2m]}h} \circ R^{[2m]}_{\bar{\gamma}^{[2m]}h} + R^{[2n]}_{\bar{\gamma}^{[2m]}h} \circ R^{[2n]}_{\gamma^{[2n]}h}\right), \tag{2.8}$$

donde en la primera iteración ($m = n$) se parte de $R_h^{[2n]} \equiv \mathcal{S}_h^{[2n]}$.

Con estas composiciones se puede alcanzar un orden dado con un número menor de etapas respecto a las composiciones que solamente usan números reales. Además, se mantiene la parte real de los coeficientes positiva. Por otro lado, estos métodos son fácilmente paralelizables debido a que la regla de recursión se puede reexpresar siempre como una combinación lineal de composiciones del método base $\mathcal{S}_h^{[2n]}$.

Para ilustrar estos hechos se realizan experimentos numéricos: primero se utiliza el oscilador armónico de manera que podemos estudiar los términos de error para la solución, para la simetría y para la simplecticidad; luego, se utiliza el problema de Kepler para ver el comportamiento en la preservación de las cantidades conservadas, y por último, se utilizan estos métodos en ecuaciones diferenciales en derivadas parciales (EDPs) de evolución. Concretamente se estudia el caso de la ecuación de Fisher [105] y la ecuación de Ginzburg–Landau [118].

Capítulo 6: High order integrators obtained by linear combinations of symmetric–conjugate compositions

A continuación presentamos un breve resumen del artículo [35] correspondiente al capítulo 6. Éste puede considerarse una continuación del anterior trabajo presentado en el capítulo 5.

Si se desarrolla el procedimiento recursivo del artículo anterior (2.8), se obtiene una combinación lineal de composiciones de esquemas tipo $\mathcal{S}_h^{[2n]}$. Por otro lado, algunas de estas composiciones son simétrico conjugadas:

$$\psi_h = \mathcal{S}^{[2n]}_{\alpha_1 h} \circ \mathcal{S}^{[2n]}_{\alpha_2 h} \circ \cdots \circ \mathcal{S}^{[2n]}_{\alpha_{s-1} h} \circ \mathcal{S}^{[2n]}_{\alpha_s h} \tag{2.9}$$

donde $\alpha_j \in \mathbb{C}$ y $\bar{\alpha}_{s+1-j} = \alpha_j$. Partiendo de esta idea, en este artículo investigamos la combinación lineal de métodos ψ_h simétrico–conjugados y su proyección sobre el eje real. Construimos una nueva familia de integradores $T_h^{(m)}$ de orden $2(n+m)$ y pseudo–simétricos de orden $4n+3$ si el método base $\mathcal{S}_h^{[2n]}$ es simétrico–temporal y de orden $2n$.

Consideramos combinaciones lineales

$$\phi_h = \frac{1}{2k} \sum_{j=1}^{k} \left(\psi_h^{(j)} + \bar{\psi}_h^{(j)} \right),$$

de forma que el método ϕ_h corresponde a la proyección sobre el eje real de todas los $\psi_h^{(j)}$. Cada $\psi_h^{(j)}$ es una composición simétrico–conjugada de métodos $\mathcal{S}_h^{[2n]}$. Con estas combinaciones lineales aumentamos el orden de la siguiente manera:

- $T_h^{(1)}$ con orden $r = 2n+2$. Para aumentar el orden necesitaremos resolver solamente dos ecuaciones de orden, y con un único método $\psi_h^{(1)}$ se pueden satisfacer:

  $$\psi_h^{(1)} = \mathcal{S}^{[2n]}_{\gamma^{[2n]}h} \circ \mathcal{S}^{[2n]}_{\bar{\gamma}^{[2n]}h},$$

  donde los coeficientes $\gamma^{[2n]}$ son los introducidos en el anterior artículo:

  $$\gamma^{[2n]} = \frac{1}{2}\left(1 + i \tan\left(\frac{\pi}{2(2n+1)}\right)\right),$$

  Nótese cómo este método corresponde con la composición *double–jump* y ademas con el primer método R (2.7):

  $$T_h^{(1)} = \frac{1}{2}\left(\mathcal{S}^{[2n]}_{\gamma^{[2n]}h} \circ \mathcal{S}^{[2n]}_{\bar{\gamma}^{[2n]}h} + \mathcal{S}^{[2n]}_{\bar{\gamma}^{[2n]}h} \circ \mathcal{S}^{[2n]}_{\gamma^{[2n]}h}\right).$$

- $T_h^{(2)}$ con orden $r = 2n+4$. En este caso se han de resolver 4 ecuaciones de orden. Estas se pueden resolver considerando los siguientes métodos $\psi_h^{(j)}$ de cuatro etapas:

  $$\begin{aligned}\psi_h^{(1)} &= \mathcal{S}^{[2n]}_{\bar{\alpha}_1 h} \circ \mathcal{S}^{[2n]}_{\bar{\alpha}_2 h} \circ \mathcal{S}^{[2n]}_{\alpha_2 h} \circ \mathcal{S}^{[2n]}_{\alpha_1 h},\\ \psi_h^{(2)} &= \mathcal{S}^{[2n]}_{\bar{\alpha}_2 h} \circ \mathcal{S}^{[2n]}_{\bar{\alpha}_1 h} \circ \mathcal{S}^{[2n]}_{\alpha_1 h} \circ \mathcal{S}^{[2n]}_{\alpha_2 h},\end{aligned}$$

  siendo $\alpha_1 = \bar{\gamma}^{[2n+2]}\bar{\gamma}^{[2n]}$ y $\alpha_2 = \bar{\gamma}^{[2n+2]}\gamma^{[2n]}$. El método obtenido coincide con las composiciones simétrico–conjugadas involucradas en la construcción del método $R_h^{(2)}$:

  $$T_h^{(2)} = \frac{1}{4}\left(\psi_h^{(1)} + \bar{\psi}_h^{(1)} + \psi_h^{(2)} + \bar{\psi}_h^{(2)}\right).$$

- $T_h^{(3)}$ con orden $r = 2n+6$. Siete son las condiciones de orden a resolver en este caso. Podemos lograrlo utilizando las siguientes composiciones $\psi_h^{(j)}$ de ocho etapas:

$$\begin{aligned}
\psi_h^{(1)} &= \mathcal{S}_{\alpha_1 h}^{[2n]} \circ \mathcal{S}_{\alpha_2 h}^{[2n]} \circ \mathcal{S}_{\alpha_3 h}^{[2n]} \circ \mathcal{S}_{\alpha_4 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_4 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_3 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_2 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_1 h}^{[2n]}, \\
\psi_h^{(2)} &= \mathcal{S}_{\alpha_2 h}^{[2n]} \circ \mathcal{S}_{\alpha_1 h}^{[2n]} \circ \mathcal{S}_{\alpha_4 h}^{[2n]} \circ \mathcal{S}_{\alpha_3 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_3 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_4 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_1 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_2 h}^{[2n]}, \\
\psi_h^{(3)} &= \mathcal{S}_{\alpha_3 h}^{[2n]} \circ \mathcal{S}_{\alpha_4 h}^{[2n]} \circ \mathcal{S}_{\alpha_1 h}^{[2n]} \circ \mathcal{S}_{\alpha_2 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_2 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_1 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_4 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_3 h}^{[2n]}, \\
\psi_h^{(4)} &= \mathcal{S}_{\alpha_4 h}^{[2n]} \circ \mathcal{S}_{\alpha_3 h}^{[2n]} \circ \mathcal{S}_{\alpha_2 h}^{[2n]} \circ \mathcal{S}_{\alpha_1 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_1 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_2 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_3 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_4 h}^{[2n]},
\end{aligned}$$

  donde los coeficientes α_j toman los valores:

$$\begin{aligned}
\alpha_1 &= \gamma^{[2n+4]}\gamma^{[2n+2]}\gamma^{[2n]}, & \alpha_2 &= \gamma^{[2n+4]}\gamma^{[2n+2]}\bar{\gamma}^{[2n]}, \\
\alpha_3 &= \gamma^{[2n+4]}\bar{\gamma}^{[2n+2]}\gamma^{[2n]}, & \alpha_4 &= \gamma^{[2n+4]}\bar{\gamma}^{[2n+2]}\bar{\gamma}^{[2n]}.
\end{aligned}$$

  Nuevamente, las composiciones involucradas en este método T son las composiciones simétrico–conjugadas presentes en el método R respectivo:

$$T_h^{(3)} = \frac{1}{8}\left(\psi_h^{(1)} + \bar{\psi}_h^{(1)} + \psi_h^{(2)} + \bar{\psi}_h^{(2)} + \psi_h^{(3)} + \bar{\psi}_h^{(3)} + \psi_h^{(4)} + \bar{\psi}_h^{(4)}\right).$$

De esta manera se obtiene el principio de una secuencia. Los métodos con orden $2n+2$, $2n+4$ y $2n+6$ corresponden a los tres primeros métodos $T_h^{(m)}$. Las composiciones involucradas en el método $T_h^{(m)}$ corresponden a las composiciones simétrico–conjugadas involucradas en el método $R_h^{(m)}$. Así pues, si cogemos un método $R_h^{(m)}$ y nos quedamos sólo con aquellas composiciones que sean simétrico–conjugadas, obtenemos el método $T_h^{(m)}$ correspondiente. Con esta idea, la construcción de los nuevos métodos se puede generalizar introduciendo la matriz de coeficientes

$$\Gamma_{2n} := \frac{1}{2}\begin{pmatrix} \gamma^{[2n]} & \bar{\gamma}^{[2n]} \\ \bar{\gamma}^{[2n]} & \gamma^{[2n]} \end{pmatrix},$$

donde cada fila representa una composición de métodos básicos $\mathcal{S}_h^{[2n]}$ y cada elemento de la fila es un método básico con el coeficiente que aparece en la matriz. El método resultante será la suma de todas las composiciones. Así pues,

$$T_h^{(1)} = \frac{1}{2}(\mathcal{S}_{\gamma^{[2n]}h}^{[2n]} \circ \mathcal{S}_{\bar{\gamma}^{[2n]}h}^{[2n]} + \mathcal{S}_{\bar{\gamma}^{[2n]}h}^{[2n]} \circ \mathcal{S}_{\gamma^{[2n]}h}^{[2n]})$$

se puede representar con la matriz Γ_{2n}, el método $T_h^{(2)}$ por $\Gamma_{2n+2} \otimes \Gamma_{2n}$, y en general:

$$T_h^{(m)} = \Gamma_{2(n+m-1)} \otimes (\Gamma_{2(n+m-2)} \otimes \cdots \otimes (\Gamma_{2n+2} \otimes \Gamma_{2n}) \cdots).$$

La secuencia que se presenta en este artículo crece como 2^m, mientras que las otras técnicas conocidas para construir métodos de orden alto con partes reales positivas crecen como 3^m en el caso del *triple–jump* (1.34) y como 4^m en el caso del *double–jump*. Este hecho ya era observado en los métodos presentados en [33], la principal diferencia en este sentido radica en que el número de ejecuciones en paralelo en este caso es menor. Mientras que los métodos R necesitan ejecutar 2^{2^m-2} composiciones a la vez, con los métodos T se necesitan 2^{m-1}. Para comprobar la mejora de eficiencia que aportan los nuevos métodos presentados, en el artículo se realizan diagramas de eficiencia comparando los nuevos métodos T con los R y con la técnica del *triple–jump* teniendo en cuenta diferentes entornos. Observándose que los métodos T presentan mejores resultados para la preservación de las cantidades conservadas, incluso en entornos que permitiesen ejecutar en paralelo todas las composiciones necesarias de los métodos R.

Capítulo 7: On symmetric–conjugate composition methods in the numerical integration of differential equations

Con el trabajo presentado en el capítulo 7 y publicado en [14] se inicia un primer análisis sistemático sobre las composiciones simétrico–conjugadas de métodos $\mathcal{S}_h^{[2]}$ y sus propiedades de preservación de estructura. Nos ceñimos solamente al caso en el que el campo de vectores asociado a la ecuación diferencial $\dot{x} = f(x)$ es real. Por tanto, aunque la utilización de métodos con coeficientes complejos implique el uso de aritmética compleja, cuando queramos obtener resultados deberemos proyectar sobre el eje real. Esto bien lo podemos hacer a cada paso de integración o bien en el instante de tiempo final. En este análisis nos centramos en el caso en el que proyectamos sobre el eje real a cada paso de integración.

Para obtener una visión completa comparamos las composiciones simétrico–conjugadas con las composiciones palindrómicas. Para el caso de las composiciones simétricas los métodos de orden $r = 2n$ tienen un orden de pseudo–simétria de $q = 4n+1$ y para el caso de las composiciones simétrico–conjugadas demostramos el siguiente resultado:

Proposición 2.1. *Dado un integrador simétrico–temporal de segundo orden* $\mathcal{S}_h^{[2]}$*, consideramos las composiciones simétrico–conjugadas*

$$\psi_h = \mathcal{S}^{[2]}_{\bar{\alpha}_1 h} \circ \mathcal{S}^{[2]}_{\bar{\alpha}_2 h} \circ \cdots \circ \mathcal{S}^{[2]}_{\alpha_2 h} \circ \mathcal{S}^{[2]}_{\alpha_1 h}$$

de orden $r \geq 3$ *y su parte real, i.e.,*

$$\hat{R}_h^{[2n]} = \frac{1}{2}\left(\psi_h^{[r]} + \bar{\psi}_h^{[r]}\right),$$

aplicadas a ecuaciones diferenciales $\dot{x} = f(x)$ *donde* $f(x)$ *es un campo vectorial real. En este caso, se cumple lo siguiente:*

(a) Si $\psi_h^{[r]}$ *es de orden impar,* $r = 2n-1$, $n = 2, 3, \dots$, *entonces* $\hat{R}_h^{[2n]}$ *es un método de orden* $2n$ *y pseudo–simétrico de orden* $q = 4n-1$. *Además, si* f *es un campo vectorial Hamiltoniano (real) y* $\mathcal{S}_h^{[2]}$ *es un integrador simpléctico, entonces* $\hat{R}_h^{[2n]}$ *es pseudo–simpléctico de orden* $p = 4n-1$.

(b) Si $\psi_h^{[r]}$ *es de orden par,* $r = 2n$, $n = 2, 3, \dots$, *entonces* $\hat{R}_h^{[2n]}$ *es un método de orden* $2n$ *y pseudo–simétrico de orden* $q = 4n+3$. *Además, si* f *es un campo vectorial Hamiltoniano (real) y* $\mathcal{S}_h^{[2]}$ *es un integrador simpléctico, entonces* $\hat{R}_h^{[2n]}$ *es pseudo–simpléctico de orden* $p = 4n+1$.

Por otro lado, mostramos que la serie de operadores $\Psi(h) = e^{V(h)}$ asociada a un método simétrico–conjugado es de la forma:

$$V(h) = h\omega_{1,1}F + \sum_{j\geq 1} h^{2j+1} \sum_{k=1}^{m(2j+1)} \omega_{2j+1,k} N_{2j+1,k} + i \sum_{j\geq 2} h^{2j} \sum_{k=1}^{m(2j)} \omega_{2j,k} N_{2j,k} \tag{2.10}$$

donde $\omega_{j,k}$ son polinomios reales, F es la derivada de Lie asociada a $f(x)$ y $m(r)$ es la dimensión de la subálgebra $\mathcal{L}^r(F, S_3, S_5, \dots)$ (ver apéndice A.1), cuyos primeros valores podemos ver en la primera fila de la tabla 2.3. De la expresión (2.10) se deduce que los términos que van con las potencias pares son imaginarios puros y los que van con las potencias impares son reales. Esto reduce el número de condiciones de orden necesarias para alcanzar un orden determinado, como se puede observar en la tabla 2.3. Veamos en cada

Orden r	1	2	3	4	5	6	7	8	9	10
$m(r)$	1	0	1	1	2	2	4	5	8	11
$n_c^{(r)}$		1		2		4		8		16
$n_c^{(r)}$ (sim-conj)		1		2		5		11(9)		24(19)
s		1		3		7		15		31
s (sim-conj)		1		2		5		11(9)		24(19)

Tabla 2.3: Dimensión de las subágebras $\mathcal{L}^r(F, S_3, S_5, \dots)$ en la primera fila, en el resto número total de condiciones de orden y de etapas para conseguir un orden r en una composición de métodos $\mathcal{S}_h^{[2]}$ utilizando coeficientes complejos y proyectando en el eje real. En la tercera y cuarta fila se expresan el número de condiciones de orden para el caso palindrómico y para el simétrico–conjugado, respectivamente. En la quinta y sexta fila se expresan el número de etapas mínimas para el caso palindrómico y para el simétrico–conjugado, respectivamente.

caso las condiciones de orden necesarias a resolver y el número de etapas para obtener un método de orden par:

- Composición palindrómica. En este caso las $\omega_{2j,k}$ son cero por construcción, así que el método deberá cumplir el siguiente número de condiciones de orden:

$$n_c^{(r)} = \sum_{i=1}^{r/2} m(2i-1),$$

y el número de etapas mínimas será $s = 2n_c^{(r)} - 1$.

- Composición simétrico-conjugada. En este caso la expresión de $V(h)$ (2.10) hace que las condiciones $\omega_{2j,k}$ sean imaginarias puras y al proyectar desaparezcan. Por eso se pueden construir métodos de orden r que cumplan el siguiente número de condiciones de orden:

$$n_c^{(r)} = \sum_{i=1}^{r} m(i) - m(r). \tag{2.11}$$

y el número de etapas mínimas será $s = n_c^{(r)}$.

Obsérvese que en la tabla 2.3 los métodos de orden 8 y 10 necesitan 11 y 24 condiciones a resolver si se aplica la formula (2.11), pero se pueden lograr métodos de estos órdenes resolviendo solamente 9 y 19 condiciones de orden. Este hecho se debe a que se pueden obtener métodos de orden 8 y 10 resolviendo el siguiente número de condiciones de orden:

$$n_c^{(r)} = \sum_{i=1}^{r} m(i) - m(r) - m(r-2).$$

Esto, en el caso de orden 8, significa que obviamos resolver las condiciones $\omega_{6,k}$, y en el caso de orden 10, significa que obviamos resolver las condiciones $\omega_{8,k}$. Respectivamente, tendremos un método de orden 5 (con las $\omega_{7,k}$ anuladas) y un método de orden 7 (con las $\omega_{9,k}$ anuladas) de forma que al proyectar se conviertan en métodos de orden 8 y 10. Este hecho tendrá consecuencias en la pseudo–simetría del método y se generaliza en la siguiente proposición:

Proposición 2.2. *Sea un integrador simétrico–conjugado de orden $r = 2n$ después de ser proyectado sobre el eje real:*

$$\psi_h^{[r]} = \mathcal{S}_{\bar{\alpha}_1 h}^{[2]} \circ \mathcal{S}_{\bar{\alpha}_2 h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_2 h}^{[2]} \circ \mathcal{S}_{\alpha_1 h}^{[2]}.$$

Si $2n > 4q + 1$ para cualquier $q \geq 0$, entonces el número de condiciones de orden que deberá verificar $\psi_h^{[r]}$ para tener un orden de pseudo–simetría $4(n-q)-1$ después de ser proyectado sobre el eje real será

$$n_c^{(r)} = \sum_{i=1}^{r} m(i) - \sum_{j=1}^{q} m(r-2j).$$

Una vez analizadas estas propiedades, proponemos nuevos integradores simétrico–conjugados hasta orden 8 y mostramos cómo los métodos de orden alto son más eficientes incluso con tamaños de paso más grandes, al contrario de lo que ocurre en el caso de composiciones con coeficientes reales. Este hecho es debido a dos factores, por un lado, como ya se ha explicado, con patrones simétrico–conjugados se puede alcanzar un orden dado con un número menor de etapas, y por otro lado, con la utilización de números complejos podemos construir métodos que tengan la parte real de los coeficientes positiva para órdenes mayores que dos. Así, a diferencia del caso real, a cada etapa, siempre se avanza en el tiempo (no hay retrocesos), dando lugar a coeficientes más pequeños y en consecuencia a errores de truncamiento mucho más pequeños.

Para finalizar, se realizan experimentos numéricos con los nuevos integradores simétrico–conjugados y se comparan con integradores palindrómicos con coeficientes complejos. Estos experimentos ilustran cómo en el caso de usar coeficientes complejos en la composición los métodos simétrico–conjugados preservan mejor las propiedades cualitativas del problema que los métodos palindrómicos.

Capítulo 8: Applying splitting methods with complex coefficients to the numerical integration of unitary problems

En el artículo anterior se muestra que los métodos simétrico–conjugados exhiben notables propiedades de conservación cuando se aplican a ecuaciones diferenciales definidas por campos vectoriales reales y la solución se proyecta sobre el eje real en cada paso de integración. Aquí hemos ampliado el análisis a problemas que evolucionan en el grupo SU(2) y en general a la integración numérica de la ecuación de Schrödinger, donde la preservación de la unitariedad es un requisito físico. En SU(2) demostramos la siguiente proposición:

Proposición 2.3. *Supongamos que un método simétrico–conjugado de la forma:*

$$\psi_h = \varphi^{[V]}_{n_1 h} \circ \varphi^{[T]}_{a_1 h} \circ \cdots \circ \varphi^{[V]}_{b_s h} \circ \varphi^{[T]}_{a_s h} \circ \varphi^{[V]}_{b_{s+1} h}.$$

con $a_{s+1-j} = \bar{a}_j$, $b_{s+2-j} = \bar{b}_j$, es aplicado a la integración numérica de la ecuación de Schrödinger:

$$i\frac{dU}{dt} = HU, \quad U(0) = I,$$

con el Hamiltoniano $H = T + V$, y $U(t) \in SU(2)$. En este caso, se cumple lo siguiente:

(a) Los valores propios de la matriz que aproxima la solución tras un paso temporal h están en en el circulo unidad del plano complejo para valores de h suficientemente pequeños.

(b) El método simétrico–conjugado es conjugado a un método unitario para valores suficientemente pequeños de h.

Por lo tanto, el error en la unitariedad no crece de forma secular con el tiempo y se puede escribir como un método procesado (ver sección 1.3.5), donde el método simétrico–conjugado sería el núcleo y el método completo sería un método unitario. Es decir, se puede escribir:

$$\Phi_{\mathrm{u}} = \pi \circ \Phi_{\mathrm{SC}} \circ \pi^{-1},$$

siendo π el procesador.

Esto nos lleva a estudiar la aplicación de estos esquemas simétrico–conjugados en un ámbito más general. Consideramos la integración numérica de la ecuación de Schrödinger dependiente del tiempo, introducida en la sección 1.4:

$$i\partial_t \Psi(x,t) = -\frac{1}{2}\Delta\Psi(x,t) + V(x)\Psi(x,t).$$

donde $\Psi(x,t)$ es la función de onda que representa el estado del sistema, $\Psi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$. Consideramos el problema unidimensional y discretizamos en el espacio tal como hemos explicado en la sección 1.4. Siendo $x \in [x_0, x_N]$ y $u_n(t) = \Psi(x_n, t)$ definimos

$$U = (u_1, u_2, \ldots, u_N),$$

y así obtenemos la siguiente EDO asociada:

$$i\dot{U} = -\frac{1}{2}AU + BU,$$

donde A es la matriz de diferenciación del operador Δ que surge al discretizar y B es la matriz diagonal del potencial $B = \mathrm{diag}(V(x_0), \cdots, V(x_{n-1}))$.

Para comparar, usamos los cuatro posibles patrones, combinando las posibilidades con $a_i \in \mathbb{C}$, $b_i \in \mathbb{C}$ y $a_i \in \mathbb{R}$, $b_i \in \mathbb{C}$ con composiciones palindrómicas o simétrico–conjugadas. Realizamos estos experimentos numéricos para dos potenciales distintos, uno cuártico y otro el de Pöschl-Teller. En ambos problemas los métodos que mantienen la estabilidad en la conservación de la energía e incluso en la conservación de la unitariedad de la norma en la función de onda son los que siguen el patrón simétrico–conjugado con $a_i \in \mathbb{R}$ y $b_i \in \mathbb{C}$.

Un hecho conocido de los métodos con coeficientes complejos es que, al componer un método simétrico–conjugado con su adjunto se obtiene un método palindrómico y al componer un método palindrómico con su adjunto se obtiene un método simétrico–conjugado. Teniendo en cuenta este hecho,

aquellos métodos simétrico–conjugados que han sido construidos de esta manera presentan buenos resultados conservativos para integraciones a tiempos largos, y aquellos simétrico–conjugados que se convierten en palindrómicos pierden esta propiedad dando lugar a peores resultados.

Con las aportaciones de este artículo se abre una nueva línea de investigación sobre la aplicación de métodos simétrico–conjugados con $a_i \in \mathbb{R}$, $b_i \in \mathbb{C}$ a problemas unitarios: primero porque se observa cómo el error en la preservación de la unitariedad está acotado y no presenta un crecimiento secular; segundo, el uso de números reales para a_i hace que el flujo asociado al operador laplaciano, e^{-iha_jA}, quede acotado; tercero, los errores de truncamiento son menores en métodos con coeficientes complejos, y cuarto, el uso de aritmética compleja en este tipo de problemas físicos no involucra mayor coste computacional porque el problema se ha de tratar en el dominio complejo igualmente.

Capítulo 3

Composition methods for dynamical systems separable into three parts

Composition Methods for Dynamical Systems Separable into Three Parts

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Abstract

New families of fourth-order composition methods for the numerical integration of initial value problems defined by ordinary differential equations are proposed. They are designed when the problem can be separated into three parts in such a way that each part is explicitly solvable. The methods are obtained by applying different optimization criteria and preserve geometric properties of the continuous problem by construction. Different numerical examples exhibit their improved performance with respect to previous splitting methods in the literature.

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1 Introduction

Splitting methods are particularly useful for the numerical integration of ordinary differential equations (ODEs)

$$\dot{x} \equiv \frac{dx}{dt} = f(x), \qquad x(t_0) = x_0 \in \mathbb{R}^D \tag{1}$$

when the vector field f can be written as $f(x) = \sum_{i=1}^{n} f_i(x)$, so that each subproblem

$$\dot{x} = f_i(x), \qquad x(t_0) = x_0, \qquad i = 1, \ldots, n$$

is explicitly solvable, with solution $x(t) = \varphi_t^{[i]}(x_0)$. Then, by composing the different flows with appropriate chosen weights it is possible to construct a numerical approximation to the exact solution $x(h)$ for a time-step h of arbitrary order [1]. Although splitting methods have a long history in numerical mathematics and have been applied, sometimes with different names, in many different contexts (partial differential equations, quantum statistical mechanics, chemical physics, molecular dynamics, etc. [2]), it is in the realm of Geometric Numerical Integration (GNI) where they play a key role, and in fact some of the most efficient geometric integrators are based on the related ideas of splitting and composition [3].

In GNI the goal is to construct numerical integrators in such a way that the approximations they furnish share one or several qualitative (often, geometric) properties with the exact solution of the differential equation [4]. In doing so, the integrator has not only an improved qualitative behavior, but also allows for a significantly more accurate long-time integration than it is the case with general-purpose methods. In this sense, symplectic integration algorithms for Hamiltonian systems constitute a paradigmatic example of geometric integrators [5, 6]. Splitting and composition methods are widely

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used in GNI because the composition of symplectic (or volume preserving, orthogonal, etc.) transformations is again symplectic (volume preserving, orthogonal, etc., respectively). In composition methods the numerical scheme is constructed as the composition of several simpler integrators for the problem at hand, so as to improve their accuracy.

When f in (1) can be separated into two parts, very efficient splitting schemes have been designed and applied to solve a wide variety of problems arising in several fields, ranging from Hamiltonian Monte Carlo techniques to the evolution of the N-body gravitational problem in Celestial Mechanics (see [3, 4] and references therein).

There are, however, relevant problems in applications where f has to be decomposed into three or more parts in order to have subproblems that are explicitly solvable. Examples include the disordered discrete nonlinear Schrödinger equation [7], Vlasov–Maxwell equations in plasma physics [8], the motion of a charged particle in an electromagnetic field according with the Lorentz force law [9] and problems in molecular dynamics [10]. In that case, although in principle methods of any order of accuracy can be built, the resulting algorithms involve such a large number of maps that they are not competitive in practice. It is the purpose of this paper to present an alternative class of efficient methods for the problem at hand and compare their performance on some non-trivial physical examples than can be split into three parts.

The paper is structured as follows. We first review how splitting methods can be directly applied to get numerical solutions (Section 2). Then the attention is turned to the application of composition methods, and we get a family of 4th-order schemes obtained by applying a standard optimization procedure (Section 3). In Section 4 we show how standard splitting methods, when formulated as a composition scheme, lead to very competitive integrators, and also propose a different optimization criterion for systems possessing invariant quantities. This allows us to get a new family of 4th-order schemes. All these integration algorithms are subsequently tested in Section 5 on a pair of numerical examples. Finally, Section 6 contains some concluding remarks.

2 First Approach: Splitting Methods

In what follows we assume that the vector field f in (1) can be split into three parts,

$$f(x) = f_a(x) + f_b(x) + f_c(x) \tag{2}$$

in such a way that the exact h-flows $\varphi_h^{[a]}$, $\varphi_h^{[b]}$, $\varphi_h^{[c]}$, corresponding to f_a, f_b, f_c, respectively, can be computed exactly.

It is clear that the composition

$$\chi_h = \varphi_h^{[a]} \circ \varphi_h^{[b]} \circ \varphi_h^{[c]} \tag{3}$$

(or any other permutation of the sub-flows) provides a first-order approximation to the exact solution $x(h) = \varphi_h(x_0)$ of (1), i.e.,

$$\chi_h(x_0) = \varphi_h(x_0) + \mathcal{O}(h^2),$$

whereas the so-called Strang splitting

$$S_h^{[2]} = \varphi_{h/2}^{[a]} \circ \varphi_{h/2}^{[b]} \circ \varphi_h^{[c]} \circ \varphi_{h/2}^{[b]} \circ \varphi_{h/2}^{[a]} \tag{4}$$

leads to a second-order approximation.

Higher order approximations to the exact solution of (1) can be obtained by generalizing (4), i.e., by considering splitting schemes of the form

$$\psi_h^{[r]} = \varphi_{c_s h}^{[c]} \circ \varphi_{b_s h}^{[b]} \circ \varphi_{a_s h}^{[a]} \circ \cdots \circ \varphi_{c_1 h}^{[c]} \circ \varphi_{b_1 h}^{[b]} \circ \varphi_{a_1 h}^{[a]}, \tag{5}$$

where the coefficients a_i, b_i, c_i, $i = 1, \ldots, s$, are chosen to achieve a prescribed order of accuracy, say, r,

$$\psi_h^{[r]}(x_0) = \varphi_h(x_0) + \mathcal{O}(h^{r+1}) \quad \text{as} \quad h \to 0. \tag{6}$$

Requirement (6) leads to a set of polynomial equations (the so-called order conditions), whose number and complexity grows enormously with the order. In particular, if $r = 1$ (i.e., for a consistency method) one has

$$\sum_{i=1}^{s} a_i = 1, \qquad \sum_{i=1}^{s} b_i = 1, \qquad \sum_{i=1}^{s} c_i = 1.$$

The specific number of order conditions is determined in fact by the dimension c_k of the homogeneous subspace of grade k, $1 \leq k \leq r$, of the free Lie algebra $\mathcal{L}(A, B, C)$ generated by the Lie derivatives A, B, C corresponding to $f^{[a]}$, $f^{[b]}$, $f^{[c]}$, respectively [1]. These dimensions are collected Table 1 for $1 \leq k \leq 8$.

Table 1: Number of order conditions to be satisfied by a splitting method of the form (5) at each order k.

Grade k	1	2	3	4	5	6	7	8
c_k	3	3	8	18	45	116	312	810

Thus, a splitting method (5) of order 4 requires solving $3 + 3 + 8 + 18 = 32$ order conditions and therefore the evaluation of at least a similar number of sub-flows to have as many parameters as equations. This number can be reduced by considering time-symmetric methods, i.e., schemes verifying

$$\psi_h^{[r]} \circ \psi_{-h}^{[r]} = \mathrm{id}, \tag{7}$$

where id is the identity map. Condition (7) is verified by left-right palindromic compositions, i.e., if

$$a_{s+1-i} = a_i, \quad b_{s+1-i} = b_i, \quad c_{s+1-i} = c_i, \qquad i = 1, 2, \ldots$$

in (5). Then all the conditions at even order are automatically satisfied. Thus, a symmetric method of order 4 requires solving 11 order conditions (instead of 32). Still, within this approach, one has to solve 56 polynomial equations to construct a method of order 6.

Methods of this class have been systematically analyzed in [11]. In particular, it has been shown that if one aims to get schemes (5) of order 2 with the minimum number of maps, then the Strang splitting (4) is recovered. With respect to order 4, the following scheme was presented:

$$\psi_\tau^{[4]} = \varphi_{c_1\tau}^{[c]} \circ \varphi_{b_1\tau}^{[b]} \circ \varphi_{a_1\tau}^{[a]} \circ \varphi_{b_2\tau}^{[b]} \circ \varphi_{c_2\tau}^{[c]} \circ \varphi_{b_3\tau}^{[b]} \circ \varphi_{a_2\tau}^{[a]} \circ \varphi_{b_3\tau}^{[b]} \circ \varphi_{c_2\tau}^{[c]} \circ \varphi_{b_2\tau}^{[b]} \circ \varphi_{a_1\tau}^{[a]} \circ \varphi_{b_1\tau}^{[b]} \circ \varphi_{c_1\tau}^{[c]} \tag{8}$$

with

$$a_1 = w_1, \; a_2 = w_0, \; b_1 = b_2 = \frac{w_1}{2}, \; b_3 = \frac{w_0}{2}, \; c_1 = \frac{w_1}{2}, \; c_2 = \frac{w_0 + w_1}{2}$$

and

$$w_1 = \frac{1}{2 - 2^{1/3}}, \qquad w_0 = 1 - 2w_1.$$

In fact, 13 is the minimum number of maps required. More efficient schemes involving 17 and 25 maps can also be found in [11]. For simplicity, we denote method (8) as $(c_1 b_1 a_1 b_2 c_2 b_3 a_2 b_3 c_2 b_2 a_1 b_1 c_1)$. More recently, in [12] a method involving 21 maps of the form

$$(a_1 b_1 c_1 a_2 b_2 c_2 a_3 b_3 c_3 a_4 b_4 a_4 c_3 b_3 a_3 c_2 b_2 a_2 c_1 b_1 a_1) \tag{9}$$

has also been proposed and tested on several numerical examples.

3 Second Approach: Composition Methods

As it is clear from the previous considerations, constructing high order splitting methods for systems separable into three parts requires solving a large number of polynomial equations involving the coefficients, and this is a very challenging task in general. For this reason, we turn our attention to another strategy based on compositions of the first order $\chi_h = \varphi_h^{[a]} \circ \varphi_h^{[b]} \circ \varphi_h^{[c]}$ and its adjoint,

$$\chi_h^* := (\chi_{-h})^{-1} = \varphi_h^{[c]} \circ \varphi_h^{[b]} \circ \varphi_h^{[a]}$$

with appropriately chosen weights. In other words, we look for integrators of the form

$$\psi_h = \chi_{\alpha_{2s}h} \circ \chi^*_{\alpha_{2s-1}h} \circ \cdots \circ \chi_{\alpha_2 h} \circ \chi^*_{\alpha_1 h}, \quad \text{with} \quad (\alpha_1, \ldots, \alpha_{2s}) \in \mathbb{R}^{2s} \tag{10}$$

verifying in addition the time-symmetry condition $\alpha_{2s+1-i} = \alpha_i$ for all i.

Remark 1 *Methods of the form*

$$\psi_h = S^{[2]}_{\alpha_m h} \circ S^{[2]}_{\alpha_{m-1}h} \circ \cdots \circ S^{[2]}_{\alpha_2 h} \circ S^{[2]}_{\alpha_1 h} \quad \textit{with} \quad (\alpha_1, \ldots, \alpha_m) \in \mathbb{R}^m \tag{11}$$

and $\alpha_{m+1-i} = \alpha_i$ (commonly referred in the literature as symmetric compositions of symmetric methods [1]) verify a much reduced number of order conditions and allows one to construct very efficient high-order schemes [3]. Notice that, since the Strang splitting (4) verifies $S_h^{[2]} = \chi_{h/2} \circ \chi^*_{h/2}$, then it is clear that when analyzing methods (10) we also recover schemes of the form (11).

3.1 Analysis in Terms of Exponentials of Operators

The analysis of the composition methods considered here can be conveniently done by considering the Lie operators associated with the vector fields involved and the graded free Lie algebra they generate.

As is well known, for each infinitely differentiable map $g : \mathbb{R}^D \longrightarrow \mathbb{R}$, the function $g(\varphi_h(x))$ admits an expansion of the form [13, 5]

$$g(\varphi_h(x)) = \exp(hF)[g](x) = g(x) + \sum_{k\geq 1} \frac{h^k}{k!} F^k[g](x), \qquad x \in \mathbb{R}^D,$$

where F is the Lie derivative associated with f,

$$F \equiv L_f = \sum_{i=1}^{D} f_i(x) \frac{\partial}{\partial x_i}. \tag{12}$$

Analogously, for the basic method χ_h one can associate a series of linear operators so that [14]

$$g(\chi_h(x)) = \exp(Y(h))[g](x), \quad \text{with} \quad Y(h) = \sum_{k\geq 1} h^k Y_k$$

for all functions g, whereas for its adjoint one has

$$g(\chi_h^*(x)) = \exp\big(-Y(-h)\big)[g](x).$$

Then the operator series associated with the integrator (10) is

$$\Psi(h) \;=\; \exp(-Y(-h\alpha_1)) \exp(Y(h\alpha_2)) \cdots \exp(-Y(-h\alpha_{2s-1})) \exp(Y(h\alpha_{2s})).$$

Notice that the order of the operators is the reverse of the maps in (10) ([3] p. 88). Now, by repeated application of the Baker–Campbell–Hausdorff formula [4] we can express formally $\Psi(h)$ as the exponential of an operator $\tilde{F}(h)$,

$$\Psi(h) = \exp(\tilde{F}(h)), \qquad \text{with} \qquad \tilde{F}(h) = \sum_{k\geq 1} h^k F_k, \tag{13}$$

$h^k F_k \in \mathcal{L}_k$ for each $k \geq 1$ and $\mathcal{L} = \bigoplus_{k\geq 1} \mathcal{L}_k$ is the graded free Lie algebra generated by the operators $\{hY_1, h^2Y_2, h^3Y_3, \ldots\}$, where, by consistency, $Y_1 = F$. One has explicitly

$$\begin{aligned} Y(h\alpha_i) &= h\alpha_i Y_1 + (h\alpha_i)^2 Y_2 + (h\alpha_i)^3 Y_3 + \cdots \\ -Y(-h\alpha_i) &= h\alpha_i Y_1 - (h\alpha_i)^2 Y_2 + (h\alpha_i)^3 Y_3 - \cdots \end{aligned}$$

so that

$$\begin{aligned} \tilde{F}(h) &= hw_1 Y_1 + h^2 w_2 Y_2 + h^3(w_3 Y_3 + w_{12}[Y_1, Y_2]) \\ &\quad + h^4(w_4 Y_4 + w_{13}[Y_1, Y_3] + w_{112}[Y_1, [Y_1, Y_2]]) \\ &\quad + h^5\big(w_5 Y_5 + w_{14}[Y_1, Y_4] + w_{113}[Y_1, Y_1, Y_3] \\ &\quad + w_{1112}[Y_1, Y_1, Y_1, Y_2] + w_{23}[Y_2, Y_3] + w_{212}[Y_2, Y_1, Y_2]\big) + \mathcal{O}(h^6), \end{aligned} \tag{14}$$

where $[Y_2, Y_1, Y_2] \equiv [Y_2, [Y_1, Y_2]]$, etc, $[\cdot, \cdot]$ refers to the usual Lie bracket and $w_1, w_2, \ldots$ are polynomials in the coefficients α_i. In particular, one has

$$\begin{aligned} w_1 &= \sum_{i=1}^{2s} \alpha_i, \qquad & w_2 &= \sum_{i=1}^{2s} (-1)^i \alpha_i^2, \\ w_3 &= \sum_{i=1}^{2s} \alpha_i^3, \qquad & w_4 &= \sum_{i=1}^{2s} (-1)^i \alpha_i^4, \\ w_{12} &= \frac{1}{2}\left(\sum_{i=1}^{2s-1} (-1)^{i+1} \alpha_i^2 \sum_{j=i+1}^{2s} \alpha_j + \sum_{i=1}^{2s-1} \alpha_i \sum_{j=i+1}^{2s} (-1)^j \alpha_j^2 \right). \end{aligned} \tag{15}$$

Thus, a time-symmetric 4th-order method has to satisfy only consistency ($w_1 = 1$) and the order conditions at order three, $w_3 = w_{12} = 0$. Notice, then, that the minimum number of maps to be considered is $s = 3$. In that case the integrator reads

$$\psi_h = \chi_{\alpha_1} \circ \chi^*_{\alpha_2} \circ \chi_{\alpha_3} \circ \chi^*_{\alpha_3} \circ \chi_{\alpha_2} \circ \chi^*_{\alpha_1} \tag{16}$$

and the unique (real) solution is given by

$$\alpha_1 = \alpha_2 = \frac{1}{2(2 - 2^{1/3})}, \qquad \alpha_3 = \frac{1}{2} - 2\alpha_1.$$

This scheme corresponds to the familiar triple-jump integrator [15]

$$\psi_h = S^{[2]}_{\alpha h/2} \circ S^{[2]}_{\beta h} \circ S^{[2]}_{\alpha h/2} \qquad \text{with} \quad \alpha = 1/(2 - 2^{1/3}). \tag{17}$$

If $\chi_h = \varphi_h^{[a]} \circ \varphi_h^{[b]} \circ \varphi_h^{[c]}$, then ψ_h involves 13 maps (the minimum number) and corresponds precisely to the splitting method (8).

It is worth remarking that the order conditions (15) are general for any composition method of the form (10), with independence of the particular basic first-order scheme χ_h considered, as long as χ_h and its adjoint χ_h^* are included in the sequence. Thus, for instance, one might take the explicit Euler method as χ_h and the implicit Euler method as χ_h^*, and also a symplectic semi-implicit method and its adjoint, leading to the symplectic partitioned Runge–Kutta schemes considered in [16].

3.2 Composition Methods of Order 4

Although one already gets a method of order 4 with only three stages, it is well known that the scheme (17) has large high-order error terms. A standard practice to construct more efficient integrators consists in adding more stages in the composition and determine the extra free parameters thus introduced

according with some optimization criteria. Although assessing the quality of a given integration method applied to all initial value problem is by no means obvious (the dominant error terms are not necessarily the same for different problems), several strategies have been proposed along the years to fix these free parameters in the composition method (10). Thus, in particular, one looks for solutions such that the absolute value of the coefficients, i.e.,

$$E_1(\boldsymbol{\alpha}) = \sum_{i=1}^{2s} |\alpha_i| \tag{18}$$

is as small as possible, the logic being that higher order terms in the expansion (14) involve powers of these coefficients. In fact, methods with small values of $E_1(\boldsymbol{\alpha})$ usually have large stability domains and small error terms [1]. In addition, for a number of problems, the dominant error term is precisely the coefficient w_5 multiplying Y_5 in the expansion (14), so that it makes sense to minimize

$$E_2(\boldsymbol{\alpha}) = 2s \Big| \sum_{i=1}^{2s} \alpha_i^5 \Big|^{1/4}, \tag{19}$$

for a given composition to take also into account the computational effort measured as the number $2s$ of basic schemes considered. Here, as in [17], we construct symmetric methods with small values of E_1 which, in addition, have also small values of E_2. For future reference, the corresponding values of the objective functions for the triple-jump (17) are $E_1 = 4.40483$ and $E_2 = 4.55004$, respectively.

Next we collect the most efficient schemes we have obtained with $s = 4, 5, 6$ by applying this strategy.

$s = 4$ **stages.** The composition is

$$\psi_h = \chi_{\alpha_1} \circ \chi_{\alpha_2}^* \circ \chi_{\alpha_3} \circ \chi_{\alpha_4}^* \circ \chi_{\alpha_4} \circ \chi_{\alpha_3}^* \circ \chi_{\alpha_2} \circ \chi_{\alpha_1}^*, \tag{20}$$

and involves 17 maps when the basic scheme χ_h is given by (3). Now we have a free parameter, which we take as α_1. The minima of both E_1 and E_2 are achieved at approximately $\alpha_1 = 0.358$, and the resulting coefficients are collected in Table 2 as method XA_4. In that case, $E_1 = 2.9084$ and $E_2 = 3.1527$.

$s = 5$ **stages.** The resulting composition

$$\psi_h = \chi_{\alpha_1} \circ \chi_{\alpha_2}^* \circ \chi_{\alpha_3} \circ \chi_{\alpha_4}^* \circ \chi_{\alpha_5} \circ \chi_{\alpha_5}^* \circ \chi_{\alpha_4} \circ \chi_{\alpha_3}^* \circ \chi_{\alpha_2} \circ \chi_{\alpha_1}^*$$

involves 21 maps when applied to a system separable into three parts. Minimum values for E_1 and E_2 are achieved when

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \frac{1}{2(4 - 4^{1/3})}, \qquad \alpha_5 = \frac{1}{2} - 4\alpha_1.$$

In consequence, the method can be written as

$$\psi_h = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]}$$

with $\alpha = 2\alpha_1$, $\beta = 2\alpha_5$. Then $E_1 = 2.3159$ and $E_2 = 2.6111$. This method, denoted XA_5, was first proposed in [18] and analyzed in detail in [19].

$s = 6$ **stages.** Analogously we have considered a composition involving three free parameters (and 25 maps when χ_h is given by (3)):

$$\psi_h = \chi_{\alpha_1} \circ \chi^*_{\alpha_2} \circ \chi_{\alpha_3} \circ \chi^*_{\alpha_4} \circ \chi_{\alpha_5} \circ \chi^*_{\alpha_6} \circ \chi_{\alpha_6} \circ \chi^*_{\alpha_5} \circ \chi_{\alpha_4} \circ \chi^*_{\alpha_3} \circ \chi_{\alpha_2} \circ \chi^*_{\alpha_1}. \tag{21}$$

The proposed solution is collected in Table 2 as method XA_6 leading to $E_1 = 2.0513$, $E_2 = 2.4078$. Notice how, by increasing the number of stages, it is possible to reduce the value of E_1 and E_2 as a measure of the efficiency of the schemes. This integrator has been tested in the numerical integration of the so-called reduced $1 + 1/2$ Vlasov–Maxwell system [20].

We could of course increase the number of stages. It turns out, however, that with $s = 7$ one has the sufficient number of parameters to satisfy all the order conditions up to order 6, resulting in a method of the form (11) [15] involving 29 maps. More efficient 6th-order schemes can be obtained indeed by increasing the number of stages. Thus, in particular, with $s = 9$ and $s = 11$ one has the methods designed in [21] (37 maps) and [22] (45 maps), respectively, when the basic scheme is given by (3).

Table 2: Fourth-order composition methods XA_s with s stages minimizing E_1 and E_2. Method S_6 corresponds to the splitting method of ([23] Table 2) expressed as a composition scheme.

XA_4	
$\alpha_1 = 0.358$	$\alpha_2 = -0.47710242361717810834$
$\alpha_3 = 0.35230499471528197958$	$\alpha_4 = 0.26679742890189612876$
XA_5	
$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \dfrac{1}{2(4 - 4^{1/3})}$	$\alpha_5 = \frac{1}{2} - 4\alpha_1$
XA_6	
$\alpha_1 = 0.16$	$\alpha_2 = 0.15$
$\alpha_3 = 0.16$	$\alpha_4 = -0.260672267225$
$\alpha_5 = 0.147945412322$	$\alpha_6 = 0.142726854903$
S_6	
$\alpha_1 = 0.0792036964311957$	$\alpha_2 = 0.1303114101821663$
$\alpha_3 = 0.22286149586760773$	$\alpha_4 = -0.36671326904742574$
$\alpha_5 = 0.32464818868970624$	$\alpha_6 = 0.10968847787674973$

4 Third Approach: Splitting via Composition

We have already seen that there exists a close relationship between composition methods of the form (10) and splitting methods. This connection can be established more precisely as follows [24]. Let us assume that f in the ODE (1) can be split into two parts, $\dot{x} = f_a(x) + f_b(x)$, which each part explicitly solvable, and take $\chi_h = \varphi^{[b]}_h \circ \varphi^{[a]}_h$. Then, the adjoint method reads $\chi^*_h = \varphi^{[a]}_h \circ \varphi^{[b]}_h$ and the composition (10) adopts the form

$$\psi_h = \left(\varphi^{[b]}_{\alpha_{2s}h} \circ \varphi^{[a]}_{\alpha_{2s}h}\right) \circ \left(\varphi^{[a]}_{\alpha_{2s-1}h} \circ \varphi^{[b]}_{\alpha_{2s-1}h}\right) \circ \cdots \circ \left(\varphi^{[b]}_{\alpha_2 h} \circ \varphi^{[a]}_{\alpha_2 h}\right) \circ \left(\varphi^{[a]}_{\alpha_1 h} \circ \varphi^{[b]}_{\alpha_1 h}\right). \tag{22}$$

Since $\varphi^{[i]}_h$, $i = a, b$ are exact flows, then they verify $\varphi^{[i]}_{\beta h} \circ \varphi^{[i]}_{\delta h} = \varphi^{[i]}_{(\beta+\delta)h}$, and (22) can be rewritten as the splitting scheme

$$\psi_h = \varphi^{[b]}_{b_{s+1}h} \circ \varphi^{[a]}_{a_s h} \circ \varphi^{[b]}_{b_s h} \circ \cdots \circ \varphi^{[b]}_{b_2 h} \circ \varphi^{[a]}_{a_1 h} \circ \varphi^{[b]}_{b_1 h} \tag{23}$$

if $b_1 = \alpha_1$ and

$$a_j = \alpha_{2j} + \alpha_{2j-1}, \qquad b_{j+1} = \alpha_{2j+1} + \alpha_{2j}, \qquad j = 1, \dots, s \tag{24}$$

(with $\alpha_{2s+1} = 0$). Conversely, any integrator of the form (23) with $\sum_{i=1}^{s} a_i = \sum_{i=1}^{s+1} b_i$ can be expressed in the form (10) with $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$ and

$$\begin{aligned} &\alpha_{2s} = b_{s+1}, \\ &\alpha_{2j-1} = a_j - \alpha_{2j}, \qquad \alpha_{2j-2} = b_j - \alpha_{2j-1}, \qquad j = s, s-1, \dots, 1, \end{aligned}$$

with $\alpha_0 = 0$ for consistency. In consequence, any splitting method in principle designed for systems of the form $\dot{x} = f_a(x) + f_b(x)$ with no further restrictions on f_a or f_b can be formulated as a composition (10) which, in turn, can also be applied when f is split into three (or more) pieces, $f = f_a + f_b + f_c$, by taking $\chi_h = \varphi_h^{[a]} \circ \varphi_h^{[b]} \circ \varphi_h^{[c]}$. The performance will be in general different, since different optimization criteria are typically used. Notice that the situation is different, however, if splitting methods of Runge–Kutta–Nyström type are considered.

A particularly efficient 4th-order splitting scheme designed for problems separated into two parts has been presented in ([23] Table 2) (method S_6) and will be used in our numerical tests. It is a time-symmetric partitioned Runge–Kutta method of the form (23), since the role played by f_a and f_b are interchangeable. When formulated as a composition method, it has six stages, i.e., it is of the form (21), with coefficients α_i listed in Table 2. For comparison, the corresponding values of E_1 and E_2 are $E_1 = 2.4668$ and $E_2 = 3.1648$.

An Optimization Criterion Based on the Error in Energy

Very often, the class of problems to integrate are derived from a Hamiltonian function. In that case, Equation (1) is formulated as

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad i = 1, \dots, d \tag{25}$$

so that $x = (q, p)^T$, $f = (\nabla_p H, -\nabla_q H)^T \equiv X_H$ and $H(q, p)$ is the Hamiltonian. The Lie derivative associated with X_H verifies, for any function $G : D \subset \mathbb{R}^{2d} \longrightarrow \mathbb{R}$,

$$L_{X_H} G = -\{H, G\} = -\sum_{j=1}^{d} \left(\frac{\partial H}{\partial q_j} \frac{\partial G}{\partial p_j} - \frac{\partial G}{\partial q_j} \frac{\partial H}{\partial p_j} \right).$$

In other words, $\{H, G\}$ is the Poisson bracket of H and G. In this context, then, the Lie bracket of operators can be replaced by the real-valued Poisson bracket of functions [13].

It is well known that the flow corresponding to (25) is symplectic and in addition preserves the total energy of the system. If H can be split as $H = A + B$, then $f^{[a]} = L_{X_A}$, $f^{[b]} = L_{X_B}$ and the splitting method (23) is also symplectic. Important as it is that the method shares this feature with the exact flow, one would like in addition that the energy be preserved as accurately as possible (since a numerical scheme cannot preserve both the symplectic form and the energy). A possible optimization criterion would be then to select the free parameters in such a way that the error in the energy (or more in general, in the conserved quantities of the continuous system) is as small as possible.

This criterion can be made more specific as follows [25]. First, we expand the modified Hamiltonian $\tilde{H}_h$ in the limit $h \to 0$ for a 4th-order splitting method (23). A straightforward calculation shows that

$$\begin{aligned} \tilde{H}_h = H &+ h^4 k_{5,1}\{A, A, A, A, B\} + h^4 k_{5,2}\{B, A, A, A, B\} + h^4 k_{5,3}\{A, A, B, A, B\} \\ &+ h^4 k_{5,4}\{A, B, B, A, B\} + h^4 k_{5,5}\{B, A, B, A, B\} + h^4 k_{5,6}\{B, B, B, A, B\} + \\ &+ h^5 \sum_{j=1}^{9} k_{6,j} E_{6,j} + \mathcal{O}(h^6), \end{aligned} \tag{26}$$

where $k_{i,j}$ are polynomials in the coefficients a_j, b_j, $\{A, A, A, A, B\}$ refers to the iterated Poisson bracket $\{A, \{A, \{A, \{A, B\}\}\}\}$, and $E_{6,j}$ are (independent) Poisson brackets involving 6 functions A and B.

Now the Lie formalism allows one to get the Taylor expansion of the energy after one time-step ([5], Section 12.2) as

$$H(q_{i+1}, p_{i+1}) = \exp(-h\mathcal{L}_{\tilde{H}_h}) H(q_i, p_i) = H(q_i, p_i) - h\mathcal{L}_{\tilde{H}_h} H(q_i, p_i) + \frac{1}{2} h^2 \mathcal{L}^2_{\tilde{H}_h} H(q_i, p_i) + \cdots,$$

where $\mathcal{L}_{\tilde{H}_h}(\cdot) = \{\tilde{H}_h, \cdot\}$.

An elementary calculation shows that

$$\begin{aligned} H(q_{i+1}, p_{i+1}) - H(q_i, p_i) = h^5 \big(& k_{51} E_{61} + (k_{51} - k_{53}) E_{62} + (k_{52} - k_{53}) E_{63} + k_{54} E_{64} \\ & + (k_{52} - \frac{1}{3} k_{53}) E_{65} + (k_{55} - \frac{1}{3} k_{53}) E_{66} + (k_{55} + k_{54}) E_{67} + (k_{56} - k_{54}) E_{68} + k_{56} E_{69} \big) \\ & + \mathcal{O}(h^6). \end{aligned}$$

Thus, for small h,

$$\begin{aligned} \Delta \equiv & \, k_{51}^2 + (k_{51} - k_{53})^2 + (k_{52} - k_{53})^2 + k_{54}^2 + (k_{52} - \frac{1}{3} k_{53})^2 \\ & + (k_{55} - \frac{1}{3} k_{53})^2 + (k_{55} + k_{54})^2 + (k_{56} - k_{54})^2 + k_{56}^2 \end{aligned} \tag{27}$$

can be taken as a measure of the energy error, and consequently,

$$E_3 = 2s\, \Delta^{1/4} \tag{28}$$

constitutes a possible objective function to minimize. The previous analysis can be also carried out for a composition method (10), resulting in

$$\Delta = w_5^2 + w_{14}^2 + w_{113}^2 + w_{1112}^2 + w_{23}^2 + w_{212}^2. \tag{29}$$

The s-stage methods XB_s whose coefficients are collected in Table 3 have been obtained by minimizing E_3 with (29) and in addition provide small values for (27) when applied with $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$.

We should emphasize again that, although methods XB_s have been obtained by minimizing (29), and thus the local error in the energy, their applicability is by no means limited to Hamiltonian systems. As a matter of fact, both classes of schemes XA_s and XB_s can be used with *any* first-order basic method and its adjoint. Their efficiency may depend, of course, of the type of problem one is approximating and the particular basic scheme taken to form the composition. Moreover, due to the close relationship between symplectic and composition methods, these schemes can also be seen as symplectic partitioned Runge–Kutta methods that, in contrast to splitting schemes, do not require the knowledge of the solution of the elementary flows.

Table 3: Fourth-order composition methods XB_s with s stages minimizing E_3.

XB_4	
$\alpha_1 = 0.1728230091082606$	$\alpha_2 = 0.43074941762060376$
$\alpha_3 = -0.5742238363039501$	$\alpha_4 = 0.4706514095750858$
XB_5	
$\alpha_1 = 0.08967664078837478$	$\alpha_2 = 0.16032335921162522$
$\alpha_3 = 0.29632291754168816$	$\alpha_4 = -0.49421908717228863$
$\alpha_5 = 0.44789616963060047$	
XB_6	
$\alpha_1 = \frac{1}{20}$	$\alpha_2 = \frac{71}{660}$
$\alpha_3 = \frac{47}{330}$	$\alpha_4 = \frac{37}{165}$
$\alpha_5 = -\frac{313}{660}$	$\alpha_6 = \frac{5}{11}$

5 Numerical Examples

Although optimization criteria based on the objective functions E_1, E_2 and E_3 allow one in principle to construct efficient composition schemes, it is clear that their overall performance depends very much on the particular problem considered, the initial conditions, etc. It is, then, worth considering some illustrative numerical examples to test the methods proposed here with respect to other integrators previously available in the literature. In particular, we take as representatives the splitting method (9) designed in [12] for problems separated into three parts (referred to as ABC_{21} in the sequel) and the splitting scheme of [23] considered as a composition (10) (referred as S_6 in Table 2).

When a specific composition method (10) is applied to a particular problem of the form $\dot{x} = f_a + f_b + f_c$ and the first-order method is $\chi_h = \varphi_h^{[a]} \circ \varphi_h^{[b]} \circ \varphi_h^{[c]}$, the implementation is in fact very similar as for a splitting method of the form (9). Thus, in particular, for the integrator (21) one has to apply the following procedure for the time step $x_n \longmapsto x_{n+1}$, where one has to take into account the symmetry of the coefficients: $\alpha_{12} = \alpha_1$, etc. and $s = 6$:

$$
\begin{aligned}
&y = x_n \\
&\text{do } j = 1 : 6 \\
&\quad y = \varphi^{[a]}_{\alpha_{2j-1}h} y \\
&\quad y = \varphi^{[b]}_{\alpha_{2j-1}h} y \\
&\quad \widetilde{\alpha} = \alpha_{2j-1} + \alpha_{2j} \\
&\quad y = \varphi^{[c]}_{\widetilde{\alpha}h} y \\
&\quad y = \varphi^{[b]}_{\alpha_{2j}h} y \\
&\quad y = \varphi^{[a]}_{\alpha_{2j}h} y \\
&\text{end} \\
&x_{n+1} = y
\end{aligned}
$$

It is worth remarking that the examples considered here have been chosen because they admit an straightforward separation into three parts that are explicitly solvable and thus may be used as a kind of testing bench to illustrate the main features of the proposed algorithms. Of course, many other systems could also be considered, including non linear oscillators and the time integration of Vlasov-Maxwell equations [8, 20]. In addition, the general technique proposed in [26] for obtaining explicit

symplectic approximations of non-separable Hamiltonians provides in a natural manner examples of systems separable into three parts.

5.1 Motion of a Charged Particle under Lorentz Force

Neglecting relativistic effects, the evolution of a particle of mass m and charge q in a given electromagnetic field is described by the Lorentz force as

$$m\,\ddot{\mathbf{x}} = q\,(\mathbf{E} + \dot{\mathbf{x}} \times \mathbf{B}), \tag{30}$$

where $\mathbf{E}$ and $\mathbf{B}$ denote the electric and magnetic field, respectively. In terms of position and velocity, the equation of motion (30) can be restated as

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{v} \\ \dot{\mathbf{v}} &= \frac{q}{m}\mathbf{E} + \omega\,\mathbf{b} \times \mathbf{v} \end{aligned} \tag{31}$$

where $\omega = -qB/m$ is the local cyclotron frequency, $B = \|\mathbf{B}\|$ and $\mathbf{b} = \mathbf{B}/B$ is the unit vector in the direction of the magnetic field. For simplicity, we assume that both $\mathbf{E}$ and $\mathbf{B}$ only depend on the position $\mathbf{x}$.

System (31) can be split into three parts in such a way that (a) each subpart is explicitly solvable and (b) the volume form in the space $(\mathbf{x}, \mathbf{v})$ is exactly preserved [9, 27]:

$$\begin{aligned} \frac{d}{dt}\begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix} &= \begin{pmatrix} \mathbf{v} \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{q}{m}\mathbf{E}(\mathbf{x}) \end{pmatrix} + \begin{pmatrix} 0 \\ \omega(\mathbf{x})\mathbf{b}(\mathbf{x}) \times \mathbf{v} \end{pmatrix} \\ &= f^{[a]}(\mathbf{x}, \mathbf{v}) + f^{[b]}(\mathbf{x}, \mathbf{v}) + f^{[c]}(\mathbf{x}, \mathbf{v}). \end{aligned} \tag{32}$$

The corresponding flows with initial condition $(\mathbf{x_0}, \mathbf{v}_0)$ are given by

$$\begin{aligned} &\varphi_t^{[a]} : \begin{cases} \mathbf{x}(t) = \mathbf{x}_0 + t\,\mathbf{v}_0 \\ \mathbf{v}(t) = \mathbf{v}_0 \end{cases}, \qquad \varphi_t^{[b]} : \begin{cases} \mathbf{x}(t) = \mathbf{x}_0 \\ \mathbf{v}(t) = \mathbf{v}_0 + t\,\frac{q}{m}\,\mathbf{E}(\mathbf{x}_0) \end{cases} \\ &\varphi_t^{[c]} : \begin{cases} \mathbf{x}(t) = \mathbf{x}_0 \\ \mathbf{v}(t) = \exp(t\omega(\mathbf{x}_0)\hat{\mathbf{b}}_0)\mathbf{v}_0 \end{cases} \end{aligned} \tag{33}$$

where $\hat{\mathbf{b}}_0 \equiv \hat{\mathbf{b}}(\mathbf{x}_0)$ is the skew-symmetric matrix

$$\hat{\mathbf{b}}(\mathbf{x}) = \begin{pmatrix} 0 & -b_3(\mathbf{x}) & b_2(\mathbf{x}) \\ b_3(\mathbf{x}) & 0 & -b_1(\mathbf{x}) \\ -b_2(\mathbf{x}) & b_1(\mathbf{x}) & 0 \end{pmatrix}$$

associated with $\mathbf{b}(\mathbf{x}) = (b_1(\mathbf{x}), b_2(\mathbf{x}), b_3(\mathbf{x}))^T$.

As in [9], we consider a static, non-uniform electromagnetic field

$$\mathbf{E} = -\nabla V = \frac{0.01}{r^3}(x\,\mathbf{e}_x + y\,\mathbf{e}_y), \qquad \mathbf{B} = \nabla \times \mathbf{A} = r\,\mathbf{e}_z \tag{34}$$

derived from the potentials

$$V = \frac{0.01}{r}, \qquad \mathbf{A} = \frac{r^2}{3}\,\mathbf{e}_\theta$$

respectively, in cylindrical coordinates (r, θ, z) and with the appropriate normalization. Then, it can be shown that both the angular momentum and energy

$$L = r^2\dot{\theta} + \frac{r^3}{3}, \qquad H = \frac{1}{2}\|\mathbf{v}\|^2 + \frac{0.01}{r}$$

are invariants of the problem [9].

With $q = -1$, $m = 1$ and starting from the initial position $\mathbf{x}_0 = (0, -1, 0)^T$ with initial velocity $\mathbf{v}_0 = (0.10, 0.01, 0)$, we integrate with the different numerical schemes until the final time $t_f = 200$ and compute the error in energy and angular momentum along the integration interval. As reference solution we take the output generated by the standard routine DOP853 based on a Runge–Kutta method of order 8 with local error estimation and step size control (with a very stringent tolerance) [28]. In this way, we obtain Figure 1 (top and bottom, respectively), where this error is depicted in terms of the number of the computed sub-flows (by taking different time-steps). For clarity, here and in the sequel, in the left panel we include the results attained by the most efficient XA_s method, whereas the right panel corresponds to the XB_s schemes. For reference and comparison, we include in all cases the splitting method (9) proposed in [12] (denoted here as ABC_{21}) and the scheme S_6, whose coefficients are collected in Table 2.

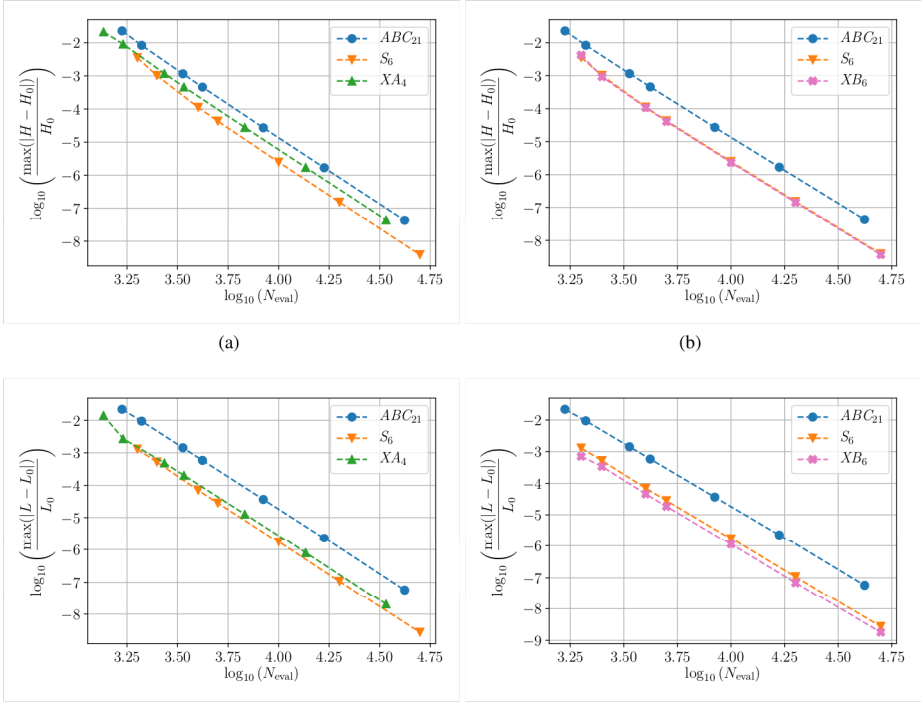
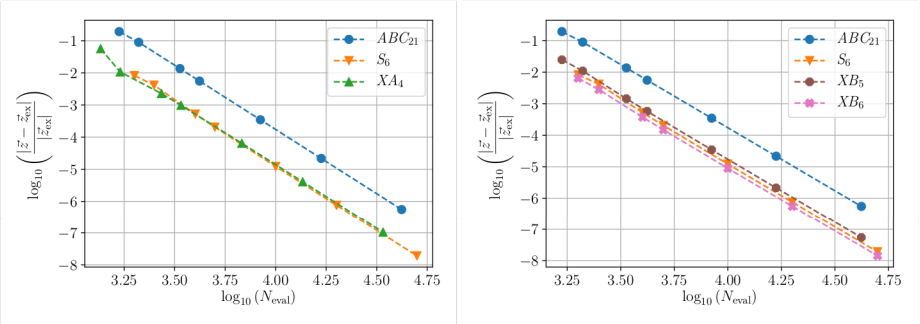


Figure 1: Relative error in conserved quantities due to each of the best numerical methods tested for charged particle under Lorentz force. (**a**) Relative error in energy for XA_4 compared to ABC_{21} and S_6. (**b**) Relative error in energy for XB_6 compared to ABC_{21} and S_6. (**c**)Relative error in angular momentum for XA_4 compared to ABC_{21} and S_6. (**d**) Relative error in angular momentum for XB_6 compared to ABC_{21} and S_6.

We notice that applying the composition methods proposed here leads to more accurate results than the direct approach based on the splitting methods of Section 2 with the same computational cost, and that the new scheme XB_6 is slightly more efficient that the the splitting scheme S_6 (the remaining composition methods of Tables 2 and 3 provide results between ABC_{21} and the best composition depicted here).

In Figure 2 we show the corresponding results obtained by each method for the error in the $(\mathbf{x}, \mathbf{v})$ space.



(a) (b)

Figure 2: Relative error in the $(\mathbf{x}, \mathbf{v})$ space for charged particle under Lorentz force. The notation is the same as in Figure 1. (**a**) Relative error in the $(\mathbf{x}, \mathbf{v})$ space for XA_4 compared to ABC_{21} and S_6. (**b**) Relative error in the $(\mathbf{x}, \mathbf{v})$ space for XB_5 and XB_6 compared to ABC_{21} and S_6.

One should notice that, although this system is Hamiltonian, the Hamiltonian function is not separable into kinetic plus potential energy, and thus general symplectic Runge–Kutta methods cannot be explicit [27]. In order to use explicit methods, one has to split the system into three parts. On the other hand, all the methods tested here are volume-preserving in the $(\mathbf{x}, \mathbf{v})$ space, just as the exact flow.

5.2 Disordered Discrete Nonlinear Schrödinger Equation

The Hamiltonian of the disordered discrete nonlinear Schrödinger equation (DDNLS)

$$\mathcal{H} = \sum_j \left(\epsilon_j |\psi_j|^2 + \frac{\beta}{2}|\psi_j|^4 - (\psi_{j+1}\overline{\psi}_j + \overline{\psi}_{j+1}\psi_j) \right) \tag{35}$$

describes a one-dimensional chain of couples nonlinear oscillators [7]. Here the sum extends over N oscillators, ψ_j are complex variables, $\beta \geq 0$ stands for the nonlinearity strength and the random energies ϵ_j are chosen uniformly from the interval $[-W/2, W/2]$, where W is related with the disorder strength. This model has two invariants: the energy (35) and the norm

$$S = \sum_j |\psi_j|^2,$$

and has been used to determine how the energy spreads in disordered systems [29]. Rather than analyzing the rich dynamics this system possesses, our interest here is to use (35) as a non-trivial test bench for the integrators we presented in previous sections. By introducing the new (real) generalized coordinates and momenta (q_j, p_j) related with ψ_j through

$$\psi_j = \frac{1}{\sqrt{2}}(q_j + ip_j), \qquad \overline{\psi}_j = \frac{1}{\sqrt{2}}(q_j - ip_j),$$

the Hamiltonian function (35) can be written as

$$H = \sum_{j=1}^{N} \left(\frac{\epsilon_j}{2}(q_j^2 + p_j^2) + \frac{\beta}{8}(q_j^2 + p_j^2)^2 - p_{j+1}\, p_j - q_{j+1}\, q_j \right) \tag{36}$$

in such a way that is the sum of three explicitly solvable parts, $H = A + B + C$, with

$$A = \sum_{j=1}^{N} \left(\frac{\epsilon_j}{2}(q_j^2 + p_j^2) + \frac{\beta}{8}(q_j^2 + p_j^2)^2 \right), \quad B = -\sum_{j=1}^{N} p_{j+1}\, p_j, \quad C = -\sum_{j=1}^{N} q_{j+1}\, q_j.$$

The corresponding flows are given, respectively, by

$$\begin{aligned}
\varphi_t^{[a]} &: \quad \begin{cases} q_j(t) = q_j(t_0)\cos(a_j t) + p_j(t_0)\sin(a_j t) \\ p_j(t) = -q_j(t_0)\sin(a_j t) + p_j(t_0)\cos(a_j t) \end{cases}, \\
\varphi_t^{[b]} &: \quad \begin{cases} q_j(t) = q_j(t_0) - t(p_{j-1}(t_0) + p_{j+1}(t_0)) \\ p_j(t) = p_j(t_0) \end{cases} \\
\varphi_t^{[c]} &: \quad \begin{cases} q_j(t) = q_j(t_0) \\ p_j(t) = p_j(t_0) + t(q_{j-1}(t_0) + q_{j+1}(t_0)) \end{cases}
\end{aligned} \tag{37}$$

with $a_j = \epsilon_j + \beta(q_j^2 + p_j^2)/2$.

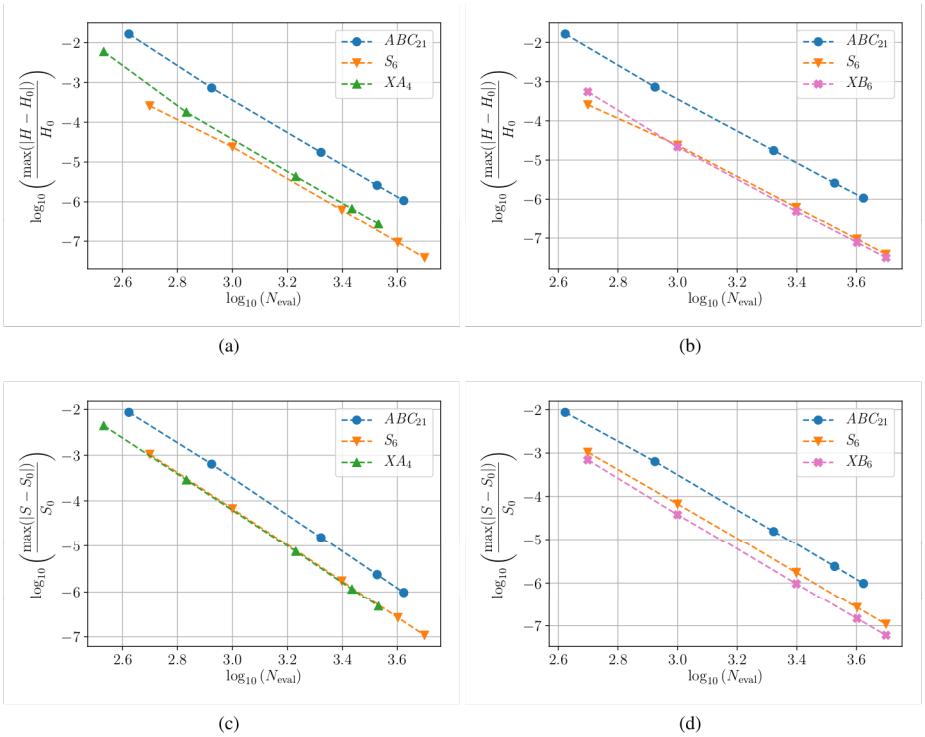
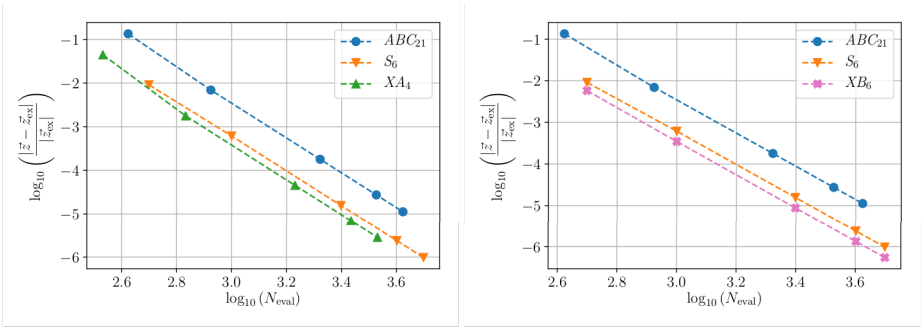


Figure 3: Relative error in conserved quantities for the DDNLS system due to each of the best numerical methods tested. (**a**) Relative error in energy for XA_4 compared to ABC_{21} and S_6. (**b**) Relative error in energy for XB_6 compared to ABC_{21} and S_6. (**c**) Relative error in norm for XA_4 compared to ABC_{21} and S_6. (**d**) Relative error in norm for XB_6 compared to ABC_{21} and S_6.

To compare the performance of the numerical integrators previously considered, we take a lattice of $N = 1000$ sites and fixed boundary conditions, $q_0 = p_0 = q_{N+1} = p_{N+1} = 0$. As in [7, 30], we excite, at the initial time $t = 0$, 21 central sites by taking the q_i at random in the interval $[0, 1]$ and

the respective p_i in such a way that each site has the same constant norm 1, so that the total norm of the system is $S = 21$. Moreover, $\beta = 0.72$, $W = 4$ and the random disorder parameters ϵ_j are chosen so that the total energy is $H \approx -29.63$. As in the previous example, we integrate until the final time $t_f = 10$ and compute the maximum relative error in energy and in norm along the integration interval. The results are depicted in Figure 3, with the top diagrams corresponding to the error in energy and the bottom to the error in norm. The same notation has been used for the tested methods. Finally, in Figure 4 we collect the error in the phase space. As before, the reference solution is obtained with the DOP853 routine. Notice that for this non trivial example the new schemes XA_4 and especially XB_6 show a better efficiency than S_6, and not only with respect to the preservation of the invariants, but also in the computation of trajectories.



(a) (b)

Figure 4: Relative error of trajectories for the DDNLS system. Same as in Figure 3. (**a**) Relative error of trajectories for XA_4 compared to ABC_{21} and S_6. (**b**) Relative error of trajectories for XB_6 compared to ABC_{21} and S_6.

6 Concluding Remarks

In this work we have presented two different families of fourth-order composition methods especially designed for problems that can be separated into three parts in such a way that each part is explicitly solvable. In addition to the usual optimization criteria applied in the literature to choose the free parameters in the composition, we have introduced another one especially oriented to problems where the energy is a constant of motion. The schemes constructed in this way show an improved behavior, and in fact one of the methods exhibits a superior performance to the familiar scheme S_6 of Table 2 on the tested examples. Other relevant examples include certain nonlinear oscillators, Poisson–Maxwell equations arising in plasma physics, and the treatment of non separable Hamiltonian dynamical systems [26].

Although only problems separable into three parts have been considered here, it is clear that the schemes we have introduced can also be applied to differential equations split into any number of pieces $n \geq 3$. The only modification one requires is to formulate the corresponding first order scheme χ_h and its adjoint χ_h^*. One should be aware, however, that augmenting the number n leads to evaluating an increasingly large number of flows for methods with large values of s, with the subsequent deterioration in performance.

An important topic not addressed in this study concerns the stability of the proposed methods. Typically, for a given method there exists a critical step size h^* such that it will be unstable for $|h| > h^*$. Of course, one is interested in methods with h^* as large as possible. The linear stability of splitting methods has been analyzed in particular in [31, 32], where highly efficient schemes

with optimal stability polynomials have presented for numerically approximating the evolution of linear problems. In the nonlinear case, however, the situation is more involved. In [19], a crude measure of the nonlinear stability of a given time symmetric scheme of order r is proposed, taking into account the error terms of orders $r+1$ and $r+3$. The stability of splitting methods in the particular setting of (semidiscretized) partial differential equations with stiff terms have been considered, in particular, in [33, 34]. A theorem is presented [34] concerning the stability of operator-splitting methods applied to linear reaction-diffusion equations with indefinite reaction terms which controls both low and high wave number instabilities. In any case, this result only affects methods up to order 2 with real and positive coefficients, whereas the application of splitting and composition methods of higher order with real coefficients in this setting leads to severe instabilities due to the existence of negative coefficients. The methods we have presented here are aimed at non-stiff problems, and they do not exhibit, at least for the examples we have considered, special step size restrictions in comparison with other splitting methods from the literature.

Finally, it is worth remarking that the local error estimators for composition methods proposed in [35] based on the construction of lower order schemes obtained at each step as a linear combination of the intermediate stages of the main integrator, can also be used in this setting. As a consequence, it is quite straightforward to implement the methods presented here with a variable step size strategy if necessary.

Acknowledgements

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Capítulo 4

Runge–Kutta–Nyström symplectic splitting methods of order 8

Runge–Kutta–Nyström symplectic splitting methods of order 8

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Abstract

Different families of Runge–Kutta–Nyström (RKN) symplectic splitting methods of order 8 are presented for second-order systems of ordinary differential equations and are tested on numerical examples. They show a better efficiency than state-of-the-art symmetric compositions of 2nd-order symmetric schemes and RKN splitting methods of orders 4 and 6 for medium to high accuracy. For some particular examples, they are even more efficient than extrapolation methods for high accuracies and integrations over relatively short time intervals.

Keywords: Runge–Kutta–Nyström splitting methods, high order symplectic integrators

1 Introduction

Second-order systems of ordinary differential equations (ODEs) of the form

$$\ddot{y} \equiv \frac{d^2 y}{dt^2} = g(y), \tag{1.1}$$

where $y \in \mathbb{R}^d$ and $g : \mathbb{R}^d \longrightarrow \mathbb{R}^d$, appear very often in applications, so that special numerical integrators have been designed for them, such as the Runge–Kutta–Nyström (RKN) class of methods. As is well known, if one introduces the new variables $x = (y, v = \dot{y})$ and the maps

$$f_a(x) = f_a(y, v) = (v, 0), \qquad f_b(x) = f_b(y, v) = (0, g(y)), \tag{1.2}$$

then eq. (1.1) is equivalent to

$$\dot{x} = f_a(x) + f_b(x) \tag{1.3}$$

and moreover each subsystem $\dot{x} = f_i(x)$, $i = a, b$, is explicitly integrable, with exact flow

$$\varphi_t^{[a]}(y, v) = (y + tv, v) \qquad \text{and} \qquad \varphi_t^{[b]}(y, v) = (y, v + tg(y)),$$

respectively. An important class of problems leading to equations of the form (1.1) corresponds to Hamiltonian dynamical systems of the form

$$H(q, p) = \frac{1}{2} p^T M^{-1} p + V(q), \tag{1.4}$$

where q and p denote coordinates and momenta, respectively, M is a symmetric positive definite square constant matrix and $V(q)$ is the potential. Then, the corresponding equations of motion can be written as (1.1) with $y = q$, $v = \dot{y} = M^{-1}p$ and $g(y) = -M^{-1}\nabla V(q)$.

Splitting methods constitute a natural option for integrating numerically the initial value problem defined by (1.3). These are schemes of the form

$$\psi_h = \varphi_{ha_s}^{[a]} \circ \varphi_{hb_s}^{[b]} \circ \cdots \circ \varphi_{ha_1}^{[a]} \circ \varphi_{hb_1}^{[b]}, \tag{1.5}$$

where the coefficients a_j, b_j are conveniently chosen so as to achieve high order approximations to the exact flow of (1.3), namely $\varphi_h(x) = \psi_h(x) + \mathcal{O}(h^{r+1})$ for a given order r and step size h. Familiar examples of splitting methods are the so-called Strang/leapfrog/Störmer–Verlet second order schemes:

$$\mathcal{S}_h^{[2]} = \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]}, \tag{1.6}$$

and

$$\mathcal{S}_h^{[2]} = \varphi_{h/2}^{[b]} \circ \varphi_h^{[a]} \circ \varphi_{h/2}^{[b]}. \tag{1.7}$$

In fact, efficient schemes of this class up to order $r = 6$ have been designed along the years (see e.g. [5] and references therein). In addition, they preserve qualitative properties of the continuous system and show a very good behavior with respect to the propagation of errors, especially for long time integrations [11].

There are situations, however, when even higher-order numerical approximations ($r = 8, 10, \ldots$) are required, for instance in problems arising in astrodynamics. In that case, although generic splitting methods exist, they involve such a large number of elementary flows $\varphi_h^{[a]}$, $\varphi_h^{[b]}$, that are not competitive with other integrators. This is so due to the exponential growth with the order r of the required number of conditions to be satisfied to achieve that order [19]. For this reason, palindromic compositions of the form

$$\mathcal{S}_{\alpha_m h}^{[2]} \circ \mathcal{S}_{\alpha_{m-1} h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_2 h}^{[2]} \circ \mathcal{S}_{\alpha_1 h}^{[2]} \qquad \text{with} \quad (\alpha_1, \ldots, \alpha_m) \in \mathbb{R}^m \tag{1.8}$$

and $\alpha_{m+1-i} = \alpha_i$, have been considered instead for order $r > 6$. In practice, schemes (1.8) are the most realistic option when one is interested in integrating (1.3) with high-order ($r = 8, 10, \ldots$) splitting methods.

It turns out, however, that the special structure of (1.2)-(1.3) corresponding to the system (1.1) leads to a reduction in the number of order conditions when $r > 4$ with respect to the generic problem. This allows one to construct highly efficient 4th- and 6th-order splitting methods especially tailored for this class of problems which show a better performance than schemes of the family (1.8) [8, 24]. They can be naturally called *RKN splitting methods*, and the question of the existence of eighth-order schemes, more efficient than methods of type (1.8), formulated some 25 years ago [21, p. 153], still remains unanswered, no doubt due to the technical difficulties involved.

It is our purpose in this note to present new RKN splitting methods of order 8 that provide higher efficiency than state-of-the-art composition methods (1.8) on a variety of examples arising in physical applications. They should then be considered as the natural option when one is interested in integrating numerically problems of the form (1.2)-(1.3) with medium to high precision whereas preserving by construction the main qualitative features of the continuous system.

Remark 1.1 *It turns out that this class of schemes can also be used to solve the slightly more general problem*

$$\ddot{y} = \alpha \dot{y} + \beta y + g(t, y), \tag{1.9}$$

where $\alpha, \beta \in \mathbb{R}^{d\times d}$ are constant: by taking time t as a new coordinate and considering $x = (y, v, t)$, it is clear that equation (1.9) can be again expressed as (1.3), this time with

$$f_a(x) = f_a(y, v, t) = (v, \alpha v + \beta y, 1), \qquad f_b(x) = f_b(y, v, t) = (0, g(t, y), 0), \tag{1.10}$$

and each sub-system being explicitly integrable.

2 Order conditions

As shown e.g. in [4], to each integrator (1.5) one can associate a series $\Psi(h)$ of differential operators given by

$$\Psi(h) = \exp(hb_1F_b)\, \exp(ha_1F_a) \cdots \exp(hb_sF_b)\, \exp(ha_sF_a), \tag{2.1}$$

where F_a, F_b are the Lie derivatives corresponding to f_a and f_b, respectively [3]: for each smooth function $g : \mathbb{R}^d \longrightarrow \mathbb{R}^d$ and $x \in \mathbb{R}^d$ one has

$$F_a\, g(x) = f_a(x) \cdot \nabla g(x), \qquad F_b\, g(x) = f_b(x) \cdot \nabla g(x), \tag{2.2}$$

so that, for the whole integrator, $g(\psi_h(x)) = \Psi(h)g(x)$. For $g(x) = (g_1(x), \ldots, g_d(x))$, we denote

$$f(x) \cdot \nabla g(x) \equiv (f(x) \cdot \nabla g_1(x), \ldots, f(x) \cdot \nabla g_d(x))$$

in eq. (2.2). The main advantage of using the series $\Psi(h)$ for representing the method ψ_h is that one can formally apply the Baker–Campbell–Hausdorff formula [28] and express $\Psi(h)$ as only one exponential,

$$\Psi(h) = \exp(F(h)), \qquad \text{with} \qquad F(h) = \sum_{j\geq 1} h^j F_j, \tag{2.3}$$

and each F_j is a linear combination of nested commutators involving j operators F_a and F_b whose coefficients are polynomials of degree j in the coefficients a_i, b_i. A method of order r requires that $F_1 = F_a + F_b$ for consistency, and $F_j = 0$ for $1 < j \leq r$. These constraints in turn lead to a set of polynomial equations to be satisfied by the coefficients of the splitting method. The number n_r of such order conditions at each r is collected in Table 1 [19]. For comparison, we also include the number s_r of order conditions for compositions of the form (1.8)

As is well known, if the composition (1.5) is left-right palindromic, then all the order conditions at even order are automatically satisfied and the method is time-symmetric. For systems of the form (1.2)-(1.3), the flow $\varphi_h^{[b]}$ is typically the most expensive part to evaluate (for the Hamiltonian (1.4), it corresponds essentially

r	1	2	3	4	5	6	7	8	9	10
s_r	1	0	1	1	2	2	4	5	8	11
n_r	2	1	2	3	6	9	18	30	56	99
ℓ_r	2	1	2	2	4	5	10	14	25	39

Table 1: Number of independent order conditions (at order r) of compositions of symmetric second order methods of the form (1.8), s_r, of splitting methods in the general case, n_r, and in the RKN case, ℓ_r.

to the force $\nabla V(q)$). It makes sense, then, to characterize a given splitting method according to the number of flows $\varphi_h^{[b]}$ involved. This is called the *number of stages* of the method. Notice that, if the Strang splitting is used as the scheme $\mathcal{S}_h^{[2]}$ in the composition (1.8), the number of stages is also m.

From Table 1 it is then straightforward to estimate the minimum number of stages to achieve an even order $r = 2k$. For the composition (1.8) and the general splitting (1.5) these values are, respectively,

$$S_r = 2\sum_{i=1}^{k} s_{2k-1} - 1, \qquad N_r = \sum_{i=1}^{k} n_{2k-1} - 1,$$

and are collected in Table 2 up to $r = 2k = 10$. Notice that, when counting the number of stages per step, we have used the so–called FSAL (First Same As Last) property: the last map in one step can be saved in the following one and does not count for the total number of stages.

r	2	4	6	8	10
S_r	1	3	7	15	31
N_r	1	3	9	27	83
L_r	1	3	7	17	42

Table 2: Minimum number of stages required to achieve order $r = 2k$ with symmetric compositions (1.8), S_r, with general splitting (1.5), N_r, and for RKN splitting methods, L_r.

The number of order conditions to be solved for each family of methods is, respectively, $(S_r + 1)/2$ and $N_r + 1$. It is clear that symmetric compositions (1.8) require to solve a considerably smaller number of order conditions to achieve high order methods. On the other hand, the space of solutions is significantly larger in the case of general splitting methods, and consequently also the chance of finding highly efficient schemes within this class. Thus, in particular, the general splitting methods of order four and six presented in [8] outperform compositions (1.8) of the same order. At order eight, however, one has to solve a system of 28 polynomial equations for general splitting methods, and although it seems quite likely that very efficient solutions exist, to carry out out a thorough analysis constitutes a formidable task.

Notice that for systems of the form (1.2)-(1.3) one has further restrictions: since $F_a = v\,\nabla_y$, and $F_b = g(y)\nabla_v$, one has for symmetric methods

$$[F_b, [F_a, F_b]] = \tilde{g}(y)\nabla_v, \qquad \text{with} \qquad \tilde{g}(y) = 2\,\nabla_y g(y)\cdot g(y),$$

where $[F_a, F_b] = F_aF_b - F_bF_a$, etc. In consequence, $[F_b, [F_b, [F_a, F_b]]] \equiv 0$, and many terms in (2.3) vanish identically, so that their order conditions can be ignored. This can be seen in the last row of Tables 1 and 2,

where we collect the order conditions ℓ_r and the the minimum number of stages,

$$L_r = \sum_{i=1}^{k} \ell_{2k-1} - 1$$

up to $r = 10$. Notice that, whereas the reduction up to $r = 6$ with respect to general splitting methods is only of two equations, for a time-symmetric method of order $r = 8$ one has to solve 18 order conditions (instead of 28). This problem, although more amenable, is still far from trivial. In addition, to get significant solutions, the relevant issue here is whether the resulting 8th-order RKN splitting schemes are competitive in terms of the number of flows involved with methods within the class (1.8).

Remark 2.1 *With respect to the more general system* (1.9)-(1.10)*, one has*

$$F_a = v\,\nabla_y + (\alpha v + \beta y)\nabla_v + 1\cdot\partial_t, \qquad F_b = g(t,y)\nabla_v,$$

so that

$$[F_b,[F_a,F_b]] = \tilde{g}(t,y)\nabla_v, \qquad \text{with} \qquad \tilde{g}(y) = 2\nabla_y g(t,y)\cdot g(t,y)$$

and therefore $[F_b,[F_b,[F_a,F_b]]] \equiv 0$ *also here.*

Before starting a systematic search of solutions to the order conditions, it seems appropriate to make explicit several considerations:

1. Due to the different qualitative character of the operators F_a and F_b, it is clear that the role of $\varphi_h^{[a]}$ and $\varphi_h^{[b]}$ in (1.5) is not interchangeable, and so two different orderings have to be considered. Specifically, we will analyze two types of composition:

$$\mathcal{A}_s = \varphi^{[a]}_{ha_{s+1}} \circ \varphi^{[b]}_{hb_s} \circ \varphi^{[a]}_{ha_s} \circ \cdots \circ \varphi^{[b]}_{hb_1} \circ \varphi^{[a]}_{ha_1}, \tag{2.4}$$

   with $a_{s+2-i} = a_i$, $b_{s+1-i} = b_i$, and

$$\mathcal{B}_s = \varphi^{[b]}_{hb_{s+1}} \circ \varphi^{[a]}_{ha_s} \circ \varphi^{[b]}_{hb_s} \circ \cdots \circ \varphi^{[a]}_{ha_1} \circ \varphi^{[b]}_{hb_1}, \tag{2.5}$$

   with $b_{s+2-i} = b_i$, $a_{s+1-i} = a_i$. Since for methods (2.4) and (2.5) one can always apply the FSAL property, we say that both schemes involve the same number s of stages.

2. Very often, compositions with a higher number of stages than the minimum required to solve the order conditions are considered in the literature. This is so because, typically, (i) methods with the minimum number of stages show a poor performance, and (ii) the presence of free parameters allows one to optimize the schemes according with some appropriate criteria, so that the extra computational cost is compensated by the reduction in the error. Thus, in particular, 8th-order methods within the class (1.8) with 17, 19 and 21 stages exist that are more efficient than schemes with the minimum number $m = 15$. Notice in this respect that the minimum number of stages for a RKN splitting method of order 8 is $s = 17$. Although one such method of the form $\mathcal{A}_s$ was proposed in [23], the numerical results collected there show no clear improvement with respect to the 8th-order method of type (1.8) with $m = 24$ presented in [9].

3. Given a method ψ_h, one may consider a near-to-identity map π_h so that the integrator $\hat{\psi}_h = \pi_h^{-1} \circ \psi_h \circ \pi_h$ is more accurate than ψ_h, for instance, by increasing its order. In this context, ψ_h is called the kernel of the processed method $\hat{\psi}_h$, and π_h is the processor or corrector. Notice that N consecutive steps correspond to $\hat{\psi}_h^N = \pi_h^{-1} \circ \psi_h^N \circ \pi_h$, i.e., the cost of applying the processed scheme is basically the cost of the kernel. This technique allows one to separate the order conditions into two sets: the conditions satisfied by the kernel itself, and those to be verified by the processor. As a result, it is possible to construct high-order RKN splitting methods involving a reduced number of stages in the kernel, although building a particular processor is far from trivial. Methods of this class have been presented in [6, 7], so that they will not be considered here.

4. For the initial value problem defined by (1.2)-(1.3), it is possible to include in the compositions (2.4) and (2.5) the flows generated by other vector fields lying in the Lie algebra generated by F_a and F_b. For instance, one could use the h-flow of the vector fields $[F_b, [F_a, F_b]]$, $[F_b, [F_b, [F_a, [F_a, F_b]]]]$, and other more general nested commutators [6, 7]. These give rise to the so-called 'modified potentials', and allow one to reduce the number of stages (although at the price of an additional computational cost to evaluate the flows). Methods of this class with and without processing have been analyzed in particular in [6] and [24]. Here, by contrast, we are only interested in standard compositions (2.4)-(2.5).

3 New methods of order 8

We next analyze families of schemes (2.4) and (2.5) involving $s = 17, 18$ and 19 stages, so that one always has enough parameters in the compositions to solve the order conditions. Of course, even with the minimum number of parameters, these order conditions possess a large number of real solutions, so that some criterion has to be adopted to select "good" methods. As is customary in the literature, and assuming h is sufficiently small and g is sufficiently smooth, we propose to take the leading term in the asymptotic expansion of the modified vector field associated with the integrator as the main contribution to the truncation error. Without any specific assumption on the function g, we take this error as $(\sum_{i=1}^{25} k_{9,i}^2)^{1/2}$. Here $k_{9,i}$ are the coefficients of the asymptotic expansion of the modified vector field at order h^9 when it is expressed as a linear combination of the 25 independent nested commutators involving 9 operators F_a and F_b. This corresponds to the subspace of the Lie algebra generated by F_a and F_b with the commutator as the Lie bracket (for more details, see [20, 18]). To take into account the computational cost, we multiply this error by the number of stages s, thus resulting in the following effective error for a method of order 8,

$$E_{\mathrm{f}} = s \cdot \left(\sqrt{\sum_{i=1}^{25} k_{9,i}^2} \right)^{1/8}, \tag{3.1}$$

which should be minimized by the integrator. One has to take into account, however, that the expression of E_{f} depends on the particular basis of nested commutators one is considering and that we are also assuming that all these commutators contribute in a similar way, something that is not guaranteed to take place in all applications. It makes sense, then, to introduce other quantities as possible estimators of the error committed. In particular, it has been noticed that large coefficients a_i, b_i in the splitting method usually leads to large truncation errors, since the expressions of $k_{\ell,j}$ for $\ell \geq 9$ depend on increasingly higher powers of these

coefficients. For this reason, we also keep track of the quantities

$$\Delta \equiv \sum_{i=1}^{s} (|a_i| + |b_i|) \qquad \text{and} \qquad \delta \equiv \max_{i=1}^{s} (|a_i|, |b_i|) \tag{3.2}$$

and eventually discard solutions with large values of Δ and/or δ. By following a similar approach as for instance in [8, 24], we will select particular schemes with small values of $E_{\rm f}$, Δ and δ, and then we will test them on an array of numerical examples to check their efficiency in practice.

$s = 17$ stages. In this case one has as many parameters as order conditions, 18 in total. Given the complexity of the problem, it is not possible to solve these nonlinear equations with a computer algebra system, and so one has to turn to numerical techniques. Specifically, they are solved with the Python [27] function `fsolve` of the *SciPy* library [29], a wrapper of the classic subroutines HYBRD and HYBRJ of MINPACK [22]. The algorithm is based on a modification of the Powell hybrid method and involves the choice of the correction as a convex combination of the Newton method and scaled gradient directions and the updating of the Jacobian by the rank-1 method (except at the starting point, where it is approximated by forward differences). Since we are not interested in methods with large values of δ, a uniform distribution in the interval $[-1, 1]$ in each variable was taken to generate about 2×10^6 initial points to start the procedure,

When a composition of type $\mathcal{A}_s$ is considered, we have obtained 376 real solutions that cannot be obtained as a composition of 2nd-order symmetric schemes (1.8), with parameters $E_{\rm f} \in [2.77, 18.05]$ and $\Delta \in [8.40, 63.05]$, respectively. Among these, we select those solutions within the more restricted range $E_{\rm f} \in [2.86, 3.45]$ and $\Delta \in [8.42, 19.30]$ and check them on the test problems of sections 4 and 5. Finally, we have chosen the scheme whose coefficients are listed in Table 4, and parameters given in Table 3. The final values of the coefficients (with 30 digits of accuracy) have been obtained by taking the solution found by `fsolve` as the starting point of the function `FindRoot` of *Mathematica*. The method can be represented in the compact form

$$\begin{aligned} \mathcal{A}_{17} \equiv (&a_1, b_1, a_2, b_2, a_3, b_3, a_4, b_4, a_5, b_5, a_6, b_6, a_7, b_7, a_8, b_8, a_9, b_9, \\ &a_9, b_8, a_8, b_7, a_7, b_6, a_6, b_5, a_5, b_4, a_4, b_3, a_3, b_2, a_2, b_1, a_1). \end{aligned} \tag{3.3}$$

For compositions of type $\mathcal{B}_s$, by applying the same methodology, we have found 149 different solutions out of more than 1.2×10^6 starting points. We have selected the four solutions in the region $E_{\rm f} \in [2.80, 3.85]$, $\Delta \in [7.30, 9.95]$ and finally we take the one whose coefficients are collected in Table 5. The method thus reads

$$\begin{aligned} \mathcal{B}_{17} \equiv (&b_1, a_1, b_2, a_2, b_3, a_3, b_4, a_4, b_5, a_5, b_6, a_6, b_7, a_7, b_8, a_8, b_9, a_9 \\ &b_9, a_8, b_8, a_7, b_7, a_6, b_6, a_5, b_5, a_4, b_4, a_3, b_3, a_2, b_2, a_1, b_1). \end{aligned} \tag{3.4}$$

$s = 18$ stages. With one more stage we have one free parameter that can be used to get in principle smaller values of the effective error and eventually more efficient schemes, as is common in the literature. Notice that the problem in this case involves solving a system of 18 polynomial equations with 19 variables. Our strategy is the following: for a composition of type $\mathcal{A}_s$ with $s = 18$, we take a_1 as the free parameter, and explore the interval $a_1 \in [0, 1]$ (since we are interested in small values of the coefficients) by fixing each time

	E_{f}	Δ	δ
$\mathcal{A}_{17}$	3.45	8.42	0.5459 ($\lvert a_9\rvert$)
$\mathcal{A}_{18}$	3.65	7.42	0.6406 ($\lvert a_9\rvert$)
$\mathcal{A}_{19}$	2.76	5.98	0.4237 ($\lvert a_4\rvert$)
$\mathcal{B}_{17}$	2.80	8.93	0.6355 ($\lvert a_5\rvert$)
$\mathcal{B}_{18}$	3.44	9.68	0.9303 ($\lvert a_4\rvert$)
$\mathcal{B}_{19}$	3.41	6.94	0.5238 ($\lvert a_6\rvert$)

Table 3: Effective error E_{f}, 1- and ∞-norm of the vector of coefficients for different 8th-order RKN splitting methods of type $\mathcal{A}_s$ and $\mathcal{B}_s$.

the value of a_1. Starting with 2×10^6 initial points, we have found 722 valid solutions, the most promising corresponding to the choice $a_1 = 0.08$. This solution is then taken as the starting point of an arc-length continuation method and follow the solution along the curve leading to a local minimum of the 1-norm of the vector of coefficients. In doing so we apply the algorithm presented in [1, 2]. After this process, we check several methods in practice and finally the solution $\mathcal{A}_{18}$ collected in Table 4, with E_{f}, Δ and δ given in Table 3.

The same technique is applied to compositions $\mathcal{B}_{18}$ leading to the solution collected in Table 5 after 1070748 initial points and the application of arc-length continuation.

$s = 19$ **stages.** Adding an additional stage and so forming the composition $\mathcal{A}_{19}$, we have explored the space of parameters in the region $a_1, a_2 \in [0.05, 0.15]$, where we have found 295 valid solutions. Then, we start from the one with best parameters and apply the following strategy: let us denote by $\mathbf{u}_0$ the vector of coefficients of this initial solution. Then we generate a random vector α verifying $\alpha \cdot (\mathbf{u} - \mathbf{u}_0) = 0$. Now we apply continuation along the curve that results from the intersection of the space of solutions (with 2 free parameters) with the random generated hyperplane. The final solution is collected in Table 5.

Concerning the composition $\mathcal{B}_{19}$, 173 solutions have been obtained out of more than 1.3×10^6 initial points. After applying the previous technique, we arrive at the solution reported in Table 5.

Although the quantities (3.1) and (3.2) provide useful information about the quality and relative performance of the methods, one should have in mind that the size of the error terms and therefore the efficiency of each scheme ultimately depends on the particular problem one is considering and even on the initial conditions. For this reason it is convenient to check the behavior of the different schemes on a variety of differential equations and initial conditions, and also to compare them with other efficient numerical integrators available in the literature. We have separated the numerical illustrations into two sections. Thus, in section 4 we compare the new schemes with symmetric compositions (1.8) of order 8, whereas in section 5 we also consider RKN splitting integrators of orders 4 and 6, as well as extrapolation methods.

	a_i	b_i
$\mathcal{A}_{17}$	$a_1 = 0.052092434384033900642603796835 3$	$b_1 = 0.14585030481264473160809660987 7$
	$a_2 = 0.225287493267702165807274831864$	$b_2 = 0.255156544139293944162028807345$
	$a_3 = 0.416276189612257117795363856737$	$b_3 = 0.018133468820831725136146068404 1$
	$a_4 = -0.384567270213950399652168569029$	$b_4 = -0.179040110299264554587007062749$
	$a_5 = 0.099727178347051481667454758936 9$	$b_5 = -0.118470801433302245053382954342$
	$a_6 = -0.108833834399100218757003157958$	$b_6 = 0.186461689273821083344937258279$
	$a_7 = 0.222010736648991680848341975522$	$b_7 = 0.459041581767136840219244627361$
	$a_8 = 0.523879522036734296002247438223$	$b_8 = -0.003660836270318358975321459399$
	$a_9 = \frac{1}{2} - \sum_{i=1}^{8} a_i$	$b_9 = 1 - 2\sum_{i=1}^{8} b_i$

	a_i	b_i
$\mathcal{A}_{18}$	$a_1 = 0.086600382271244592013580595446 2$	$b_1 = -0.08$
	$a_2 = -0.023157273542438807022871469375 3$	$b_2 = 0.209460550048243262121199483001$
	$a_3 = 0.191410576083774088999564416369$	$b_3 = 0.274887805875735483503233064415$
	$a_4 = 0.378895558692931579545387584925$	$b_4 = -0.224214208870409561366168655624$
	$a_5 = -0.046735956636455611159948552605 1$	$b_5 = 0.347657740563761656321390026010$
	$a_6 = -0.156198111997810415438979605642$	$b_6 = -0.168783183866211679175007668385$
	$a_7 = 0.156025836895094823718831871041$	$b_7 = 0.144209344805460873709120777707$
	$a_8 = 0.252844012473796333586850465807$	$b_8 = 0.011685112136026548338140505424 4$
	$a_9 = -0.640644212172254239866860564270$	$b_9 = \frac{1}{2} - \sum_{i=1}^{8} b_i$
	$a_{10} = 1 - 2\sum_{i=1}^{9} a_i$	

	a_i	b_i
$\mathcal{A}_{19}$	$a_1 = 0.0505805$	$b_1 = 0.12947860656053673066249379439 5$
	$a_2 = 0.149999$	$b_2 = 0.222257260092671143423043559581$
	$a_3 = -0.055179551077161557351102695036 1$	$b_3 = -0.057751489332514720475702324632 0$
	$a_4 = 0.423755898835337951482264998051$	$b_4 = -0.057831226210392491022134503276 3$
	$a_5 = -0.213495353584659048059672194633$	$b_5 = 0.103087297437175356747933252265$
	$a_6 = -0.068076977457403261911163073627 4$	$b_6 = -0.140819612554090768205554103887$
	$a_7 = 0.227917056974013435948887201671$	$b_7 = 0.023446260349282627669971371862 6$
	$a_8 = -0.235373619381058906524740047732$	$b_8 = 0.134854517356684096617882205068$
	$a_9 = 0.387413869179878047816794031058$	$b_9 = 0.028797382107377930634517216021 1$
	$a_{10} = \frac{1}{2} - \sum_{i=1}^{9} a_i$	$b_{10} = 1 - 2\sum_{i=1}^{9} b_i$

Table 4: Coefficients of 8th-order RKN splitting methods of type $\mathcal{A}_s$, with $s = 17$, 18 and 19 stages.

4 Numerical tests I: 8th-order schemes

The first set of examples is intended to illustrate the performance of the new RKN splitting methods in comparison with the most efficient symmetric compositions of the form (1.8) we have found in the literature. In addition, we also include in the tests the only 8th-order RKN splitting method with 17 stages. Specifically, in addition to the previous $\mathcal{A}_s$ and $\mathcal{B}_s$ schemes, we consider the following 8th-order integrators:

	a_i	b_i
$\mathcal{B}_{17}$	$a_1 = 0.160227696073839513690970240076$	$b_1 = 0.051419614253721007343152693459$
	$a_2 = 0.306354507436867319879440957100$	$b_2 = 0.250497030318342871458417941091$
	$a_3 = 0.308395508895171191756544975556$	$b_3 = 0.512412268300327350035492806653$
	$a_4 = 0.120362086566233408450063177659$	$b_4 = -0.231597138650894401279645184364$
	$a_5 = -0.622888687549183872072186218718$	$b_5 = 0.116091323536875759881216298975$
	$a_6 = 0.635560951632990078378672016548$	$b_6 = -0.009836517324696576398576303428 3$
	$a_7 = -0.144226974795419229640437363913$	$b_7 = -0.108032771466281638634277563747$
	$a_8 = -0.284867527074173816678992817545$	$b_8 = 0.249039864198023642002940910070$
	$a_9 = 1 - 2\sum_{i=1}^{8} a_i$	$b_9 = \frac{1}{2} - \sum_{i=1}^{8} b_i$

	a_i	b_i
$\mathcal{B}_{18}$	$a_1 = 0.144410089394373457971755553148$	$b_1 = 0.045$
	$a_2 = 0.911935520865154315536815857376$	$b_2 = 0.459016679491512416807266107555$
	$a_3 = -0.000729329098373926551611999968 44$	$b_3 = -0.045655344559433315322365535275 7$
	$a_4 = -0.930317101800698721159455541447$	$b_4 = 0.045703102040184100319264809655 9$
	$a_5 = 0.253804074671714046593439154323$	$b_5 = -0.216814341025322492810152535338$
	$a_6 = 0.147948981530918626913598733391$	$b_6 = 0.163168264552484857133047358600$
	$a_7 = -0.448814759614614928125216243784$	$b_7 = -0.085708031981437621938985003943 0$
	$a_8 = 0.082412398079458010675123719541 8$	$b_8 = 0.026574581065052346614292209359 1$
	$a_9 = \frac{1}{2} - \sum_{i=1}^{8} a_i$	$b_9 = -0.036553833299289322014709615067 5$
		$b_{10} = 1 - 2\sum_{i=1}^{9} b_i$

	a_i	b_i
$\mathcal{B}_{19}$	$a_1 = 0.337548675291317241942440116575$	$b_1 = 0.036132460472136313416730168194$
	$a_2 = -0.223647977575409990331768222380$	$b_2 = 0.012697863961074113381675193011$
	$a_3 = 0.168949714872223740906385138015$	$b_3 = 0.201318391240629276109068041836$
	$a_4 = 0.171179938816205886154783136334$	$b_4 = 0.135683350134504233201330671671$
	$a_5 = -0.349765168067292877221144631312$	$b_5 = -0.057907183399996304150474066301 5$
	$a_6 = 0.523808861006312397712070357524$	$b_6 = -0.077250950179264954946387493182 1$
	$a_7 = -0.194208871063049124066394765282$	$b_7 = -0.002647582664099259528222161203471$
	$a_8 = -0.323496751337931087309823477561$	$b_8 = -0.032984438494560306532079753735 5$
	$a_9 = 0.322817287614899749216601693799$	$b_9 = 0.047678156095036692753064628975 5$
	$a_{10} = 1 - 2\sum_{i=1}^{9} a_i$	$b_{10} = \frac{1}{2} - \sum_{i=1}^{9} b_i$

Table 5: Coefficients of 8th-order RKN splitting methods of type $\mathcal{B}_s$, with $s = 17$, 18 and 19 stages.

- $\mathcal{O}_{17}$: the RKN splitting method of type $\mathcal{A}_s$ presented in [23], with $s = 17$ stages.
- $\mathcal{SS}_{17}$: the symmetric composition of $m = 17$ symmetric 2nd-order methods of the form (1.8) obtained in [15] (the coefficients are also collected in [11, p. 157]).
- $\mathcal{SS}_{19}$ and $\mathcal{SS}_{21}$: schemes (1.8) with $m = 19$ and $m = 21$, respectively, presented in [25].

These $\mathcal{SS}_m$ methods have been shown to be the most efficient 8th-order schemes within the family of compo-

sition methods (1.8). We collect in Table 6 the corresponding values of the quantities $E_{\rm f}$ and Δ for methods $\mathcal{SS}_m$ when they are used with $\mathcal{S}_h^{[2]}$ as in (1.6) (ABA) or (1.7) (BAB). The values of $E_{\rm f}$ are always greater when the basic scheme is (1.7).

The implementation of all the integrators has been done in Python 3.7 [27] running on Debian GNU/Linux 10 [16] and the array operations have been coded using the *NumPy* library [13].

	$E_{\rm f}$		Δ
	ABA	BAB	
$\mathcal{O}_{17}$	4.78	–	16.63
$\mathcal{SS}_{17}$	3.12	3.30	8.33
$\mathcal{SS}_{19}$	2.66	2.68	6.84
$\mathcal{SS}_{21}$	2.59	2.88	6.43

Table 6: Effective error $E_{\rm f}$ and 1-norm of the vector of coefficients for 8th-order symmetric compositions of symmetric methods $\mathcal{SS}_m$ and the RKN splitting method of [23].

Example 1: Kepler problem. We take the 2-body gravitational problem with Hamiltonian

$$H(q,p) = \frac{1}{2}p^T p - \mu\frac{1}{r}, \tag{4.1}$$

where $q = (q_1, q_2), p = (p_1, p_2)$, $\mu = GM$, G is the gravitational constant and M is the sum of the masses of the two bodies. We take $\mu = 1$ and initial conditions

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \tag{4.2}$$

so that the trajectory corresponds to an ellipse of eccentricity e, with period 2π and energy $E = -\frac{1}{2}$. We first check the order of the new RKN splitting methods and compare their efficiency with respect to $\mathcal{O}_{17}$. Thus, Figure 1 (left panel) shows the relative error in energy with respect to s/h (which is proportional to the number of force evaluations) for $e = 0.5$ and a final time $t_f = 1000$ for methods of type $\mathcal{A}_s$, whereas in the right panel we explore the range of eccentricities $0 \le e \le 0.8$. All schemes involve the same number of evaluations of the potential in this case. Figure 2 shows analogous results for methods of type $\mathcal{B}_s$. Notice that the order 8 is clearly visible in the figures and that the new methods are more efficient than $\mathcal{O}_{17}$. The improvement is particularly prominent for $\mathcal{A}_{17}$ and specially $\mathcal{A}_{19}$ (up to four orders of magnitude for the same value of h/s) and is more moderate for methods $\mathcal{B}_s$. In fact, all of them show essentially the same performance, which is lower than that of $\mathcal{A}_{19}$.

We next carry out the same experiment, but in this case we compare the performance of the new schemes $\mathcal{A}_{17}$ and $\mathcal{A}_{19}$ with the previous state-of-the-art symmetric compositions of the Strang splitting $\mathcal{SS}_m$, $m = 17, 19, 21$. We take the composition (1.6) as the basic $\mathcal{S}_h^{[2]}$ method because it shows the best performance in the numerical experiments. The corresponding results are shown in Figure 3. We notice that $\mathcal{A}_{19}$ is the more efficient method for the whole range of eccentricities explored.

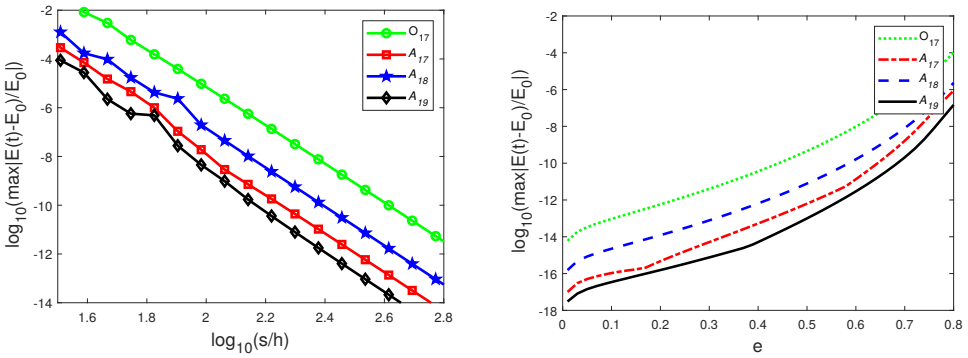


Figure 1: (a) Efficiency diagram for the Kepler problem with $e = 0.5$ for all RKN splitting methods of $\mathcal{A}_s$ type. The final time is $t_f = 1000$. (b) Maximum error in energy for different values of the eccentricity with $t_f = 1000$ and $s/h = 340$.

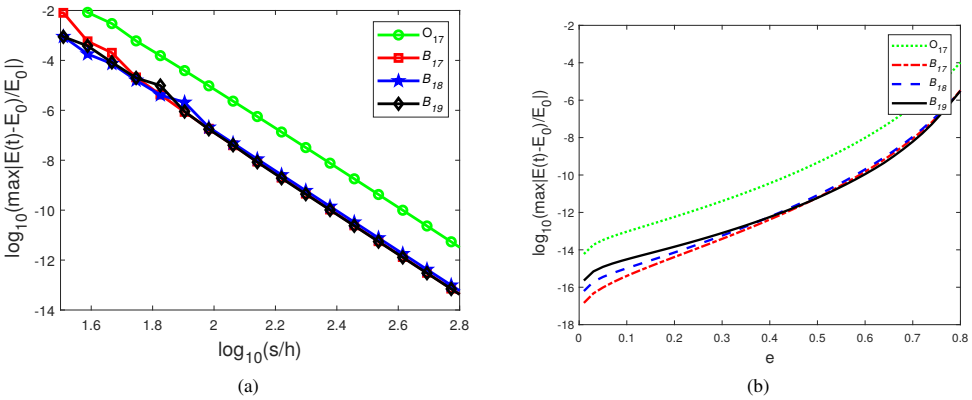
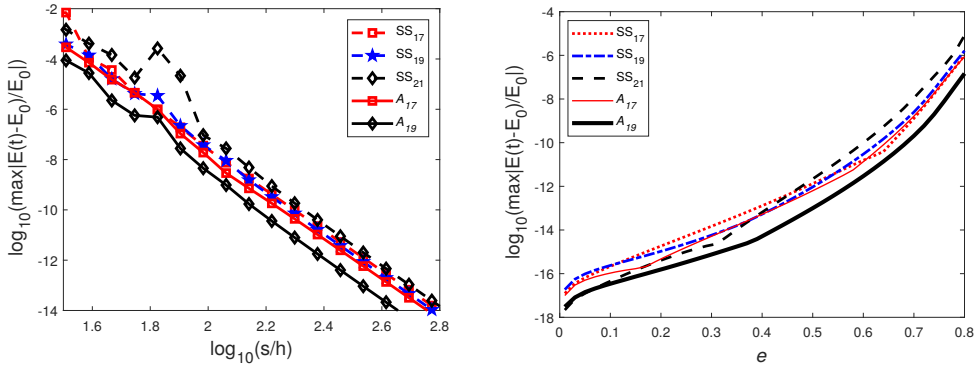


Figure 2: (a) Efficiency diagram for the Kepler problem with $e = 0.5$ for all RKN splitting methods of $\mathcal{B}_s$ type. The final time is $t_f = 1000$. (b) Maximum error in energy for different values of the eccentricity with $t_f = 1000$ and $s/h = 340$.

Example 2: simple pendulum. Our next example is the simple mathematical pendulum. In appropriate units, it corresponds to the 1-degree-of-freedom Hamiltonian system with

$$H(q,p) = \frac{1}{2}p^2 - \cos q. \tag{4.3}$$



(a) (b)

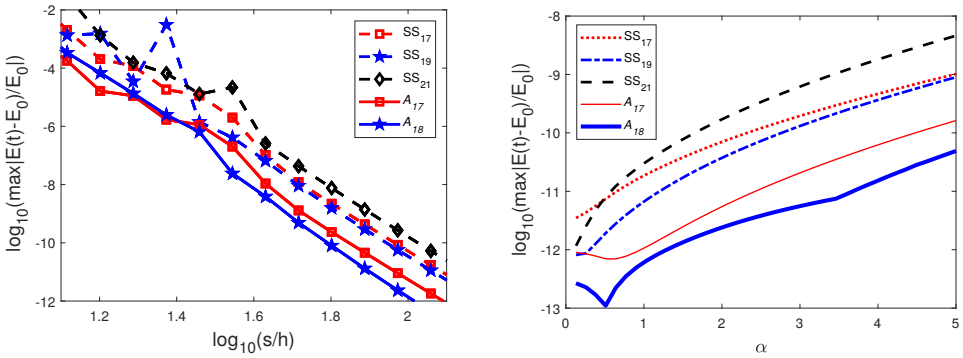
Figure 3: (a) Efficiency diagram for the Kepler problem with $e = 0.5$ for composition $\mathcal{SS}_m$ and the new RKN splitting methods $\mathcal{A}_{17}$ and $\mathcal{A}_{19}$. Final time $t_f = 1000$. (b) Maximum error in energy for different values of the eccentricity with $t_f = 1000$ and $s/h = 340$.

We explore the set of initial conditions $(q, p) = (0, \alpha)$, with $0 \leq \alpha \leq 5$, integrate until the final time $t_f = 1000$ and check the error in energy along the integration. Since the error achieved by $\mathcal{O}_{17}$ is always 3-4 orders of magnitude larger than the new schemes, we no longer include them in the diagrams, so that we only compare with symmetric compositions $\mathcal{SS}_m$. Figure 4 shows the efficiency diagram corresponding to $\alpha = 3$ (panel (a)) and the maximum of the relative error in the energy along the integration interval. In this case, the new schemes $\mathcal{A}_{17}$ and $\mathcal{A}_{18}$ are the most efficient. Scheme $\mathcal{A}_{19}$ shows a similar behavior as $\mathcal{SS}_{19}$, and thus it has not been included in the diagrams. On the other hand, the most efficient scheme of the BAB type in this case is $\mathcal{B}_{18}$ (not shown), providing similar results as $\mathcal{A}_{18}$.

Example 3: Hénon–Heiles potential. For our next experiment we choose the well known two-degrees of freedom Hénon–Heiles Hamiltonian [14]

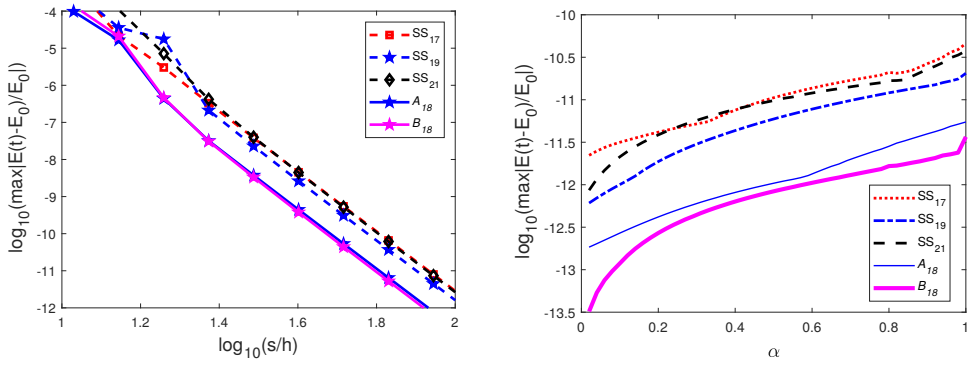
$$H = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3. \tag{4.4}$$

It has been the subject of extensive numerical experimentation and is considered, in particular, as a model problem to characterize the transition to Hamiltonian chaos. In this case we take the same initial conditions as in [8], the set $(q_1, q_2, p_1, p_2) = (\alpha/2, 0, 0, \alpha/4)$, with $0 \leq \alpha \leq 1$. The corresponding results are depicted in Figure 5. In this case $\mathcal{B}_{18}$ and $\mathcal{A}_{18}$ are the most efficient schemes, whereas $\mathcal{A}_{17}$ is similar as $\mathcal{A}_{18}$ and it is not shown in the figure.



(a) (b)

Figure 4: Simple pendulum. (a) Efficiency diagram for $\alpha = 3.0$ and final time $t_f = 1000$. (b) Maximum error in energy for initial conditions $(q_0, p_0) = (0, \alpha)$ for $\mathcal{SS}$ and the best RKN methods at final time $t_f = 1000$ with $s/h = 85$.



(a) (b)

Figure 5: Hénon–Heiles Hamiltonian. (a) Efficiency diagram with initial condition corresponding to $\alpha = 0.2$ and final time $t_f = 1000$. (b) Maximum error in energy for $0 \leq \alpha \leq 1$ at final time $t_f = 1000$ with $s/h = 85$.

Example 4: Schrödinger equation with Pöschl–Teller potential. Finally, we apply our integrators to the one-dimensional Schrödinger equation ($\hbar = 1$)

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t), \tag{4.5}$$

with the well known Pöschl–Teller potential [10],

$$V(x) = -\frac{\lambda(\lambda+1)}{2}\mathrm{sech}^2(x), \tag{4.6}$$

with $\lambda(\lambda+1) = 10$. When a Fourier spectral collocation method is used for discretizing in space [26], one ends up with the N-dimensional linear ODE

$$i\frac{d}{dt}u(t) = H\,u(t) \equiv (T+V)\,u(t), \qquad u(0) = u_0 \in \mathbb{C}^N, \tag{4.7}$$

where T is a (full) differentiation matrix related with the kinetic energy, V is a diagonal matrix associated with the potential and the components of the vector u are the approximations to the wave function at the nodes, $u_n \approx \psi(x_n, t)$. The action of T on the wave function vector u is then carried out by the forward and backward discrete Fourier transform (computed with the FFT algorithm) [17]. The initial condition is taken as $\psi_0(x) = \sigma\,\mathrm{e}^{-x^2/2}$, with σ a normalizing constant, the interval is $x \in [-8, 8]$ with $N = 256$ nodes, and the integration is done until the final time $t_f = 1000$. In this case we check the error in the expected value of the energy,

$$\text{energy error:} \quad |u^*_{\mathrm{ap}}(t)\cdot(Hu_{\mathrm{ap}}(t)) - u_0^*\cdot(Hu_0)|, \tag{4.8}$$

where $u_{\mathrm{ap}}(t)$ stands for the numerical approximation obtained by each method. The results are shown in Figure 6. Observe that the new RKN splitting method $\mathcal{A}_{19}$ is also the most efficient in this setting.

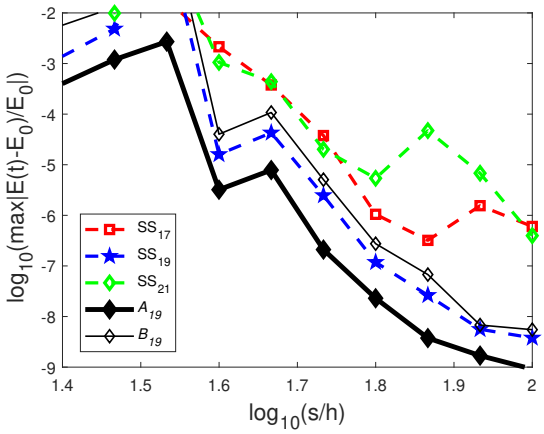


Figure 6: Efficiency diagram of different methods. Schrödinger equation with Pöschl–Teller potential.

5 Numerical tests II: RKN splitting and extrapolation methods

Given the observed improvement of the new 8th-order RKN splitting methods with respect to the symmetric compositions of a basic 2nd-order symmetric scheme, it seems appropriate to carry out further comparisons

with other lower-order RKN splitting methods when medium to high accuracy is desired. Specifically we consider the following optimized 4th- and 6th-order methods of type $\mathcal{B}_s$ presented in [8]:

- RKN4_6: order 4 with 6 stages (the scheme SRKN$_6^b$ in [8]).
- RKN6_{11}: order 6 with 11 stages (the scheme SRKN$_{11}^b$ in [8]).

On the other hand, extrapolation methods constitute one of the most efficient classes of schemes for the numerical integration of the second order differential equation (1.1) when high accuracy is required [12]. Notice, however, that in contrast with RKN splitting methods, they do not preserve by construction geometric properties of the exact solution. To carry out our comparisons, we take (1.6) as the symmetric second order basic method (which corresponds to *Störmer's rule* [12, eq. (14.32)]) and apply the harmonic sequence to construct by extrapolation schemes of orders 4, 6 and 8 with only 3, 6 and 10 stages, respectively. For completeness, the resulting methods can be written explicitly as

$$\Psi_{(r=2k)} = \sum_{\ell=1}^{k} \alpha_\ell^{(k)} \prod_{i=1}^{\ell} \mathcal{S}_{h/\ell}^{[2]}, \qquad k = 2, 3, 4,$$

with $\alpha^{(k)} = (\alpha_1^{(k)}, \ldots, \alpha_k^{(k)})$ and

$$\alpha^{(2)} = \left(-\frac{1}{3}, \frac{4}{3}\right), \qquad \alpha^{(3)} = \left(\frac{1}{24}, -\frac{16}{15}, \frac{81}{40}\right), \qquad \alpha^{(4)} = \left(-\frac{1}{360}, \frac{16}{45}, -\frac{729}{280}, \frac{1024}{315}\right). \tag{5.1}$$

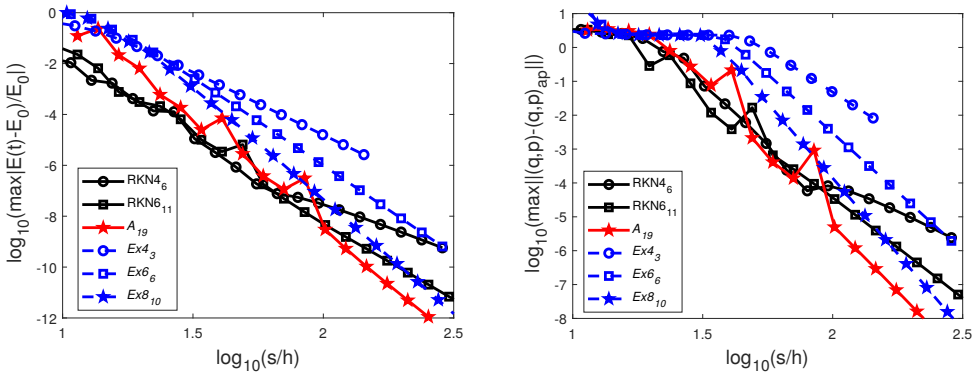
Example 5: Kepler problem revisited. For the Hamiltonian (4.1) with initial conditions (4.2) we compare the most efficient 8th-order RKN splitting method $\mathcal{A}_{19}$ with the 4th- and 6th-order schemes RKN4_6 and RKN6_{11}, and the previous extrapolation methods of orders 4, 6 and 8 for the final time $t_f = 1000$. The results achieved for the maximum error in energy and positions are displayed in Figure 7. To reduce round-off errors when computing the linear combinations in extrapolation methods, instead of evaluating directly the numerical solution as $y_{n+1} = \Psi_{(r=2k)} y_n$, we express $y_{n+1}^{(\ell)} \equiv \prod_{i=1}^{\ell} \mathcal{S}_{h/\ell}^{[2]}\, y_n$ as $y_{n+1}^{(\ell)} = y_n + \Delta y_{n+1}^{(\ell)}$. In this way we compute only $\Delta y_{n+1}^{(\ell)}$, then extrapolation is used only for these increments, namely,

$$\Delta y_{n+1} = \sum_{\ell=1}^{k} \alpha_\ell^{(k)} \Delta y_{n+1}^{(\ell)}$$

and finally we form $y_{n+1} = y_n + \Delta y_{n+1}$. In doing so, round-off errors are reduced by two or more digits.

Figure 7 shows that the new RKN splitting methods are competitive with extrapolation methods and, in particular, $\mathcal{A}_{19}$ is the most efficient when medium to high accuracy is desired.

Example 6: simple pendulum revisited. Let us consider again the simple pendulum, this time with initial conditions $(q, p) = (0, 0.3)$. We measure the error in energy along the integration for the schemes RKN4_6, RKN6_{11}, $\mathcal{A}_{18}$ and the extrapolation methods until the final time $t_f = 1000$. Figure 8 shows the efficiency diagram corresponding to the maximum of the relative error in the energy along the integration interval. In this case, the new scheme $\mathcal{A}_{18}$ is the most efficient when high accuracy is desired. There are initial conditions, however, for which RKN6_{11} provides better results up to round-off.



(a) (b)

Figure 7: (a) Maximum error in the energy for the Kepler problem with $e = 0.5$ obtained by RKN splitting methods RKN4$_6$, RKN6$_{11}$, $\mathcal{A}_{19}$ (solid lines), and extrapolation (dashed lines) of orders 4 (circles), 6 (squares) and 8 (stars). (b) Same for the maximum error in position.

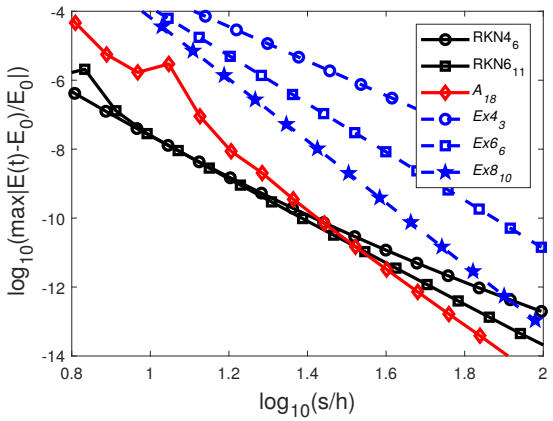


Figure 8: Simple pendulum. Maximum error in the energy for the simple pendulum with initial conditions $(q, p) = (0, 0.3)$ and final time $t_f = 1000$ obtained by RKN splitting methods RKN4$_6$, RKN6$_{11}$, $\mathcal{A}_{19}$ (solid lines), and extrapolation (dashed lines) of orders 4 (circles), 6 (squares) and 8 (stars).

Very similar results are obtained for the Hénon-Heiles potential, and for this reason they are not shown here. From the previous experiments, we can conclude that the new scheme $\mathcal{A}_{19}$ outperforms the symplectic

methods of order 4 and 6 from medium to high accuracy when the potential has a singularity, whereas $\mathcal{A}_{17}$, $\mathcal{A}_{18}$ and $\mathcal{B}_{18}$ deliver the best results only at high accuracy for smooth potentials. To provide further evidence to this class, we next consider a slightly more involved example.

Example 7: the restricted three body problem. In this case we have two bodies of masses $1-\mu$ and μ in circular rotation in a plane and a third body of negligible mass moving around in the same plane. The equations of motion in a fixed coordinate system read [12, p. 129]

$$\begin{aligned} \ddot{y}_1 &= y_1 + 2\dot{y}_2 - \mu' \frac{y_1+\mu}{D_1} - \mu \frac{y_1-\mu'}{D_2} \\ \ddot{y}_2 &= y_2 - 2\dot{y}_1 - \mu' \frac{y_2}{D_1} - \mu \frac{y_2}{D_2}, \end{aligned} \tag{5.2}$$

where $D_1 = ((y_1+\mu)^2 + y_2^2)^{3/2}$, $D_2 = ((y_1-\mu')^2 + y_2^2)^{3/2}$, and $\mu' = 1-\mu$. This system can be split as in (1.9)-(1.10). Alternatively, in a rotating system the equations of motion become

$$\begin{aligned} \ddot{y}_1 &= \mu' \frac{a_1(t)-y_1}{D_1} + \mu \frac{b_1(t)-y_1}{D_2} \\ \ddot{y}_2 &= \mu' \frac{a_2(t)-y_2}{D_1} + \mu \frac{b_2(t)-y_2}{D_2}, \end{aligned} \tag{5.3}$$

where now

$$D_1 = ((y_1-a_1(t))^2 + (y_2-a_2(t))^2)^{3/2}, \quad D_2 = ((y_1-b_1(t))^2 + (y_2-b_2(t))^2)^{3/2},$$

and the motion of the massive bodies is described by

$$a_1(t) = -\mu\cos(t), \quad a_2(t) = -\mu\sin(t); \quad b_1(t) = \mu'\cos(t), \quad b_2(t) = \mu'\sin(t).$$

We take, as in [12], $\mu = 0.012277471$ and the following initial conditions in the rotating system:

$$y_1(0) = 0.994, \quad \dot{y}_1(0) = 0, \quad y_2(0) = 0, \quad \dot{y}_2(0) = -1.00758510637908252240.$$

The resulting closed trajectory corresponds to the so-called Arenstorf orbit in the fixed coordinate system, with period $T = 17.06521656015796255889$.

In this case we integrate for one period with the RKN splitting methods of order 4 and 6, and the new 8th-order scheme $\mathcal{A}_{19}$. We measure the error with respect to the initial conditions (taking into account that we are integrating in the rotating system) and display the corresponding errors in Figure 9. Again, $\mathcal{A}_{19}$ is the most efficient scheme even for medium accuracies.

6 Conclusions

We have presented new RKN splitting methods of order 8 that show a better efficiency than the best existing symmetric compositions of 2nd-order symmetric schemes on a variety of examples. We have thus answered in the affirmative the question formulated by [21] in 1996 and filled the existing gap in the classification of the most efficient splitting and composition methods [5, 19]. The technical difficulties involved in the process

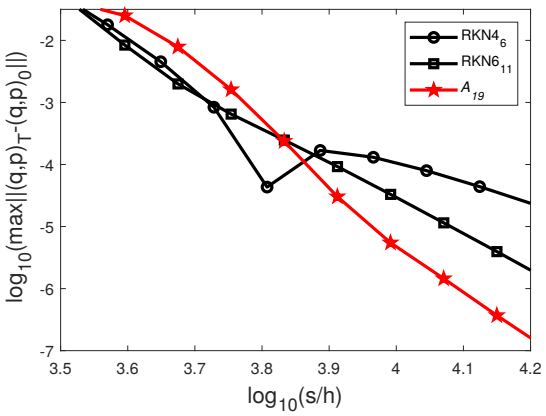


Figure 9: Error with respect to the initial conditions after one period, T, of the Arenstorf orbit versus the number of force evaluations for the 4th-, 6th- and 8th-order RKN splitting methods, RK4N$_6$ (circles), RKN6$_{11}$ (squares) and $\mathcal{A}_{19}$ (stars).

have been overcome by applying standard techniques for solving nonlinear polynomial equations and free software on a personal computer. Whereas previous 8th-order RKN splitting methods require the evaluation of 'modified potentials' or force-gradients [24], the schemes collected here only involve the evaluation of the force $g(y)$, just as compositions (1.8) and thus they should be considered as the natural option when one is interested in integrating the system (1.1) with high precision and the evaluation of modified potentials is computationally expensive or not feasible.

Both types of compositions (2.4) and (2.5) have been analyzed and different schemes with up to two free parameters have been constructed and tested on different numerical examples. These show that $\mathcal{A}_{18}$ and $\mathcal{B}_{18}$ provide better efficiencies when the force is derived from a smooth, singularity-free potential, whereas for problems involving singularities $\mathcal{A}_{19}$ exhibits the best results. As representatives of the first situation (i.e., singularity-free potentials), we have examined the simple pendulum, the Hénon–Heiles potential and the quantum treatment of the Pöschl–Teller potential. The second case, involving singularities, corresponds to the Kepler problem and the restricted planar three body problem. Moreover, the new schemes are more efficient than lower order RKN splitting methods for medium to high accuracies, and provide better results than extrapolation methods of order 8 even for relatively short time integrations.

Acknowledgements

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Capítulo 5

Compositions of pseudo–symmetric integrators with complex coefficients for the numerical integration of differential equations

Compositions of pseudo-symmetric integrators with complex coefficients for the numerical integration of differential equations

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Yong Zhang[§]

May 27, 2020

Abstract

In this paper, we are concerned with the construction and analysis of a new class of methods obtained as double jump compositions with complex coefficients and projection on the real axis. It is shown in particular that the new integrators are symmetric and symplectic up to high orders if one uses a symmetric and symplectic basic method. In terms of efficiency, the aforementioned technique requires fewer stages than standard compositions of the same orders and is thus expected to lead to faster methods.

Keywords: Composition methods, projection on the real-axis, pseudo-symmetry, pseudo-symplecticity.

1 Introduction

Given a differential equation

$$\dot{x} \equiv \frac{dx}{dt} = f(x), \qquad x(0) = x_0, \tag{1}$$

composition methods constitute a powerful technique to raise the order of a given integrator ψ_τ applied to (1) with time-step τ, as high as might be required, by considering expressions of the form

$$\phi_\tau = \psi_{\gamma_1\tau} \circ \psi_{\gamma_2\tau} \circ \cdots \circ \psi_{\gamma_s\tau}, \tag{2}$$

where the coefficients $\gamma_1, \gamma_2, \ldots, \gamma_s$ are appropriately chosen so as to satisfy some *universal algebraic conditions* [HLW06, MSS99, CM09]. It is known in particular that if ψ_τ is of order k, i.e. satisfies

$$\varphi_\tau(x_0) - \psi_\tau(x_0) = \mathcal{O}(\tau^{k+1}),$$

where φ_τ denotes the exact flow of (1), then ϕ_τ will be at least of order $k+1$ (i.e., local error $k+2$) if the following two conditions are satisfied

$$(i)\ \sum_{i=1}^{s} \gamma_i = 1 \qquad \text{and} \qquad (ii)\ \sum_{i=1}^{s} \gamma_i^{k+1} = 0. \tag{3}$$

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Given that these two equations have no real solution for odd k and arbitrary s, a series of authors (e.g. [Suz90, Yos90]) suggested to start from a second-order method and to consider *symmetric compositions* only, i.e., schemes with coefficients satisfying the additional condition

$$\gamma_{s+1-i} = \gamma_i, \qquad i = 1, \dots, s.$$

This has led to so-called triple-jump compositions ($s = 3$, $\gamma_3 = \gamma_1$) obtained by iterating the process described above to construct a sequence of symmetric methods with even orders (see, e.g., [HLW06] pp. 44).

In spite of its simplicity, the triple-jump rationale leads to inefficiencies for high orders as compared to methods obtained by solving directly the order conditions [HLW06]. On top of this, it also suffers from the occurrence of negative time-steps, although this fact is not specific to triple-jump methods and concerns all composition or splitting methods of orders higher than two. This, of course, is a severe limiting factor for equations where the vector field (usually an operator) is not reversible, the prototypical example of which being the heat equation. To circumvent this difficulty, several authors have suggested to use complex time-steps (or complex coefficients) in the context of parabolic equations [CCDV09, HO09]. One indeed easily sees that, already for $s = 2$, solutions of equations $(i) - (ii)$ exist in $\mathbb{C}$.

Generally speaking, suppose that ψ_τ is an integrator of order k, denoted $\mathcal{S}_\tau^{[k]}$ in the sequel for clarity, and consider the composition (2) with $s = 2$,

$$\mathcal{S}_\tau^{[k+1]} = \mathcal{S}_{\gamma_1\tau}^{[k]} \circ \mathcal{S}_{\gamma_2\tau}^{[k]}. \tag{4}$$

Then, if the coefficients verify conditions $(i) - (ii)$, that is to say if

$$\gamma_1 = \bar{\gamma}_2 \equiv \gamma = \frac{1}{2} + \frac{i}{2}\frac{\sin(\frac{2\ell+1}{k+1}\pi)}{1+\cos(\frac{2\ell+1}{k+1}\pi)} \quad \text{for} \quad \begin{cases} -\frac{k}{2} \le \ell \le \frac{k}{2} - 1 & \text{if } k \text{ is even} \\ -\frac{k+1}{2} \le \ell \le \frac{k-1}{2} & \text{if } k \text{ is odd} \end{cases}, \tag{5}$$

then (4) results in a method of order $k + 1$, which can subsequently be used to generate recursively higher order composition schemes by applying the same procedure. The choice $\ell = 0$,

$$\gamma = \gamma^{[k]} := \frac{1}{2} + \frac{i}{2}\frac{\sin\left(\frac{\pi}{k+1}\right)}{1+\cos\left(\frac{\pi}{k+1}\right)} = \frac{1}{2} + \frac{i}{2}\tan\left(\frac{\pi}{2(k+1)}\right) = \frac{1}{2\cos\left(\frac{\pi}{2(k+1)}\right)} e^{\frac{\pi}{2(k+1)}} \tag{6}$$

gives the solutions with the smallest phase. If we start with a symmetric method of order 2, $\mathcal{S}_\tau^{[2]}$, and apply composition (4) with corresponding coefficients (6), we can construct the following sequence of methods:

$$\mathcal{S}_\tau^{[2]} \longrightarrow \mathcal{S}_\tau^{[3]} \longrightarrow \mathcal{S}_\tau^{[4]} \longrightarrow \mathcal{S}_\tau^{[5]} \longrightarrow \mathcal{S}_\tau^{[6]},$$

all of which have coefficients with positive real part [HO09]. The final method of order 6 involves 16 evaluations of the basic scheme $\mathcal{S}_\tau^{[2]}$. By contrast, there are composition methods of order 6 (both with real and complex coefficients) involving just 7 evaluations of $\mathcal{S}_\tau^{[2]}$ [BCCM13, Yos90]. It is thus apparent that this direct approach does not lead to cost-efficient high-order schemes.

One should remark that the composition (4) does not provide a time-symmetric method, i.e., $\mathcal{S}_{-\tau}^{[k+1]} \circ \mathcal{S}_\tau^{[k+1]}$ is *not* the identity map, even if $\mathcal{S}_\tau^{[k]}$ happens to be symmetric. As we have mentioned before, symmetry allows to raise the order by two at each iteration by considering the triple-jump composition

$$\mathcal{S}_\tau^{[2k+2]} = \mathcal{S}_{\gamma_1\tau}^{[2k]} \circ \mathcal{S}_{\gamma_2\tau}^{[2k]} \circ \mathcal{S}_{\gamma_1\tau}^{[2k]} \tag{7}$$

starting from a symmetric method. Apart from the real solution, the complex one with the smallest phase is

$$\gamma_1 = \frac{\mathrm{e}^{i\pi/(k+1)}}{2^{1/(k+1)} - 2\,\mathrm{e}^{i\pi/(k+1)}}, \qquad \gamma_2 = 1 - 2\gamma_1, \tag{8}$$

and symmetric methods up to order 8 with coefficients having positive real part are possible if one starts with a symmetric second-order scheme[1]. These order barriers has been rigorously proved in [BCCM13].

The simple third-order scheme (4) corresponding to $k = 2$ has been in fact rediscovered several times in the literature [BS91, CCDV09, Cha03, HO09, Suz92]. In particular, it was shown in [Cha03] that the method, when applied to the two-body Kepler problem, behaves indeed as a fourth-order integrator, the reason being attributed to the fact that the main error term in the asymptotic expansion is purely imaginary. In this note we elaborate further the analysis and provide a comprehensive study of the general composition (4), paying special attention to the qualitative properties the method shares with the continuous system (1). In addition, we show how it is possible to combine compositions and a trivial linear combination to raise the order, while still preserving the qualitative properties of the basic integrator up to an order higher than of the method itself.

2 Composition and pseudo-symmetry or pseudo-symplecticity

In what follows, we will assume for convenience that all values of x in (1) lie in a compact set K where the function f is *smooth*. Before starting the analysis, it is worth recalling the notions of adjoint method and symplectic flow.

The *adjoint method* ψ_τ^* of a given method is the inverse map of the original integrator with reversed time step $-\tau$, i.e., $\psi_\tau^* := \psi_{-\tau}^{-1}$. A symmetric method satisfies $\psi_\tau^* = \psi_\tau$ [Cha15, HLW06].

The vector field f in (1) is Hamiltonian if there exists a function $H(x)$ such that $f = J\nabla_x H(x)$, where $x = (q, p)^T$ and J is the basic canonical matrix. Then, the exact flow of (1) is a symplectic transformation, $\varphi_t'(x)^T J \varphi_t'(x) = J$ for $t \geq 0$ [BC16, SSC94].

It then makes sense introducing the following definitions, taken from [CL98] and [AC98]:

Definition 1 *Let ψ_τ be a smooth and consistent integrator:*

1. *it is* pseudo-symmetric *of* pseudo-symmetry order *q if for all sufficiently small τ, the following relation holds true:*

$$\psi_\tau^* = \psi_\tau + \mathcal{O}(\tau^{q+1}), \tag{9}$$

   where the constant in the $\mathcal{O}$-term depends on bounds of derivatives of ψ on K.

2. *it is* pseudo-symplectic *of* pseudo-symplecticity order *r if for all sufficiently small τ, the following relation holds true when ψ_τ is applied to a Hamiltonian system:*

$$(\psi_\tau')^T \, J \, \psi_\tau' = J + \mathcal{O}(\tau^{r+1}), \tag{10}$$

   where the constant in the $\mathcal{O}$-term depends on bounds of derivatives of ψ on K.

Remark 1 *A symmetric method is pseudo-symmetric of any order $q \in \mathbb{N}$, whereas a method of order k is pseudo-symmetric of order $q \geq k$. A similar statement holds for symplectic methods.*

As a first illustration of Definition 1, let us consider again a symmetric 2nd-order method $\mathcal{S}_\tau^{[2]}$ and form the composition

$$\psi_\tau^{[3]} = \mathcal{S}_{\gamma\tau}^{[2]} \circ \mathcal{S}_{\bar\gamma\tau}^{[2]}$$

with $\gamma = \frac{1}{2} + i\frac{\sqrt{3}}{6}$. Then, if the vector field f under consideration is real-valued, its real part

$$\Re(\psi_\tau^{[3]}) = \frac{1}{2}\left(\psi_\tau^{[3]} + \overline{\psi}_\tau^{[3]}\right) = \frac{1}{2}\left(\mathcal{S}_{\gamma\tau}^{[2]} \circ \mathcal{S}_{\bar\gamma\tau}^{[2]} + \mathcal{S}_{\bar\gamma\tau}^{[2]} \circ \mathcal{S}_{\gamma\tau}^{[2]}\right).$$

[1] It is actually possible to reach order 14 if, in the construction, one uses formula (7) alternatively with coefficients γ_1, γ_2 and coefficients $\bar\gamma_1, \bar\gamma_2$ [CCDV09].

is a method of order 4 and pseudo-symmetric of pseudo-symmetry order 7. This result is a consequence of the fact that

$$(\psi_\tau^{[3]})^* = \overline{\psi}_\tau^{[3]}$$

and the following general statement, which lies at the core of the construction procedure described in this paper.

Proposition 1 *Let ψ_τ be any consistent smooth method for equation (1) and consider the new method*

$$R_\tau = \frac{1}{2}\left(\psi_\tau + \psi_\tau^*\right).$$

Assume also that ψ_τ is pseudo-symmetric of order q. Then R_τ is of pseudo-symmetry order $2q+1$. If ψ_τ is furthermore of pseudo-symplecticity order r, then R_τ is of pseudo-symplecticity order $\min(2q+1, r)$.

Proof: By assumption, there exists a smooth function $(\tau, x) \mapsto \delta_\tau(x)$, defined for all x in a compact set K and for all sufficiently small real τ, such that

$$\psi_\tau^* = \psi_\tau + \tau^{q+1}\delta_\tau \quad \text{or} \quad \psi_{-\tau}^{-1} = \psi_\tau + \tau^{q+1}\delta_\tau \quad \text{or} \quad \psi_\tau^{-1} = \psi_{-\tau} + (-\tau)^{q+1}\delta_{-\tau}, \tag{11}$$

so that

$$R_\tau = \psi_\tau + \frac{1}{2}\tau^{q+1}\delta_\tau.$$

Composing the third relation of (11) from the left by ψ_τ, we obtain

$$\mathrm{id} = \psi_\tau \circ \psi_{-\tau} + (-\tau)^{q+1}\psi_\tau' \circ \psi_{-\tau} \cdot \delta_{-\tau} + \mathcal{O}(\tau^{2(q+1)}), \tag{12}$$

where the $\mathcal{O}$-term depends on bounds of the derivatives of ψ_τ and δ_τ on K. Similarly, composing the second relation of (11) from the right by $\psi_{-\tau}$, we get

$$\mathrm{id} = \psi_\tau \circ \psi_{-\tau} + \tau^{q+1}\delta_\tau \circ \psi_{-\tau}. \tag{13}$$

As a consequence, we have

$$\tau^{q+1}\delta_\tau \circ \psi_{-\tau} = (-\tau)^{q+1}\psi_\tau' \circ \psi_{-\tau} \cdot \delta_{-\tau} + \mathcal{O}(\tau^{2(q+1)}).$$

We are then in position to write

$$\begin{aligned} R_\tau \circ R_{-\tau} &= \left(\psi_\tau + \frac{1}{2}\tau^{q+1}\delta_\tau\right) \circ \left(\psi_{-\tau} + \frac{1}{2}(-\tau)^{q+1}\delta_{-\tau}\right) \\ &= \psi_\tau \circ \psi_{-\tau} + \frac{1}{2}(-\tau)^{q+1}\psi_\tau' \circ \psi_{-\tau} \cdot \delta_{-\tau} + \frac{1}{2}\tau^{q+1}\delta_\tau \circ \psi_{-\tau} + \mathcal{O}(\tau^{2(q+1)}) \\ &= \mathrm{id} + \mathcal{O}(\tau^{2(q+1)}), \end{aligned}$$

which proves the first statement. Now, if ψ_τ is in addition of pseudo-symplecticity order r, then its adjoint ψ_τ^* is also of pseudo-symplecticity order r, so that relation (11) leads to

$$\begin{aligned} J + \mathcal{O}(\tau^{r+1}) &= (\partial_x \psi_\tau^*)^T J\, \partial_x \psi_\tau^* = (\psi_\tau' + \tau^{q+1}\delta_\tau')^T J (\psi_\tau' + \tau^{q+1}\delta_\tau') \\ &= J + \mathcal{O}(\tau^{r+1}) + \tau^{q+1}\left((\delta_\tau')^T J\, \psi_\tau' + (\psi_\tau')^T J\, \delta_\tau'\right) + \mathcal{O}(\tau^{2(q+1)}), \end{aligned}$$

which implies that

$$\tau^{q+1}\left((\delta_\tau')^T J\, \psi_\tau' + (\psi_\tau')^T J\, \delta_\tau'\right) = \mathcal{O}(\tau^{\min(2(q+1), r+1)}).$$

As an immediate consequence, we have that

$$(R_\tau')^T J\, R_\tau' = J + \mathcal{O}(\tau^{\min(2(q+1), r+1)})$$

which proves the second statement. □

This result can be rendered more specific as follows:

Proposition 2 *Let $S_\tau^{[2n]}$ be a smooth method of order $2n \geq 2$ and pseudo-symmetry order $q \geq 2n+1$. Let us consider the composition method*

$$\psi_\tau^{[2n+1]} = S_{\gamma_1\tau}^{[2n]} \circ S_{\gamma_2\tau}^{[2n]}, \tag{14}$$

where the coefficients γ_1 and γ_2 satisfy both relations $\gamma_1 + \gamma_2 = 1$ and $\gamma_1^{2n+1} + \gamma_2^{2n+1} = 0$. Then the method

$$\hat{R}_\tau = \frac{1}{2}\left(\psi_\tau^{[2n+1]} + \overline{\psi}_\tau^{[2n+1]}\right) \tag{15}$$

is of order

$$\begin{cases} 2n+1 & \text{if } q = 2n+1, \\ 2n+2 & \text{if } q \geq 2n+2 \end{cases} \tag{16}$$

when the vector field f in (1) is real, and of pseudo-symmetry order

$$\begin{cases} 2n+1 & \text{if } q = 2n+1, \\ \min(q, 4n+3) & \text{if } q \geq 2n+2. \end{cases} \tag{17}$$

If in addition, f is a (real) Hamiltonian vector field and $S_\tau^{[2n]}$ is of pseudo-symplecticity order r, then $\hat{R}_\tau$ is of pseudo-symplecticity order

$$\begin{cases} \min(r, 2n+1) & \text{if } q = 2n+1, \\ \min(q, r, 4n+3) & \text{if } q \geq 2n+2. \end{cases} \tag{18}$$

Remark 2 *Note that in Proposition 2, one has necessarily $q \geq 2n+1$. This can be seen straightforwardly by a direct computation of $S_{-\tau}^{[2n]} \circ S_\tau^{[2n]}(x)$ with $S_\tau^{[2n]}(x) = \varphi_\tau(x) + \tau^{2n+1}C(x) + \mathcal{O}(\tau^{2n+2})$.*

Proof: Noticing that γ_1 and γ_2 are complex conjugate and (1) is real, and taking into account that $S_\tau^{[2n]}$ is of pseudo-symmetry order q, we have

$$\begin{aligned} \overline{\psi}_\tau^{[2n+1]} &= S_{\gamma_2\tau}^{[2n]} \circ S_{\gamma_1\tau}^{[2n]} = \left((S_{\gamma_2\tau}^{[2n]})^* + \mathcal{O}(\tau^{q+1})\right) \circ \left((S_{\gamma_1\tau}^{[2n]})^* + \mathcal{O}(\tau^{q+1})\right) \\ &= (S_{\gamma_2\tau}^{[2n]})^* \circ (S_{\gamma_1\tau}^{[2n]})^* + \mathcal{O}(\tau^{q+1}) = (\psi_\tau^{[2n+1]})^* + \mathcal{O}(\tau^{q+1}). \end{aligned} \tag{19}$$

Moreover, by construction, $\psi_\tau^{[2n+1]}$ is at least of order $2n+1$, so that

$$\psi_\tau^{[2n+1]} + \mathcal{O}(\tau^{2n+2}) = \overline{\psi}_\tau^{[2n+1]} = (\psi_\tau^{[2n+1]})^* + \mathcal{O}(\tau^{2n+2}), \tag{20}$$

and altogether

$$\hat{R}_\tau = R_\tau + \mathcal{O}(\tau^{\max(2n+2, q+1)}). \tag{21}$$

Now, since the pseudo-symmetry order of $\psi_\tau^{[2n+1]}$ is at least $2n+1$, the method

$$R_\tau = \frac{1}{2}\left(\psi_\tau^{[2n+1]} + (\psi_\tau^{[2n+1]})^*\right)$$

is, according to Proposition 1, of pseudo-symmetry order $4n+3$ and of pseudo-symplecticity order $\min(4n+3, q)$. The first (16), second (17) and third (18) statements on orders then follow from (21). □

In the Appendix we provide an alternative proof of Proposition 2 based on the Lie formalism, which allow us, in addition, to generalise the previous result on pseudo-symplecticity to other geometric properties the continuous system may possess (such as in volume preserving flows, isospectral flows, differential equations evolving on Lie groups, etc.).

Notice that, according with Proposition 2, if we start from $n = 1$, that is to say from a basic symmetric ($q = +\infty$) and symplectic ($r = +\infty$) method of order 2, we get a method of order 4 that is pseudo-symmetric and pseudo-symplectic of order 7 just by considering the simple composition (14) and taking the real part of the output at each time step. If this technique is applied to a symmetric and symplectic method of order 4, i.e. with $n = 2$, then $\hat{R}_\tau$ is of order 6 and pseudo-symmetric and pseudo-symplectic of order 11.

Let us consider, in particular, the 4^{th}-order symmetric scheme (7) with $k = 2$ as basic scheme. Then, the resulting 6^{th}-order integrator $\hat{R}_\tau$ only requires the evaluation of 6 second-order methods $S_\tau^{[2]}$, whereas the corresponding 6^{th}-order scheme obtained by the triple-jump technique involves 9 evaluations. This number is reduced to 7 by considering general compositions of $S_\tau^{[2]}$ [BCCM13]. If we take this 6^{th}-order composition of 7 schemes as the basic method $S_\tau^{[6]}$, the resulting integrator of order 8, $\hat{R}_\tau$, involves the evaluation of 14 $S_\tau^{[2]}$, whereas 15 evaluations are required by pure composition methods. Notice that $\hat{R}_\tau$ is pseudo-symmetric and pseudo-symplectic of order 15, so that for values of τ sufficiently small, it preserves effectively the symmetry up to round-off error while the drift in energy for Hamiltonian systems is hardly noticeable.

3 Families of pseudo-symplectic methods

There is another possibility to increase the order, though, and it consists in applying the technique of Proposition 2 recursively. Thus, if denote by $\hat{R}_\tau^{(1)} \equiv \hat{R}_\tau$ the method of eq. (15), we propose to apply the following recurrence:

$$\begin{aligned} &\text{For } i = 2, 3, \dots \\ &\qquad \Phi_\tau^{(i)} = \hat{R}^{(i-1)}_{\gamma^{[2i]}\tau} \circ \hat{R}^{(i-1)}_{\bar{\gamma}^{[2i]}\tau} \\ &\qquad \hat{R}_\tau^{(i)} = \frac{1}{2}\left(\Phi_\tau^{(i)} + \overline{\Phi}_\tau^{(i)}\right) \end{aligned} \tag{22}$$

where $\gamma^{[2i]}$ is given by (6). Then, according with Proposition 2, it is possible to raise the order up to the pseudo-symmetry order of the underlying basic method $S_\tau^{[2n]}$. Thus, in particular, the maximum order one can achieve by applying this technique to the basic symmetric method $S_\tau^{[2]}$ is 7, whereas if we start with a basic symmetric method of order 4, $S_\tau^{[4]}$, the maximum order is 11. It is 15 from a symmetric method $S_\tau^{[6]}$ of order 6 and so on and so forth.

To give an assessment of the computational cost of the methods obtained by applying this type of composition, we notice that the computation of $\Phi_\tau^{(i)}$ and $\overline{\Phi}_\tau^{(i)}$ required to form $\hat{R}_\tau^{(i)}$ by (22) at the intermediate stages can be done in parallel, whereas at the final stage it only requires taking the real part. Thus, the method of order 6 constructed recursively from $S_\tau^{[2]}$ only requires the effective computation of 4 basic methods $S_\tau^{[2]}$.

Starting from a symmetric second-order method $S_\tau^{[2]}$, say Strang splitting for instance, it is important to monitor the sign of the real part of all coefficients involved in the previous iteration. It is immediate to see that in the recursive construction

$$S_\tau^{[2]} \to \hat{R}_\tau^{(1)} \to \hat{R}_\tau^{(2)} \to \hat{R}_\tau^{(3)}$$

envisaged in the recurrence (22), the basic method $S_\tau^{[2]}$ is used with the following coefficients

$i = 1 : \gamma^{[2]}, \quad \bar{\gamma}^{[2]}$

$i = 2 : \gamma^{[4]}\gamma^{[2]}, \quad \bar{\gamma}^{[4]}\gamma^{[2]}, \quad \gamma^{[4]}\bar{\gamma}^{[2]}, \quad \bar{\gamma}^{[4]}\bar{\gamma}^{[2]}$

$i = 3 : \gamma^{[6]}\gamma^{[4]}\gamma^{[2]}, \ \gamma^{[6]}\bar{\gamma}^{[4]}\gamma^{[2]}, \ \gamma^{[6]}\gamma^{[4]}\bar{\gamma}^{[2]}, \ \gamma^{[6]}\bar{\gamma}^{[4]}\bar{\gamma}^{[2]}, \ \bar{\gamma}^{[6]}\gamma^{[4]}\gamma^{[2]}, \ \bar{\gamma}^{[6]}\bar{\gamma}^{[4]}\gamma^{[2]}, \ \bar{\gamma}^{[6]}\gamma^{[4]}\bar{\gamma}^{[2]}, \ \bar{\gamma}^{[6]}\bar{\gamma}^{[4]}\bar{\gamma}^{[2]}$

Given the expression of $\gamma^{[k]}$ (see (6)), these coefficients have arguments of the form

$$\frac{\pi}{2}\sum_{j=1}^{i} \pm\frac{1}{2j+1} = \frac{\pi}{2}\Big(\pm\frac{1}{3} \pm \frac{1}{5} \pm \cdots \pm \frac{1}{2i+1}\Big), \qquad i = 1, 2, 3,$$

so that their maximum argument is

$$\frac{\pi}{2}\sum_{j=1}^{3}\frac{1}{2j+1}.$$

For all the coefficients to have positive real parts, a necessary and sufficient condition is thus that

$$\sum_{j=1}^{3}\frac{1}{2j+1}\leq 1.$$

It clearly holds for methods $\hat{R}_\tau^{(1)}$, $\hat{R}_\tau^{(2)}$ and $\hat{R}_\tau^{(3)}$, of respective orders 4, 6 and 7, since $1/3+1/5+1/7 = 71/105$. Similarly, starting form a symmetric method of order 4 having real or complex coefficients with maximum argument θ_4, the condition becomes

$$\frac{2\theta_4}{\pi}+\sum_{j=1}^{4}\frac{1}{2j+3}=\frac{2\theta_4}{\pi}+\frac{1888}{3465}\leq 1.$$

For instance, suppose that f in (1) can be split as $f(x) = f_a(x) + f_b(x)$, so that the exact τ-flows $\varphi_\tau^{[a]}$ and $\varphi_\tau^{[b]}$ corresponding to f_a and f_b, respectively, can be computed exactly. Then, the following composition

$$S_\tau^{[4]} = \varphi_{b_1\tau}^{[b]}\circ\varphi_{a_1\tau}^{[a]}\circ\varphi_{b_2\tau}^{[b]}\circ\varphi_{a_2\tau}^{[a]}\circ\varphi_{b_3\tau}^{[b]}\circ\varphi_{a_2\tau}^{[a]}\circ\varphi_{b_2\tau}^{[b]}\circ\varphi_{a_1\tau}^{[a]}\circ\varphi_{b_1\tau}^{[b]} \tag{23}$$

with

$$b_1=\frac{1}{10}-\frac{1}{30}i,\quad b_2=\frac{4}{15}+\frac{2}{15}i,\quad b_3=\frac{4}{15}-\frac{1}{5}i\quad\text{and}\quad a_1=a_2=a_3=a_4=\frac{1}{4}$$

provides a 4th-order symmetric scheme (see [CCDV09]). Taking (23) as basic method we get $\max_{i=1,2,3}\mathrm{Arg}(b_i) = \arccos(4/5)$ so that

$$\frac{2\theta_4}{\pi}+\frac{1888}{3465}<0.409666+\frac{1888}{3465}<0.96<1$$

and thus all methods

$$S_\tau^{[4]}\to\hat{R}_\tau^{(1)}\to\hat{R}_\tau^{(2)}\to\hat{R}_\tau^{(3)}\to\hat{R}_\tau^{(4)}$$

of respective orders 4, 6, 8, 10 and 11 obtained by the procedure (22) have all their coefficients with positive real parts. As far as the f_a part is concerned, the maximum argument is less than $0.55\frac{\pi}{2}$.

4 Numerical experiments

In this section we illustrate the previous results on several numerical examples, comprising Hamiltonian systems and partial differential equations of evolution previously discretised in space.

4.1 Harmonic oscillator

We first consider the simple harmonic oscillator, with Hamiltonian

$$H = T(p)+V(q)=\frac{1}{2}p^2+\frac{1}{2}q^2.$$

If we denote by $M_X(\tau)$ the exact matrix evolution associated with the Hamiltonians $X = H, T$ and V, i.e., $(q(\tau), p(\tau))^T = M_X(\tau)(q(0), p(0))^T$, then

$$M_H(\tau)=\begin{pmatrix}\cos(\tau) & \sin(\tau)\\ -\sin(\tau) & \cos(\tau)\end{pmatrix},\quad M_T(\tau)=\begin{pmatrix}1 & \tau\\ 0 & 1\end{pmatrix},\quad M_V(\tau)=\begin{pmatrix}1 & 0\\ -\tau & 1\end{pmatrix},$$

ψ_τ	$M_H(\tau) - \psi_\tau$	$\psi_\tau \circ \psi_{-\tau} - I_2$	$\det(\psi_\tau)$
$\hat{R}_\tau^{(1)}$	$\begin{pmatrix} 0 & -\frac{1}{180} \\ -\frac{1}{120} & 0 \end{pmatrix} \tau^5$	$\begin{pmatrix} -\frac{1}{1728} & 0 \\ 0 & -\frac{1}{1728} \end{pmatrix} \tau^8$	$1 - \frac{1}{1728}\tau^8$
$\hat{R}_\tau^{(2)}$	$\begin{pmatrix} 0 & 3.8\times10^{-5} \\ 5.1\times10^{-5} & 0 \end{pmatrix} \tau^7$	$\begin{pmatrix} 5.4\times10^{-6} & 0 \\ 0 & 5.4\times10^{-6} \end{pmatrix} \tau^8$	$1 + 5.4\times10^{-6}\,\tau^8$
$\hat{R}_\tau^{(3)}$	$\begin{pmatrix} 5.8\times10^{-9} & 0 \\ 0 & 5.8\times10^{-9} \end{pmatrix} \tau^8$	$\begin{pmatrix} -1.1\times10^{-8} & 0 \\ 0 & -1.1\times10^{-8} \end{pmatrix} \tau^8$	$1 - 1.1\times10^{-8}\,\tau^8$

Table 1: Main term in the truncation error, degree of symmetry and symplecticity for schemes $\hat{R}_\tau^{(i)}$ obtained from the basic leapfrog integrator for the simple harmonic oscillator. I_2 stands for the 2×2 identity matrix.

respectively. We take as basic symmetric (and symplectic) scheme the leapfrog/Strang splitting:

$$S_\tau^{[2]} = M_T(\tau/2) M_V(\tau) M_T(\tau/2) \tag{24}$$

and compute the first three iterations in (22). In Table 1 we collect the main term in the truncation error for the resulting integrators $\hat{R}_\tau^{(i)}$, $i = 1, 2, 3$. We also check their time-symmetry and the preservation of the symplectic character of the approximate solution matrix by computing its determinant (a 2×2 matrix A is symplectic iff $\det(A) = 1$). One can observe that these results are in agreement with the previous estimates.

Next we take initial conditions $(q, p) = (2.5, 0)$, integrate until the final time $t_f = 10^4$ with $S_\tau^{[2]}$, $\hat{R}_\tau^{(1)}$, and $\hat{R}_\tau^{(2)}$ and compute the relative error in energy along the evolution. The result is depicted in Figure 1. We see that for $\hat{R}_\tau^{(1)}$ and $\hat{R}_\tau^{(2)}$ the error in energy is almost constant for a certain period of time, and then there is a secular growth proportional to $\mathcal{O}(\tau^7)$.

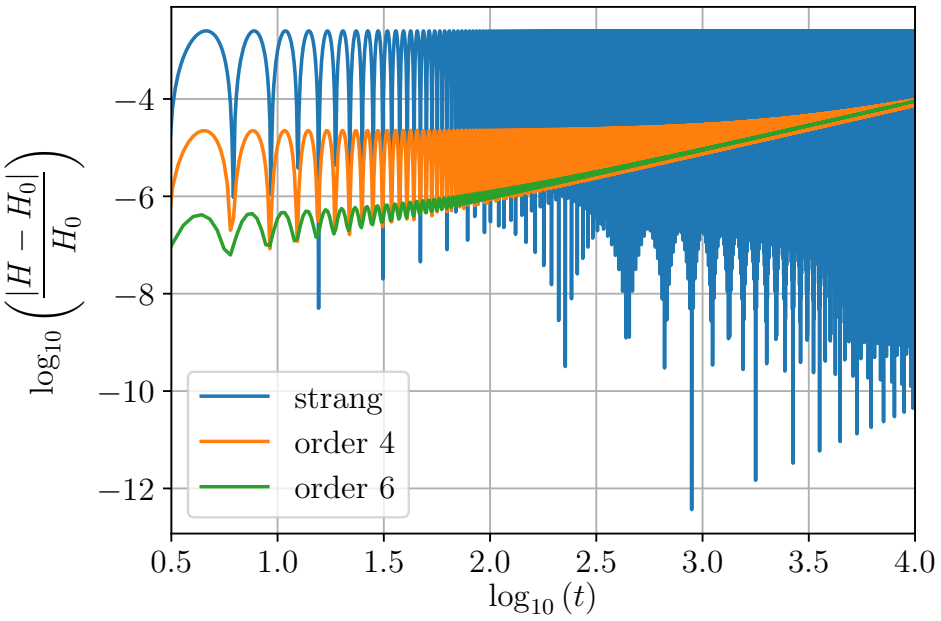

Figure 1: Error in energy along the integration for the harmonic oscillator taking (24) as the basic integrator in the sequence (22).

4.2 Kepler problem

Next, we consider the two-dimensional Kepler problem with Hamiltonian

$$H(q,p) = T(p) + V(q) = \frac{1}{2}p^T p - \mu\frac{1}{r}. \tag{25}$$

Here $q = (q_1, q_2), p = (p_1, p_2)$, $\mu = GM$, G is the gravitational constant and M is the sum of the masses of the two bodies. Taking $\mu = 1$ and initial conditions

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \tag{26}$$

if $0 \le e < 1$, then the solution is periodic with period 2π, and the trajectory is an ellipse of eccentricity e. Note that the gradient function must here be implemented carefully so as to be analytic for complex values of $z = q_1^2 + q_2^2$. Here, we define it using the following determination of the complex logarithm (analytic on the complex plane outside the negative real axis):

$$\forall\,(x,y) \in \mathbb{R}^2 \text{ s.t. } x + iy \notin \mathbb{R}_-, \qquad L(x+iy) = \log|x+iy| + 2i\arctan\left(\frac{y}{x+|x+iy|}\right).$$

As a consequence, the analytic continuation of the function $1/r^3 = 1/(q_1^2+q_2^2)^{3/2}$ writes

$$\exp\Big(-\frac{3}{2}L(x+iy)\Big),$$

where $x = \Re(q_1^2+q_2^2)$ and $y = \Im(q_1^2+q_2^2)$.

Here, as with the harmonic oscillator, we take as basic method the 2nd-order Strang splitting

$$S_\tau^{[2]} = \varphi_{\tau/2}^{[a]} \circ \varphi_\tau^{[b]} \circ \varphi_{\tau/2}^{[a]}, \tag{27}$$

where $\varphi_\tau^{[a]}$ (respectively, $\varphi_\tau^{[b]}$) corresponds to the exact solution obtained by integrating the kinetic energy $T(p)$ (resp., potential energy $V(q)$) in (25).

We take $e = 0.6$, integrate until the final time $t = 20$ with Strang and the schemes obtained by the recursion (22) with $i = 1, 2, 3$ for several time steps and compute the relative error in energy at the final time. Figure 2 show this error as a function of the inverse of the step size $1/\tau$ to illustrate the order of convergence: order 2 for Strang, order 4 for $\hat{R}_\tau^{(1)}$ and order 6 for $\hat{R}_\tau^{(2)}$. For $\hat{R}_\tau^{(3)}$, and contrary to what happens to the harmonic oscillator, the observed numerical order is higher than expected, varying between 7 and 8. We do not have at present a theoretical explanation for this phenomenon. Figure 2 (right) depicts the time evolution of this error when the final time is $t = 10^4$.

4.3 The semi-linear reaction-diffusion equation of Fisher

Our third test-problem is the scalar equation in one-dimension

$$\frac{\partial u(x,t)}{\partial t} = \Delta u(x,t) + F(u(x,t)), \tag{28}$$

with periodic boundary conditions on the interval $[0, 1]$. Here $F(u)$ is a *nonlinear* reaction term. For the purpose of testing our methods, we take Fisher's potential [Sar15]

$$F(u) = u(1-u)$$

as considered for example in [BCCM13].

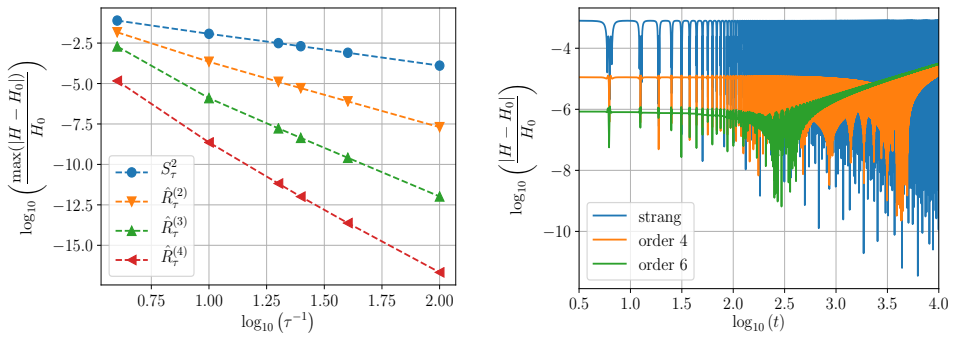

Figure 2: Left figure: Relative error in energy vs. the inverse of the step size τ after approximately 3.183 periods ($t = 20$) for the Kepler problem for the schemes obtained by the recurrence (22). Right figure: Evolution of this error along the integration.

The splitting corresponds here to solving, on the one hand, the linear equation with the Laplacian (as f_a), and on the other hand, the non-linear ordinary differential equation

$$\frac{\partial u(x,t)}{\partial t} = u(x,t)(1-u(x,t)),$$

with initial condition $u(x,0) = u_0(x)$, whose analytical solution is given by the well-defined (for small enough complex time t) formula

$$u(x,t) = u_0(x) + u_0(x)(1-u_0(x))\frac{(\mathrm{e}^t-1)}{1+u_0(x)(\mathrm{e}^t-1)}.$$

Here we aim to solve Eq. (28) with periodic boundary conditions on the interval $[0,1]$, and initial condition $u_0(x) = \sin(2\pi x)$. Numerically, the interval is discretised on a uniform grid, i.e., $x_j = j/N, j = 0,\ldots,N-1$, $N \in \mathbb{N}$, and $u(x,t)$ is approximated by Fourier pseudo-spectral methods. In this way we construct a vector $\mathbf{u}$ with components $(\mathbf{u})_j \approx u(x_{j-1},t)$, $j = 1,2,\ldots,N$. If we denote by $\mathbf{u}_\tau$ the whole numerical solution computed by a certain integrator with step size τ from $t = 0$ until the final time, and by $\mathbf{u}_{\tau/2}$ the corresponding numerical solution computed by the same integrator with step size $\tau/2$, then the quantity $E_\tau := \|\mathbf{u}_\tau - \mathbf{u}_{\tau/2}\|_\infty$ is a good indicator of the convergence order.

Numerical simulations were carried out in quadruple precision (with Intel Fortran) such that roundoff errors are suppressed. Figure 3 shows the successive errors E_τ, at final time $T = 10$, of the methods obtained with the sequence (22) with the Strang splitting as the basic method $S_\tau^{[2]}$ (left) and the fourth order scheme $S_\tau^{[4]}$ given by (23) (right) with different time steps $\tau_j = 0.1/2^j$, $j = 1,\ldots,7$. One can clearly observe that the convergence order matches the previous analysis with a slightly better performance for the highest order, analogously to the Kepler problem. Figure 4 shows the successive errors versus the number of basic integrators in each case.

4.4 The semi-linear complex Ginzburg–Landau equation

Our final test problem is the complex Ginzburg–Landau equation on the domain $(x,t) \in [-100,100]\times[0,100]$,

$$\frac{\partial u(x,t)}{\partial t} = \alpha\Delta u(x,t) + \varepsilon u(x,t) - \beta|u(x,t)|^2 u(x,t), \tag{29}$$

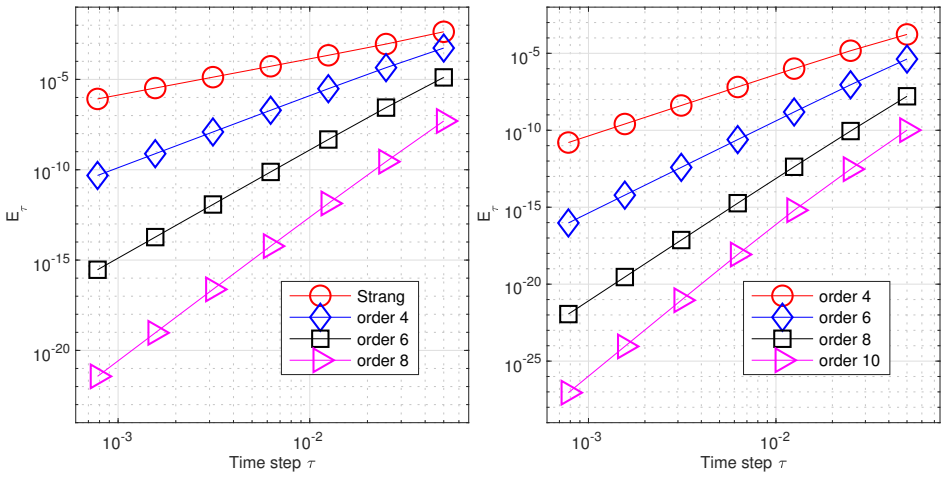

Figure 3: Successive errors E_τ versus time step τ for Eq. (28) of the composition methods starting from the Strang scheme (left) and the fourth order scheme $S_\tau^{[4]}$ (right).

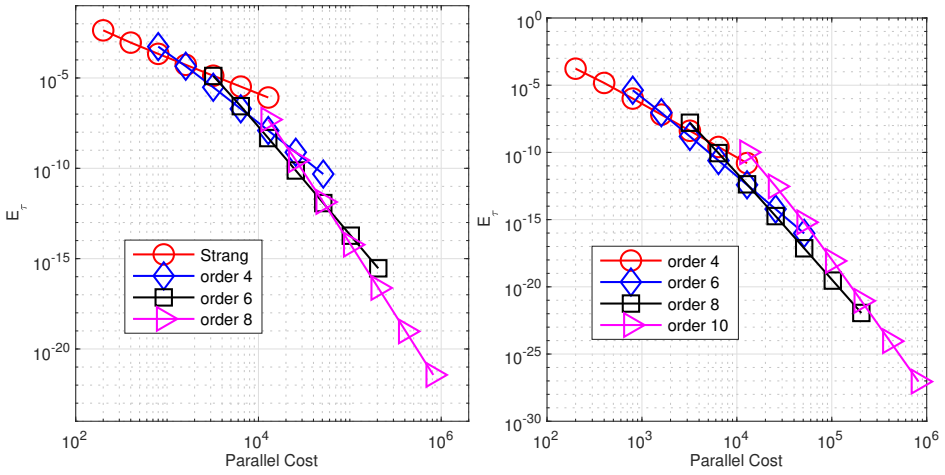

Figure 4: Successive errors E_τ versus number of basic integrators for Eq. (28) of the composition methods starting from the Strang scheme (left) and the fourth order scheme $S_\tau^{[4]}$ (right).

with $\alpha = 1 + ic_1$, $\beta = 1 - ic_3$ and initial condition $u(x,0) = u_0(x)$. Here, ε, c_1 and c_3 denote *real* coefficients. In physics, the Ginzburg-Landau appears in the mathematical theory used to model superconductivity. For a broad introduction to the rich dynamics of this equation, we refer to [vS95]. Here, we will use the values $c_1 = 1$, $c_3 = -2$ and $\varepsilon = 1$, for which plane wave solutions establish themselves quickly after a transient phase (see [WMC05]). In addition, we set

$$u_0(x) = \frac{0.8}{\cosh(x-10)^2} + \frac{0.8}{\cosh(x+10)^2},$$

so that the solution can be represented in Figure 5.

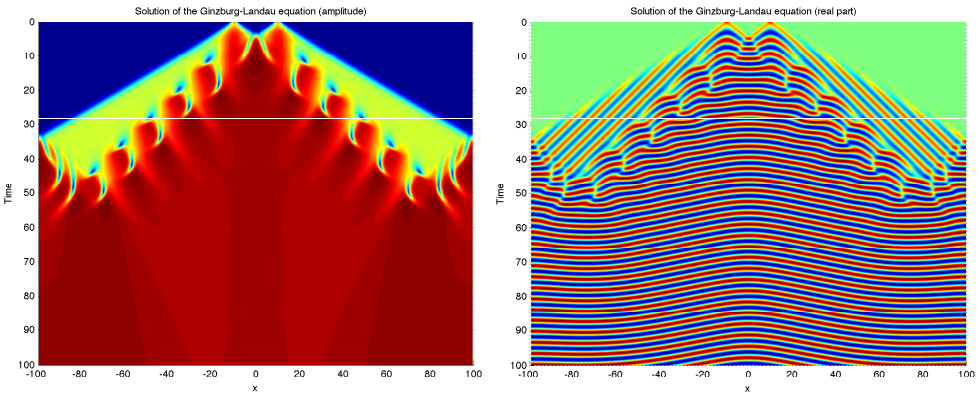

Figure 5: Colormaps of the amplitude $|u(x,t)|^2$ (left) and real part $\Re(u(x,t))$ (right) of the solution of (29).

To apply the composition methods presented in previous sections, it seems natural to split equation (29) as

$$\frac{\partial u(x,t)}{\partial t} = (1 + ic_1)\Delta u(x,t) + \varepsilon u(x,t), \tag{30}$$

whose solution is $u(x,t) = \mathrm{e}^{\varepsilon t}\mathrm{e}^{t(1+ic_1)\Delta}u_0(x)$ for $t \geq 0$, and

$$\frac{\partial u(x,t)}{\partial t} = -(1 - ic_3)|u(x,t)|^2 u(x,t) \tag{31}$$

with solution is for $t \geq 0$

$$u(x,t) = \mathrm{e}^{-(1-ic_3)\int_0^t M(x,s)ds}u_0(x) = \mathrm{e}^{-\frac{\beta}{2}\log(1+2tM_0(x))}u_0(x).$$

Here we have first solved the equation for $M(x,t) := |u(x,t)|^2$, given by

$$\frac{\partial M(x,t)}{\partial t} = -2M^2(x,t),$$

with solution

$$M\,(x,t) = \frac{M_0(x)}{1 + 2M_0(x)t}.$$

Considering t now as a complex variable with positive real part does not raise any difficulty for the first part, since $\mathrm{e}^{\varepsilon t}\mathrm{e}^{t(1+ic_1)\Delta}$ is well-defined. More care has to be taken for the second part, since $u \mapsto |u|^2 u$ is *not* a holomorphic function, and this prevents us from solving (29) in its current form.

As a consequence, we first rewrite (29) as a system for $(v(x,t), w(x,t))$ where $v(x,t) = \mathfrak{R}(u(x,t))$ and $w(x,t) = \mathfrak{I}(u(x,t))$:

$$\left\{ \begin{array}{rcl} \dfrac{\partial v(x,t)}{\partial t} & = & \Delta v(x,t) - c_1 \Delta w(x,t) + \varepsilon v(x,t) - (v^2(x,t) + w^2(x,t))(v(x,t) + c_3 w(x,t)) \\ \dfrac{\partial w(x,t)}{\partial t} & = & c_1 \Delta v(x,t) + \Delta w(x,t) + \varepsilon w(x,t) - (v^2(x,t) + w^2(x,t))(-c_3 v(x,t) + w(x,t)) \end{array} \right. \tag{32}$$

and now solve it for complex time $t \in \mathbb{C}$ with $\mathfrak{R}(t) \geq 0$. Observing that

$$\begin{pmatrix} -1 & -c_3 \\ c_3 & -1 \end{pmatrix} = P D_3 P^{-1} \text{ and } \begin{pmatrix} 1 & -c_1 \\ c_1 & 1 \end{pmatrix} = P D_1 P^{-1},$$

with

$$D_1 = \begin{pmatrix} \alpha & 0 \\ 0 & \bar{\alpha} \end{pmatrix}, D_3 = \begin{pmatrix} -\beta & 0 \\ 0 & -\bar{\beta} \end{pmatrix}, P = \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \text{ and } P^{-1} = \begin{pmatrix} -\frac{i}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{i}{2} \end{pmatrix},$$

system (32) can be rewritten as

$$\left\{ \begin{array}{rcl} \dfrac{\partial \tilde{v}(x,t)}{\partial t} & = & \Big(\alpha \Delta \tilde{v}(x,t) + \varepsilon \tilde{v}(x,t)\Big) - \Big(\beta \tilde{M}(x,t) \tilde{v}(x,t)\Big) \\ \dfrac{\partial \tilde{w}(x,t)}{\partial t} & = & \Big(\bar{\alpha} \Delta \tilde{w}(x,t) + \varepsilon \tilde{w}(x,t)\Big) - \Big(\bar{\beta} \tilde{M}(x,t) \tilde{w}(x,t)\Big) \end{array} \right. \tag{33}$$

where $\tilde{M}(x,t) = 4i\tilde{v}(x,t)\tilde{w}(x,t)$ and where

$$\begin{pmatrix} \tilde{v} \\ \tilde{w} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}.$$

It is not difficult to see that the exact solution of the second part of (33) is given by

$$\left\{ \begin{array}{rcl} \tilde{v}(x,t) & = & \tilde{v}_0(x) \mathrm{e}^{-\frac{\beta}{2} \log(1 + 2t\tilde{M}_0(x))} \\ \tilde{w}(x,t) & = & \tilde{w}_0(x) \mathrm{e}^{-\frac{\bar{\beta}}{2} \log(1 + 2t\tilde{M}_0(x))} \end{array} \right. \tag{34}$$

where $\tilde{M}_0(x)$ is now defined as $\tilde{M}_0(x) := 4i\tilde{v}_0(x)\tilde{w}_0(x)$. Note that here, by convention, the logarithm refers to the principal value of $\log(z)$ for complex numbers: if $z = (a + ib) = re^{i\theta}$ with $-\pi < \theta \leq \pi$, then

$$\log z := \ln r + i\theta = \ln |z| + i \arg z = \ln(|a + ib|) + 2i \arctan\left(\frac{b}{a + \sqrt{a^2 + b^2}} \right).$$

Since $\log(z)$ is *not defined* for $z \in \mathbb{R}^-$, this means that the solution $(\tilde{v}(x,t), \tilde{w}(x,t))$ is defined only as long as $1 + 2\tilde{M}_0(x)t \notin \mathbb{R}^-$. Finally, the solution $(v(x,t), w(x,t))$ is of the form

$$\left\{ \begin{array}{rcl} v(x,t) & = & v_0(x) \frac{(\mathrm{e}^{-\beta L(x,t)} + \mathrm{e}^{-\bar{\beta} L(x,t)})}{2} - w_0(x) \frac{(\mathrm{e}^{-\beta L(x,t)} - \mathrm{e}^{-\bar{\beta} L(x,t)})}{2i} \\ w(x,t) & = & v_0(x) \frac{(\mathrm{e}^{-\beta L(x,t)} - \mathrm{e}^{-\bar{\beta} L(x,t)})}{2i} + w_0(x) \frac{(\mathrm{e}^{-\beta L(x,t)} + \mathrm{e}^{-\bar{\beta} L(x,t)})}{2} \end{array} \right.$$

where $L(x,t) := \log(1 + 2t\tilde{M}_0(x)) = \log(1 + 2tM_0(x))$ with $M_0(x) = v_0^2(x) + w_0^2(x)$.

Denoting $V = (v_1, \ldots, v_N) \in \mathbb{R}^N$ and $W = (w_1, \ldots, w_N) \in \mathbb{R}^N$, we eventually have to numerically solve the following system:

$$\left\{ \begin{array}{rcl} \dot{V} & = & AV - c_1 AW + \varepsilon V - G(V + c_3 W) \\ \dot{W} & = & c_1 AV + AW + \varepsilon W - G(-c_3 V + W) \end{array} \right.$$

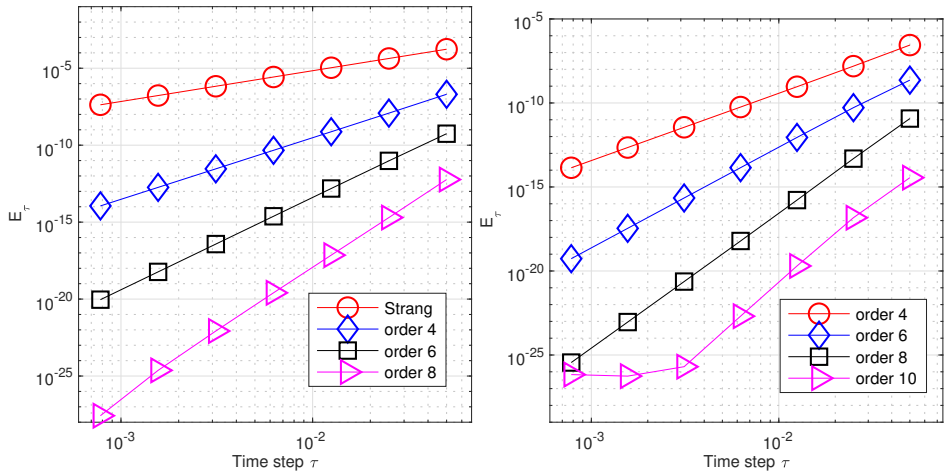

Figure 6: Successive errors E_τ versus time step τ for Eq. (29) of the composition methods starting from the Strang scheme (left) and the fourth order scheme $S_\tau^{[4]}$ (right).

where G is the diagonal matrix with $G_{i,i} = v_i^2 + w_i^2$.

Equation (29) is solved with periodic boundary conditions on the interval $[-100, 100]$. Now, in the previous example, the interval is discretised on a uniform grid, i.e., $x_j = j/N, j = 0, \dots, N-1$, $N \in \mathbb{N}$ with $N = 512$, and $u(x,t)$ is approximated by Fourier pseudo-spectral methods. The successive errors $E_\tau := \|\mathbf{u}_\tau - \mathbf{u}_{\tau/2}\|_\infty$ are shown also here to confirm the convergence order. Figure 6 shows the successive errors, at final time $T = 10$, of the schemes obtained by applying the sequence (22) from the basic Strang splitting and the fourth-order scheme (23) with $\tau_j = 0.1/2^j$, $j = 1, \dots, 7$. The observed order of convergence matches the previous analysis with a slightly better performance for the highest order. Figure 7 shows the successive errors versus the number of basic integrators.

Acknowledgements

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Appendix

In this Appendix we provide an alternative proof of Proposition 2 via Lie formalism. This allows us not only to gain some additional insight into the structure of the methods, but also to generalize the result on pseudo-symplecticity to other properties of geometric character, very often related to Lie groups, the differential equation may possess.

To begin with, if φ_τ is the exact flow of the equation (1), then for each infinitely differentiable map g, the function $g(\varphi_\tau(x))$ admits an expansion of the form [Arn89, SSC94]

$$g(\varphi_\tau(x)) = \exp(\tau F)[g](x) = g(x) + \sum_{k\geq 1} \frac{\tau^k}{k!} F^k[g](x),$$

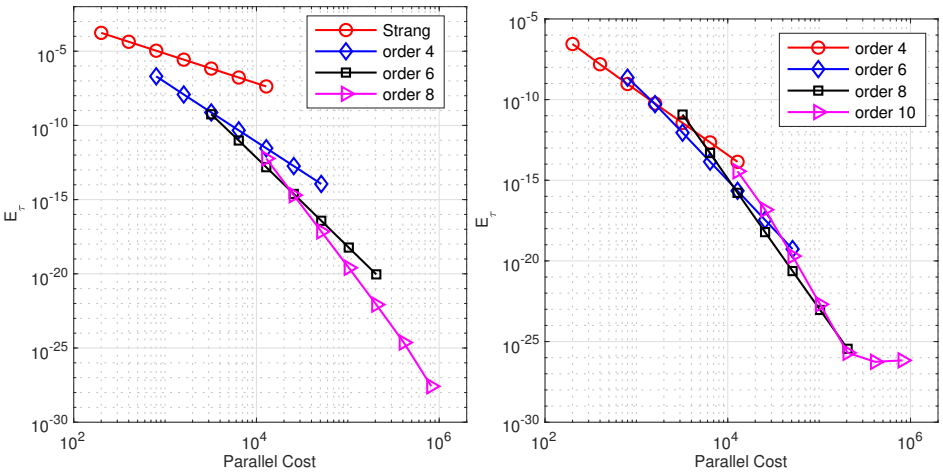

Figure 7: Successive errors E_τ versus number of basic integrators for Eq. (29) of the composition methods starting from the Strang scheme (left) and the fourth order scheme $S_\tau^{[4]}$ (right).

where F is the Lie derivative associated with f,

$$F = \sum_{i\geq 1} f_i(x)\,\frac{\partial}{\partial x_i}. \tag{35}$$

Analogously, for a given integrator ψ_τ one can associate a series of linear operators so that

$$g(\psi_\tau(x)) = \exp(Y(\tau))[g](x), \qquad \text{with} \qquad Y(\tau) = \sum_{j\geq 1} \tau^j Y_j$$

for all functions g [BCM08]. The integrator ψ_τ is of order k if

$$Y_1 = F \qquad \text{and} \qquad Y_j = 0 \quad \text{for} \quad 2 \leq j \leq k.$$

For the adjoint integrator $\psi_\tau^* = \psi_\tau^{-1}$, one clearly has

$$g(\psi_\tau^*(x)) = \exp\big(-Y(-\tau)\big)[g](x).$$

This shows that ψ_τ is symmetric if and only if $Y(\tau) = \tau Y_1 + \tau^3 Y_3 + \cdots$, and in particular, that symmetric methods are of even order.

An integrator $S_\tau^{[2n]}$ of order $2n \geq 2$ can be associated with the series

$$\Phi(\tau) = \exp\left(\tau F + \tau^{2n+1} N_{2n+1} + \tau^{2n+2} N_{2n+2} + \cdots\right) \tag{36}$$

for certain operators N_k. Then, the adjoint method $(S_\tau^{[2n]})^*$ has the associated series

$$\Phi^*(\tau) = \exp\left(\tau F + \tau^{2n+1} N_{2n+1} - \tau^{2n+2} N_{2n+2} + \cdots\right).$$

In consequence, $S_\tau^{[2n]}$ is pseudo-symmetric of order $q \geq 2n+1$.

(i) Let us analyse first the case $q > 2n+1$. Then, $N_{2n+2} = \cdots = N_q = 0$ in (36) and the series of operators associated with the composition $\psi_\tau^{[2n+1]} = S_{\gamma_1\tau}^{[2n]} \circ S_{\gamma_2\tau}^{[2n]}$ is

$$\Psi(\tau) = \Phi(\gamma_2\tau)\,\Phi(\gamma_1\tau) \equiv \exp(V(\tau)),$$

where $V(\tau)$ can be formally determined by applying the Baker–Campbell–Hausdorff formula [BC16] as

$$V(\tau) = (\gamma_1+\gamma_2)\tau F + (\gamma_1^{2n+1}+\gamma_2^{2n+1})\tau^{2n+1}N_{2n+1} + \frac{1}{2}(\gamma_2\gamma_1^{2n+1}-\gamma_1\gamma_2^{2n+1})\tau^{2n+2}[F,N_{2n+1}] + (\gamma_1^{2n+3}+\gamma_2^{2n+3})\tau^{2n+3}N_{2n+3} + \mathcal{O}(\tau^{2n+4}).$$

Here $[\cdot,\cdot]$ denotes the usual Lie bracket. Clearly, the order of $\psi_\tau^{[2n+1]}$ is $2n+1$ if

$$\gamma_1+\gamma_2 = 1, \qquad \gamma_1^{2n+1}+\gamma_2^{2n+1} = 0, \tag{37}$$

so that $\gamma_2 = \bar{\gamma}_1 \equiv \gamma$ is given by eq. (5) (with $k = 2n$). In that case we can write

$$V(\tau) = \tau F + \tau^{2n+2}G(\tau), \qquad \text{with} \qquad G(\tau) = \sum_{i=0}^{\infty}\tau^i G_i,$$

whereas for the adjoint method one has

$$\Psi^*(\tau) = \exp(-V(-\tau)) = \exp\left(\tau F + \tau^{2n+2}\widetilde{G}(\tau)\right), \qquad \text{with} \qquad \widetilde{G}(\tau) = \sum_{i=0}^{\infty}(-1)^{i+1}\tau^i G_i.$$

In particular, $G_0 = \frac{1}{2}(\gamma_2\gamma_1^{2n+1}-\gamma_1\gamma_2^{2n+1})[F,N_{2n+1}]$, and $G_1 = (\gamma_1^{2n+3}+\gamma_2^{2n+3})N_{2n+3}$.

The series $\Psi(\tau)$ can also be written as

$$\Psi(\tau) = \exp\left(\frac{\tau}{2}F\right)\exp W(\tau)\exp\left(\frac{\tau}{2}F\right),$$

where $W(\tau)$ is determined by applying the symmetric BCH formula [BC16] as

$$\begin{aligned} W(\tau) &= \tau^{2n+2}G(\tau) + \frac{1}{24}\tau^{2n+4}[F,[F,G(\tau)]] + \mathcal{O}(\tau^{4n+4}) \\ &= \tau^{2n+2}G_0 + \tau^{2n+3}G_1 + \tau^{2n+4}\big(G_2 + \frac{1}{24}[F,[F,G_0]]\big) + \mathcal{O}(\tau^{2n+5}). \end{aligned}$$

By the same token,

$$\Psi^*(\tau) = \exp\left(\frac{\tau}{2}F\right)\exp\big(-W(-\tau)\big)\exp\left(\frac{\tau}{2}F\right).$$

Consider now the method

$$R_\tau = \frac{1}{2}\big(\psi_\tau^{[2n+1]} + (\psi_\tau^{[2n+1]})^*\big). \tag{38}$$

Clearly, its associated series of operators,

$$\mathcal{R}(\tau) = \frac{1}{2}\Psi(\tau) + \frac{1}{2}\Psi^*(\tau),$$

can be expressed as

$$\mathcal{R}(\tau) = \exp\left(\frac{\tau}{2}F\right)\mathcal{Y}\exp\left(\frac{\tau}{2}F\right),$$

where

$$\mathcal{Y} = \frac{1}{2}\exp\left(W(\tau)\right) + \frac{1}{2}\exp\left(-W(-\tau)\right).$$

By expanding, we have

$$\mathcal{Y} = I + \frac{1}{2}\big(W(\tau)-W(-\tau)\big) + \frac{1}{4}\big(W^2(\tau)+W^2(-\tau)\big) + \cdots,$$

but

$$W(\tau)-W(-\tau) = 2\tau^{2n+3}\sum_{i=0}^{\infty}\tau^{2i}z_{2i} \equiv 2\tau^{2n+3}Z(\tau),$$

with $z_0 = G_1$, $z_2 = G_3 + \frac{1}{24}[F,[F,G_1]]$, etc. In general, z_{2i} is a linear combination of the operators $\{F, N_{2n+1}, N_{2n+2}, \dots\}$ and their nested Lie brackets. In addition, $W^2(\tau) + W^2(-\tau) = \mathcal{O}(\tau^{4n+4})$, so that we can write

$$\mathcal{Y} = I + \tau^{2n+3} Z + \mathcal{O}(\tau^{4n+4}) = \exp\left(\tau^{2n+3} Z\right) + \mathcal{O}(\tau^{4n+4})$$

and

$$\mathcal{R}(\tau) = \exp\left(\frac{\tau}{2} F\right) \exp\left(\tau^{2n+3} Z\right) \exp\left(\frac{\tau}{2} F\right) + \mathcal{O}(\tau^{4n+4}),$$

whence the following statements follow at once:

- Method (38) is of order $2n+2$, since $\mathcal{R}(\tau) = \exp(\tau F) + \mathcal{O}(\tau^{2n+3})$.
- Since $Z(\tau)$ only contains even powers of τ (up to $\tau^{q+1} N_{q+1}$), then $\mathrm{e}^{\frac{\tau}{2}F} \mathrm{e}^{\tau^{2n+3} Z} \mathrm{e}^{\frac{\tau}{2}F}$ is a symmetric composition and R_τ is pseudo-symmetric of order $\min(q, 4n+3)$.
- Let us suppose that scheme (38) is applied to a Hamiltonian system and that $S_\tau^{[2n]}$ is of pseudo-symplecticity order r. Since Z is an operator in the free Lie algebra generated by $\{F, N_{2n+1}, N_{2n+2}, \dots\}$, clearly the composition $\mathrm{e}^{\frac{\tau}{2}F} \mathrm{e}^{\tau^{2n+3} Z} \mathrm{e}^{\frac{\tau}{2}F}$ is symplectic (at least up to terms $\mathcal{O}(\tau^r)$). As a matter of fact, this can be extended to any geometric property the differential equation (1) has: volume-preserving, unitary, etc., as long as the basic scheme $S_\tau^{[2n]}$ preserves this property up to order r.

Finally, in view of (19)-(21) and recalling that $q \geq 2n+2$, the same considerations apply if we take the complex conjugate instead of the adjoint, i.e., to the scheme

$$\hat{R}_\tau = \mathfrak{R}(\psi_\tau^{[2n+1]}) = \frac{1}{2}\left(\psi_\tau^{[2n+1]} + \overline{\psi}_\tau^{[2n+1]}\right). \tag{39}$$

(ii) We analyse next the case $q = 2n+1$. Then $N_{2n+2} \neq 0$ in (36) and, if γ_1 and γ_2 verify equations (37), then $V(\tau)$ read

$$V(\tau) = \tau F + \tau^{2n+2} V_0 + \mathcal{O}(\tau^{2n+3})$$

with

$$V_0 = (\gamma_1^{2n+2} + \gamma_2^{2n+2}) N_{2n+2} + \frac{1}{2}(\gamma_2 \gamma_1^{2n+1} - \gamma_1 \gamma_2^{2n+1})[F, N_{2n+1}].$$

Notice that, whereas $\gamma_1^{2n+2} + \gamma_2^{2n+2}$ is a real number, $\gamma_2 \gamma_1^{2n+1} - \gamma_1 \gamma_2^{2n+1}$ has non-vanishing real and imaginary parts. In any event, the same procedure as in the previous case can be carried out, leading to the conclusion that method (38) is still of order $2n+2$.

The situation is different, however, for method (39), since relations (19)-(21) do not provide further information. We have to analyse instead

$$\mathfrak{R}(\Psi(\tau)) = \exp\left(\frac{\tau}{2} F\right) \mathfrak{R}\left(\exp W(\tau)\right) \exp\left(\frac{\tau}{2} F\right),$$

with $W(\tau) = \tau^{2n+2} V_0 + \mathcal{O}(\tau^{2n+3})$. Noting that

$$\mathfrak{R}\left(\exp W(\tau)\right) = I + \mathfrak{R}\left(W(\tau)\right) + \mathcal{O}(\tau^{4n+4}) = I + \tau^{2n+2} \mathfrak{R}(V_0) + \mathcal{O}(\tau^{2n+3})$$

then we can write

$$\mathfrak{R}(\Psi(\tau)) = \exp\left(\frac{\tau}{2} F\right) \exp\left(\tau^{2n+2} \mathfrak{R}(V_0) + \mathcal{O}(\tau^{2n+3})\right) \exp\left(\frac{\tau}{2} F\right) + \mathcal{O}(\tau^{4n+4}).$$

In consequence, $\hat{R}_\tau$ is a method of order $2n+1$, pseudo-symmetric of order $2n+1$ and pseudo-symplectic of order $\min(r, 2n+1)$.

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Capítulo 6

High order integrators obtained by linear combinations of symmetric–conjugate compositions

High order integrators obtained by linear combinations of symmetric-conjugate compositions

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Abstract

A new family of methods involving complex coefficients for the numerical integration of differential equations is presented and analyzed. They are constructed as linear combinations of symmetric-conjugate compositions obtained from a basic time-symmetric integrator of order $2n$ ($n \geq 1$). The new integrators are of order $2(n+k)$, $k = 1, 2, \ldots$, and preserve time-symmetry up to order $4n+3$ when applied to differential equations with real vector fields. If in addition the system is Hamiltonian and the basic scheme is symplectic, then they also preserve symplecticity up to order $4n+3$. We show that these integrators are well suited for a parallel implementation, thus improving their efficiency. Methods up to order 10 based on a 4th-order integrator are built and tested in comparison with other standard procedures to increase the order of a basic scheme.

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1 Introduction

Composition methods constitute a standard tool to construct high-order numerical integrators for the initial value problem

$$\dot{x} = f(x), \qquad x(t_0) = x_0 \in \mathbb{R}^d, \tag{1.1}$$

in particular when the vector field f possesses some qualitative property whose preservation by numerical approximations is deemed relevant [6, 16]. Let $\mathcal{S}_h^{[2n]}$ denote a $2n$-th order method, so that $\mathcal{S}_h^{[2n]}(x_0) = \varphi_h(x_0) + \mathcal{O}(h^{2n+1})$, where $x(h) = \varphi_h(x_0)$ is the exact solution of Eq. (1.1) for a time step h. Then, if the

coefficients $\alpha_1, \alpha_2, \ldots, \alpha_s$ satisfy some algebraic conditions, the composition of the basic scheme with step sizes $\alpha_1 h, \alpha_2 h, \ldots, \alpha_s h$, i.e.,

$$\psi_h = \mathcal{S}^{[2n]}_{\alpha_1 h} \circ \mathcal{S}^{[2n]}_{\alpha_2 h} \circ \cdots \circ \mathcal{S}^{[2n]}_{\alpha_{s-1} h} \circ \mathcal{S}^{[2n]}_{\alpha_s h} \tag{1.2}$$

is a new method of higher order $2n+m$ [9]. If in particular f is Hamiltonian and $\mathcal{S}^{[2n]}_h$ is symplectic, then the composition method (1.2) is also symplectic [16]. In general, any geometric property the basic method has in common with the exact solution is still shared by the higher-order scheme (1.2) if this property is preserved by composition [18]. Moreover, suppose $\mathcal{S}^{[2n]}_h$ is time-symmetric, namely, it satisfies

$$\mathcal{S}^{[2n]}_h \circ \mathcal{S}^{[2n]}_{-h} = \mathrm{id},$$

where id is the identity map, for any h. Then, method (1.2) is also time-symmetric if the composition is left-right palindromic, i.e., $\alpha_{s+1-j} = \alpha_j$, $j = 1, 2, \ldots$.

A well known class of composition methods is obtained by applying the triple-jump procedure [21, 24]:

$$\mathcal{S}^{[2n+2]}_h = \mathcal{S}^{[2n]}_{\alpha_1 h} \circ \mathcal{S}^{[2n]}_{\alpha_2 h} \circ \mathcal{S}^{[2n]}_{\alpha_1 h}, \tag{1.3}$$

with

$$\alpha_1 = \frac{1}{2 - 2^{1/(2n+1)}}, \qquad \alpha_2 = 1 - 2\alpha_1, \tag{1.4}$$

is a new method of order $2n+2$. The same technique can be applied again to $\mathcal{S}^{[2n+2]}_h$, so that one can construct recursively time-symmetric methods of any order $2n+2k$, $k = 1, 2, \ldots$.

When constructing high-order composition methods, real coefficients $\alpha_1, \ldots, \alpha_s$ are not the only option, however. In fact, the unavoidable existence of negative α_j in (1.2) when the order is higher than two [5, 15, 20, 22] typically imposes stability restrictions on the step size. This occurs in particular when Eq. (1.1) is the outcome of a parabolic differential equation discretized in space. In that case, considering complex coefficients with positive real part is also a valid alternative [12, 17]. Even for problems where the presence of some $\alpha_j < 0$ is not particularly troublesome, composition methods with complex coefficients have also been proposed and analyzed from the preservation of properties viewpoint [10, 7, 13].

In the particular case of the triple-jump composition (1.3), in addition to the real solution (1.4), the complex one with the smallest phase is

$$\alpha_1 = \frac{\mathrm{e}^{i\pi/(2n+1)}}{2^{1/(2n+1)} - 2\mathrm{e}^{i\pi/(2n+1)}}, \qquad \alpha_2 = 1 - 2\alpha_1, \tag{1.5}$$

and the resulting method has in fact smaller truncation errors than its real counterpart (1.4). If the basic scheme is time-symmetric and of order 2, then time-symmetric methods up to order 14 with coefficients having positive real part are possible by applying this technique [8].

The order can be raised by one instead with the simplest composition [3, 22]

$$\psi^{[2n+1]}_h = \mathcal{S}^{[2n]}_{\alpha_1 h} \circ \mathcal{S}^{[2n]}_{\alpha_2 h} \tag{1.6}$$

if

$$\alpha_1 = \bar{\alpha}_2 = \frac{1}{2} + \frac{i}{2} \frac{\sin \frac{2\ell+1}{2n+1}\pi}{1 + \cos \frac{2\ell+1}{2n+1}\pi} \qquad \text{for} \qquad -n \le \ell \le n-1.$$

The choice $\ell = 0$ gives the solution with the smallest phase, which we denote by $\gamma^{[2n]}$:

$$\alpha_1 = \gamma^{[2n]} := \frac{1}{2} + \frac{i}{2}\frac{\sin\frac{\pi}{2n+1}}{1+\cos\frac{\pi}{2n+1}}, \qquad n = 1, 2, \ldots \tag{1.7}$$

When the vector field f in (1.1) is real, then $x_1 = \psi_h^{[2n+1]}(x_0)$ is complex, and so it is quite natural to project x_1 on the real axis and proceed to the next step only with $\Re(x_1)$. This is equivalent of course to integrating with the scheme

$$R_h^{(1)} = \frac{1}{2}\left(\psi_h^{[2n+1]} + \overline{\psi}_h^{[2n+1]}\right). \tag{1.8}$$

Method (1.8) is not time-symmetric, even when $\mathcal{S}_h^{[2n]}$ is. Nevertheless, it has been shown in [11] that $R_h^{(1)}$ is *pseudo-symmetric* of order $4n+3$, in the sense that

$$R_h^{(1)} \circ R_{-h}^{(1)} = \mathrm{id} + \mathcal{O}(h^{4n+4})$$

if the vector field f in (1.1) is real. If in addition f is Hamiltonian and $\mathcal{S}_h^{[2n]}$ is symplectic, then $R_h^{(1)}$ is also *pseudo-symplectic* of order $4n+3$. In other words, projecting $\psi_h^{[2n+1]}$ at each integration step leads to a numerical method that preserves geometric properties of the exact solution up to an order that is much higher than the order of the method itself. Pseudo-symplectic integrators have been previously considered in the literature, both in the context of Runge–Kutta [2] and polynomial extrapolation methods [4, 14].

Moreover, as shown in [11], $R_h^{(1)}$ can be taken as the basis of the recursion

$$R_h^{(k)} = \frac{1}{2}\left(R_{\gamma^{[2k]}h}^{(k-1)} \circ R_{\bar{\gamma}^{[2k]}h}^{(k-1)} + R_{\bar{\gamma}^{[2k]}h}^{(k-1)} \circ R_{\gamma^{[2k]}h}^{(k-1)}\right), \qquad k = 2, 3\ldots, \tag{1.9}$$

producing methods of order $2(n+k)$, also pseudo-symmetric of order $4n+3$. Here the coefficients $\gamma^{[2k]}$ are given by Eq. (1.7). For future reference, we call (1.9) **R-methods**.

Scheme (1.6) is a particular example of a *symmetric-conjugate* composition. These are composition methods of the form

$$\psi_h = \mathcal{S}_{\alpha_1 h}^{[2n]} \circ \mathcal{S}_{\alpha_2 h}^{[2n]} \circ \cdots \circ \mathcal{S}_{\bar{\alpha}_2 h}^{[2n]} \circ \mathcal{S}_{\bar{\alpha}_1 h}^{[2n]}, \tag{1.10}$$

i.e., compositions (1.2) with $\alpha_j \in \mathbb{C}$ and

$$\bar{\alpha}_{s+1-j} = \alpha_j, \qquad j = 1, 2, \ldots.$$

Methods of this class, as shown in [7], possess remarkable preservation properties when considering its real part,

$$\Re(\psi_h) = \frac{1}{2}\left(\psi_h + \overline{\psi}_h\right).$$

In particular, if one takes a time-symmetric 2nd-order scheme as the basic method and the coefficients $\alpha_1, \alpha_2, \ldots$ are chosen in such a way that ψ_h is of order $2n-1$, then $\Re(\psi_h)$ is of order $2n$ and pseudo-symmetric of order $4n-1$ when the vector field f in (1.1) is real. If in addition f is a (real) Hamiltonian vector field and $\mathcal{S}_h^{[2]}$ is a symplectic integrator, then $\Re(\psi_h)$ is pseudo-symplectic of order $4n-1$.

Since taking the real part of a symmetric-conjugate method is just a very special linear combination, it is quite natural to ask what happens when one considers a more general linear combination of symmetric-conjugate compositions and their complex-conjugate, $\psi_h^{(j)}$, $\overline{\psi}_h^{(j)}$: is it possible to construct new methods

of higher order whereas still preserving time-symmetry (and symplecticity) up to the order prescribed by the composition $\psi_h^{(j)}$? If yes, how the new methods are built? Addressing these questions is precisely the subject of the present paper. In doing so, we present a new family of schemes of increasingly higher order well adapted for implementation in a parallel environment, requiring less computational effort than the R-methods (1.9) but with the same qualitative properties.

If we denote for simplicity the symmetric-conjugate composition (1.10) by its sequence of coefficients,

$$\psi_h^{(j)} = (\alpha_1, \alpha_2, \ldots, \alpha_{s-1}, \alpha_s),$$

with $\bar{\alpha}_{s+1-j} = \alpha_j$, these new schemes have the basic structure

$$T_h^{(k)} = \frac{1}{2^k} \sum_{j=1}^{2^{k-1}} \Big((\alpha_{j_{2^k}}, \ldots, \alpha_{j_1}) + \text{c.c.} \Big) \tag{1.11}$$

and are of order $2(n+k) \leq 4n+3$ and pseudo-symmetric of order $4n+3$. We designate them as T**-methods**.

2 Construction of the family of T-methods

In this section we construct the new family of integrators $T_h^{(k)}$ and show explicitly that they are of order $2(n+k)$ and pseudo-symmetric of order $4n+3$ for $k = 1, 2, 3$. The same procedure can be formally extended to any $k > 3$. The analysis is based on the Lie formalism applied to the series of differential operators associated to the integrators.

2.1 Series of differential operators

As is well known, given a time-symmetric integrator $\mathcal{S}_h^{[2n]}$ of order $2n \geq 2$ one can associate a series of linear operators $\exp(Y(h))$ so that

$$g(\mathcal{S}_h^{[2n]}(x)) = \exp(Y(h))[g](x)$$

for all functions g [9], with

$$Y(h) = hY_1 + h^{2n+1}Y_{2n+1} + h^{2n+3}Y_{2n+3} + \cdots .$$

Here Y_k are certain operators depending on the particular method and, for consistency, $Y_1 = F$, where F is the Lie derivative associated with f:

$$F = \sum_{i \geq 1} f_i(x) \, \frac{\partial}{\partial x_i}. \tag{2.1}$$

The composition (1.2) then has the associated series

$$\Psi(h) = \exp(Y(h\alpha_s)) \, \exp(Y(h\alpha_{s-1})) \cdots \exp(Y(h\alpha_2)) \, \exp(Y(h\alpha_1)), \tag{2.2}$$

which can be formally written as $\Psi(h) = \exp(V(h))$ by repeated application of the Baker–Campbell–Hausdorff formula, with

$$V(h) = hF + h^{2n+1}V_{2n+1} + h^{2n+2}V_{2n+2} + \cdots .$$

Here $V_{2n+1}, V_{2n+2}, \dots$ are linear combinations of Lie brackets involving the operators $Y_1, Y_{2n+1}, Y_{2n+3}, \dots$ [18]. In the particular case of a symmetric-conjugate composition (1.10), terms V_{2k} in $V(h)$ of even powers in h are pure imaginary, whereas terms V_{2k+1} are real [7].

For a consistent symmetric-conjugate composition (1.10), i.e., verifying

$$\sum_{j=1}^{s} \alpha_j = \alpha_1 + \alpha_2 + \cdots + \bar{\alpha}_2 + \bar{\alpha}_1 = 1, \tag{2.3}$$

we get explicitly

$$V(h) = hE_{1,1} + h^{2n} \sum_{j\geq 0} h^{2j+1} \sum_{k=1}^{\ell_{2j+1}} \mu_{2n+2j+1,k} E_{2j+1,k} + i\, h^{2n} \sum_{j\geq 1} h^{2j} \sum_{k=1}^{\ell_{2j}} \sigma_{2n+2j,k} E_{2j,k}, \tag{2.4}$$

where $\mu_{n,k}$, $\sigma_{n,k}$ are homogeneous real polynomials of degree n in the coefficients α_l, $l = 1, \dots, s$, and $E_{n,k}$ are elements Y_j and independent Lie brackets involving these operators. In particular

$$\mu_{2n+2j+1,1} = \sum_{l=1}^{s} \alpha_l^{2(n+j)+1}, \qquad j \geq 0$$

and

$$E_{1,1} = Y_1, \quad E_{2n+2n+2j+1,1} = Y_{2n+2j+1}, \quad E_{2n+2j,1} = [E_{1,1}, E_{2n+(2j-1),1}], \quad j = 1, 2, \dots$$

2.2 Linear combinations of symmetric-conjugate compositions

Let us now consider the linear combination

$$\phi_h = \frac{1}{2k} \sum_{j=1}^{k} \left(\psi_h^{(j)} + \overline{\psi}_h^{(j)} \right), \tag{2.5}$$

where each $\psi_h^{(j)}$ is a consistent symmetric-conjugate composition of the form (1.10) with different coefficients $\alpha_k^{(j)}$. Then, clearly, ϕ_h has

$$\Phi(h) \equiv \frac{1}{2k} \sum_{j=1}^{k} \left(\Psi^{(j)}(h) + \overline{\Psi}^{(j)}(h) \right) = \frac{1}{2k} \sum_{j=1}^{k} \left(\mathrm{e}^{V_j(h)} + \mathrm{e}^{\overline{V}_j(h)} \right) \tag{2.6}$$

as the associated series of operators, where each $V_j(h)$ is of the form (2.4). Now, by following the same approach as in [11], we express $\Phi(h)$ as

$$\Phi(h) = \frac{1}{2k} \mathrm{e}^{\frac{h}{2}F} \sum_{j=1}^{k} \left(\mathrm{e}^{W_j(h)} + \mathrm{e}^{\overline{W}_j(h)} \right) \mathrm{e}^{\frac{h}{2}F},$$

where

$$
\begin{aligned}
W_j(h) = {} & h^{2n+1}\mu^{(j)}_{2n+1,1}E_{2n+1,1} + i\,h^{2n+2}\sigma^{(j)}_{2n+2,1}E_{2n+2,1} \\
& + h^{2n+3}\left(\mu^{(j)}_{2n+3,1}E_{2n+3,1} + \left(\mu^{(j)}_{2n+3,2} + \frac{1}{24}\mu^{(j)}_{2n+1,1}\right)E_{2n+3,2}\right) \\
& + i\,h^{2n+4}\left(\sigma^{(j)}_{2n+4,1}E_{2n+4,1} + \left(\sigma^{(j)}_{2n+4,2} + \frac{1}{24}\sigma^{(j)}_{2n+2,1}\right)E_{2n+4,2}\right) \\
& + h^{2n+5}\left(\mu^{(j)}_{2n+5,1}E_{2n+5,1} + \left(\mu^{(j)}_{2n+5,2} + \frac{1}{24}\mu^{(j)}_{2n+3,1}\right)E_{2n+5,2} + \right. \\
& \qquad \left. \left(\mu^{(j)}_{2n+5,3} + \frac{1}{24}\mu^{(j)}_{2n+3,2} + \frac{1}{1920}\mu^{(j)}_{2n+1,1}\right)E_{2n+5,3}\right) \\
& + i\,h^{2n+6}\left(\sigma^{(j)}_{2n+6,1}E_{2n+6,1} + \left(\sigma^{(j)}_{2n+6,2} + \frac{1}{24}\sigma^{(j)}_{2n+4,1}\right)E_{2n+6,2} + \right. \\
& \qquad \left. \left(\sigma^{(j)}_{2n+6,3} + \frac{1}{24}\sigma^{(j)}_{2n+4,2} + \frac{1}{1920}\sigma^{(j)}_{2n+2,1}\right)E_{2n+6,3}\right) \\
& + \mathcal{O}(h^{2n+7}).
\end{aligned}
\tag{2.7}
$$

Here

$$
\begin{aligned}
&E_{2n+3,2} = [E_{1,1}, E_{2n+2,1}], \quad E_{2n+4,2} = [E_{1,1}, E_{2n+3,2}], \quad E_{2n+5,2} = [E_{1,1}, E_{2n+4,1}], \\
&E_{2n+6,2} = [E_{1,1}, E_{2n+5,1}], \quad E_{2n+5,3} = [E_{1,1}, E_{2n+4,2}], \quad E_{2n+6,2} = [E_{1,1}, E_{2n+5,2}].
\end{aligned}
$$

This is done by applying the symmetric Baker–Campbell–Hausdorff formula to each product $\mathrm{e}^{-\frac{h}{2}F}\,\mathrm{e}^{V_j(h)}\,\mathrm{e}^{-\frac{h}{2}F}$. From (2.7), a straightforward calculation shows that

$$
\begin{aligned}
(W_j + \overline{W}_j)^2 &= 4h^{4n+2}(\mu^{(j)}_{2n+1,1})^2\,E^2_{2n+1,1} + \mathcal{O}(h^{4n+4}) \\
W_j^2 + \overline{W}_j^2 &= 2h^{4n+2}(\mu^{(j)}_{2n+1,1})^2\,E^2_{2n+1,1} + \mathcal{O}(h^{4n+4}).
\end{aligned}
$$

Therefore,

$$
\frac{1}{2}\left(\mathrm{e}^{W_j} + \mathrm{e}^{\overline{W}_j}\right) - \mathrm{e}^{\frac{1}{2}(W_j+\overline{W}_j)} = \frac{1}{4}(W_j^2 + \overline{W}_j^2) - \frac{1}{8}(W_j + \overline{W}_j)^2 + \cdots = \mathcal{O}(h^{4n+4})
$$

and $\Phi(h)$ can also be written as

$$
\Phi(h) = \frac{1}{k}\sum_{j=1}^{k} \mathrm{e}^{\frac{h}{2}F}\,\mathrm{e}^{\frac{1}{2}(W_j(h)+\overline{W}_j(h))}\,\mathrm{e}^{\frac{h}{2}F} + \mathcal{O}(h^{4n+4}).
$$

In consequence, each term in ϕ_h is time-symmetric up to terms h^{4n+3}, with independence of the polynomials $\mu^{(j)}_{k,l}$, $\sigma^{(j)}_{k,l}$, since the sum $W_j(h) + \overline{W}_j(h)$ only contains odd powers of h.

On the other hand, one has

$$\begin{aligned}
&\frac{1}{2k}\sum_{j=1}^{k}\left(\mathrm{e}^{W_j}+\mathrm{e}^{\overline{W}_j}\right)-\exp\left(\frac{1}{2k}\sum_{j=1}^{k}(W_j+\overline{W}_j)\right)\\
&=\frac{1}{4k}\sum_{j=1}^{k}(W_j^2+\overline{W}_j^2)-\frac{1}{8k^2}\left(\sum_{j=1}^{k}(W_j+\overline{W}_j)\right)^2+\cdots\\
&=h^{4n+2}\,\frac{1}{2k}\left(\sum_{j=1}^{k}(\mu_{2n+1}^{(j)})^2-\frac{1}{k}\Big(\sum_{j=1}^{k}\mu_{2n+1,1}^{(j)}\Big)^2\right)E_{2n+1,1}^2+\mathcal{O}(h^{4n+4}),
\end{aligned}$$

so that it is also true that

$$\Phi(h)=\exp\left(\frac{h}{2}F\right)\exp\left(\frac{1}{2k}\sum_{j=1}^{k}\big(W_j(h)+\overline{W}_j(h)\big)\right)\exp\left(\frac{h}{2}F\right)+\mathcal{O}(h^{4n+2}). \tag{2.8}$$

2.3 Order conditions

It is thus possible to obtain the order conditions for the method ϕ_h in (2.5) by analyzing just the exponent of the central term in (2.8). From (2.7) it follows that

$$\begin{aligned}
\frac{1}{2}\sum_{j=1}^{k}\big(W_j(h)+\overline{W}_j(h)\big)&=h^{2n+1}\,c_{2n+1,1}\,E_{2n+1,1}+h^{2n+3}c_{2n+3,1}E_{2n+3,1}\\
&+h^{2n+3}\left(c_{2n+3,2}+\frac{1}{24}c_{2n+1,1}\right)E_{2n+3,2}+h^{2n+5}\,c_{2n+5,1}\,E_{2n+5,1}\\
&+h^{2n+5}\left(c_{2n+5,2}+\frac{1}{24}c_{2n+3,1}\right)E_{2n+5,2}\\
&+h^{2n+5}\left(c_{2n+5,3}+\frac{1}{24}c_{2n+3,2}+\frac{1}{1920}c_{2n+1,1}\right)E_{2n+5,3}+\mathcal{O}(h^{2n+7}),
\end{aligned}$$

with

$$\begin{aligned}
c_{2n+1,1}&=\sum_{j=1}^{k}\mu_{2n+1,1}^{(j)}, & c_{2n+3,1}&=\sum_{j=1}^{k}\mu_{2n+3,1}^{(j)}, & c_{2n+3,2}&=\sum_{j=1}^{k}\mu_{2n+3,2}^{(j)}\\
c_{2n+5,1}&=\sum_{j=1}^{k}\mu_{2n+5,1}^{(j)}, & c_{2n+5,2}&=\sum_{j=1}^{k}\mu_{2n+5,2}^{(j)}, & c_{2n+5,3}&=\sum_{j=1}^{k}\mu_{2n+5,3}^{(j)}
\end{aligned}$$

In consequence, for consistent compositions $\psi_h^{(j)}$, $j=1,\ldots,k$, the conditions to be satisfied so that ϕ_h is a method of order r are the following:

- $r=2n+2$: $c_{2n+1,1}=0$
- $r=2n+4$: $c_{2n+1,1}=c_{2n+3,1}=c_{2n+3,2}=0$
- $r=2n+6$: $c_{2n+1,1}=c_{2n+3,1}=c_{2n+3,2}=c_{2n+5,1}=c_{2n+5,2}=c_{2n+5,3}=0$

2.4 New schemes

Once identified the relevant order conditions, our next goal is to solve these equations with the minimum number of basic schemes in the compositions $\psi_h^{(j)}$ and the minimum value of k in the linear combination (2.5).

Order $r = 2n + 2$. One needs to solve two equations to get a method ϕ_h of order $2n + 2$: consistency and $c_{2n+1,1} = 0$. These can be satisfied by taking $k = 1$ and the simplest composition $\psi_h = \mathcal{S}^{[2n]}_{\alpha_1 h} \circ \mathcal{S}^{[2n]}_{\bar\alpha_1 h}$, in which case one has

$$\alpha_1 + \bar\alpha_1 = 1, \qquad \alpha_1^{2n+1} + \bar\alpha_1^{2n+1} = 0.$$

In other words, we recover the composition (1.6) and the R-method (1.8). Our first T-method (1.11) is thus

$$T_h^{(1)} = \frac{1}{2}\Big((\gamma^{[2n]}, \bar\gamma^{[2n]}) + (\bar\gamma^{[2n]}, \gamma^{[2n]})\Big) \tag{2.9}$$

or in more detail

$$T_h^{(1)} = \frac{1}{2}\Big(\mathcal{S}^{[2n]}_{\gamma^{[2n]}h} \circ \mathcal{S}^{[2n]}_{\bar\gamma^{[2n]}h} + \mathcal{S}^{[2n]}_{\bar\gamma^{[2n]}h} \circ \mathcal{S}^{[2n]}_{\gamma^{[2n]}h}\Big).$$

Order $r = 2n+4$. Now we have to solve 3 order conditions in addition to consistency for the compositions $\psi_h^{(j)}$ involved. As before, one could take in principle $k = 1$. In that case, the minimum number of basic maps in $\psi_h^{(1)}$ is 4, just to have enough parameters to satisfy the order conditions. It turns out, however, that there are no solutions with the required symmetry $\alpha_4 = \bar\alpha_1$, $\alpha_3 = \bar\alpha_2$. In fact, if we take

$$\psi_h^{(1)} = (\bar\alpha_1, \bar\alpha_2, \alpha_2, \alpha_1), \qquad \text{with} \qquad \alpha_1 = \bar\gamma^{[2n+4]}\bar\gamma^{[2n+2]}, \quad \alpha_2 = \bar\gamma^{[2n+4]}\gamma^{[2n]},$$

then $\mu^{(1)}_{2n+1,1} = \mu^{(1)}_{2n+3,1} = 0$, but $\mu^{(1)}_{2n+3,2} \neq 0$. On the other hand, if we take

$$\psi_h^{(2)} = (\bar\alpha_2, \bar\alpha_1, \alpha_1, \alpha_2)$$

with the *same* values of α_1, α_2 as before, then $\mu^{(2)}_{2n+3,2} = -\mu^{(1)}_{2n+3,2}$, whereas still verifying that $\mu^{(2)}_{2n+1,1} = \mu^{(2)}_{2n+3,1} = 0$. In consequence, by combining both compositions,

$$\phi_h = \frac{1}{4}\left(\psi_h^{(1)} + \overline{\psi}_h^{(1)} + \psi_h^{(2)} + \overline{\psi}_h^{(2)}\right),$$

one gets a method of order $2n + 4$ and pseudo-symmetric of order $4n + 3$. This corresponds to our second T-method, which reads explicitly

$$\begin{aligned} T_h^{(2)} \;=\; & \frac{1}{4}\Big((\gamma^{[2n+2]}\gamma^{[2n]}, \gamma^{[2n+2]}\bar\gamma^{[2n]}, \bar\gamma^{[2n+2]}\gamma^{[2n]}, \bar\gamma^{[2n+2]}\bar\gamma^{[2n]}) \\ & + (\gamma^{[2n+2]}\bar\gamma^{[2n]}, \gamma^{[2n+2]}\gamma^{[2n]}, \bar\gamma^{[2n+2]}\bar\gamma^{[2n]}, \bar\gamma^{[2n+2]}\gamma^{[2n]}) \\ & + (\bar\gamma^{[2n+2]}\bar\gamma^{[2n]}, \bar\gamma^{[2n+2]}\gamma^{[2n]}, \gamma^{[2n+2]}\bar\gamma^{[2n]}, \gamma^{[2n+2]}\gamma^{[2n]}) \\ & + (\bar\gamma^{[2n+2]}\gamma^{[2n]}, \bar\gamma^{[2n+2]}\bar\gamma^{[2n]}, \gamma^{[2n+2]}\gamma^{[2n]}, \gamma^{[2n+2]}\bar\gamma^{[2n]})\Big). \end{aligned} \tag{2.10}$$

Again, the coefficients $\gamma^{[2m]}$ are given by Eq. (1.7).

Order $r = 2n + 6$**.** A total of 7 equations (including consistency) have to be solved in this case, so that we take a symmetric-conjugate composition involving $s = 8$ basic maps,

$$\psi_h^{(1)} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4, \bar{\alpha}_4, \bar{\alpha}_3, \bar{\alpha}_2, \bar{\alpha}_1).$$

With the choice

$$\begin{aligned} \alpha_1 &= \gamma^{[2n+4]}\gamma^{[2n+2]}\gamma^{[2n]}, & \alpha_2 &= \gamma^{[2n+4]}\gamma^{[2n+2]}\bar{\gamma}^{[2n]}, \\ \alpha_3 &= \gamma^{[2n+4]}\bar{\gamma}^{[2n+2]}\gamma^{[2n]}, & \alpha_4 &= \gamma^{[2n+4]}\bar{\gamma}^{[2n+2]}\bar{\gamma}^{[2n]} \end{aligned}$$

it turns out that conditions $c_{2n+1} = c_{2n+3,1} = c_{2n+5,1} = 0$ are automatically satisfied. By following the same approach as before, we permute the position of the coefficients and take the composition

$$\psi_h^{(2)} = (\alpha_2, \alpha_1, \alpha_4, \alpha_3, \bar{\alpha}_3, \bar{\alpha}_4, \bar{\alpha}_1, \bar{\alpha}_2).$$

Then, one has $\mu_{2n+3,2}^{(2)} = -\mu_{2n+3,2}^{(1)}$, so that $\psi_h^{(1)} + \psi_h^{(2)}$ leads to a method of order $2n+4$. More composition have to be incorporated, however, in order to verify conditions $c_{2n+5,2} = 0$ and $c_{2n+5,3} = 0$. The former is accomplished by both sums $\psi_h^{(1)} + \psi_h^{(4)}$ and $\psi_h^{(2)} + \psi_h^{(3)}$, where

$$\begin{aligned} \psi_h^{(3)} &= (\alpha_3, \alpha_4, \alpha_1, \alpha_2, \bar{\alpha}_2, \bar{\alpha}_1, \bar{\alpha}_4, \bar{\alpha}_3) \\ \psi_h^{(4)} &= (\alpha_4, \alpha_3, \alpha_2, \alpha_1, \bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, \bar{\alpha}_4), \end{aligned}$$

but the later is satisfied only by adding up the four compositions. In summary, the linear combination

$$\frac{1}{4}\Re(\psi_h^{(1)} + \psi_h^{(2)} + \psi_h^{(3)} + \psi_h^{(4)})$$

leads to a method of order $2n + 6$, denoted as $T_h^{(3)}$. More explicitly,

$$T_h^{(3)} = \frac{1}{8}\Big(\psi_h^{(1)} + \psi_h^{(2)} + \psi_h^{(3)} + \psi_h^{(4)} + \overline{\psi}_h^{(1)} + \overline{\psi}_h^{(2)} + \overline{\psi}_h^{(3)} + \overline{\psi}_h^{(4)}\Big). \tag{2.11}$$

The same procedure can be carried out in general, although more order conditions (and consequently more compositions involving more basic maps) have to be dealt with. This class of methods can be represented in a convenient way as follows. If we introduce the matrix of coefficients

$$\Gamma_{2n} := \frac{1}{2}\begin{pmatrix} \gamma^{[2n]} & \bar{\gamma}^{[2n]} \\ \bar{\gamma}^{[2n]} & \gamma^{[2n]} \end{pmatrix}$$

then, according with the previous results, method $T_h^{(1)}$ (of order $2n + 2$) can be represented by Γ_{2n},

$$T_h^{(1)} \rightsquigarrow \Gamma_{2n},$$

whereas $T_h^{(2)}$ (of order $2n + 4$) can be associated with the matrix

$$\Gamma_{2n+2} \otimes \Gamma_{2n} = \frac{1}{4}\begin{pmatrix} \gamma^{[2n+2]}\gamma^{[2n]} & \gamma^{[2n+2]}\bar{\gamma}^{[2n]} & \bar{\gamma}^{[2n+2]}\gamma^{[2n]} & \bar{\gamma}^{[2n+2]}\bar{\gamma}^{[2n]} \\ \gamma^{[2n+2]}\bar{\gamma}^{[2n]} & \gamma^{[2n+2]}\gamma^{[2n]} & \bar{\gamma}^{[2n+2]}\bar{\gamma}^{[2n]} & \bar{\gamma}^{[2n+2]}\gamma^{[2n]} \\ \bar{\gamma}^{[2n+2]}\gamma^{[2n]} & \bar{\gamma}^{[2n+2]}\bar{\gamma}^{[2n]} & \gamma^{[2n+2]}\gamma^{[2n]} & \gamma^{[2n+2]}\bar{\gamma}^{[2n]} \\ \bar{\gamma}^{[2n+2]}\bar{\gamma}^{[2n]} & \bar{\gamma}^{[2n+2]}\gamma^{[2n]} & \gamma^{[2n+2]}\bar{\gamma}^{[2n]} & \gamma^{[2n+2]}\gamma^{[2n]} \end{pmatrix},$$

in the sense that each file of Γ_{2n+2} corresponds to a particular symmetric-conjugate composition entering into the formulation of $T_h^{(2)}$. We can write analogously

$$T_h^{(2)} \rightsquigarrow \Gamma_{2n+2} \otimes \Gamma_{2n},$$

and moreover

$$T_h^{(3)} \rightsquigarrow \Gamma_{2n+4} \otimes (\Gamma_{2n+2} \otimes \Gamma_{2n}).$$

In general, the coefficients in the T-method of order $r = 2n + 2k$ are distributed according with the pattern

$$T_h^{(k)} \rightsquigarrow \Gamma_{2(n+k-1)} \otimes (\Gamma_{2(n+k-2)} \otimes \cdots \otimes (\Gamma_{2n+2} \otimes \Gamma_{2n}) \cdots).$$

3 Numerical examples

We illustrate next the behavior of some of the previously constructed T-methods on a pair of numerical examples. The first one (the 2-dimensional Kepler problem) allows one to check preservation properties, whereas the second (a simple diffusion equation) is used as a test of their relative performance. In all cases we take as basic scheme $\mathcal{S}_h^{[2n]}$ the 4th-order ($n = 2$) time-symmetric splitting method

$$\mathcal{S}_h^{[4]} = \varphi_{b_1 h}^{[b]} \circ \varphi_{a_1 h}^{[a]} \circ \varphi_{b_2 h}^{[b]} \circ \varphi_{a_2 h}^{[a]} \circ \varphi_{b_3 h}^{[b]} \circ \varphi_{a_2 h}^{[a]} \circ \varphi_{b_2 h}^{[b]} \circ \varphi_{a_1 h}^{[a]} \circ \varphi_{b_1 h}^{[b]} \tag{3.1}$$

with coefficients

$$\begin{aligned} b_1 &= 0.060078275263542357774 - 0.060314841253378523039\, i, \\ a_1 &= 0.18596881959910913140, \\ b_2 &= 0.27021183913361078161 + 0.15290393229116195895\, i, \\ a_2 &= 0.31403118040089086860, \\ b_3 &= 0.33941977120569372122 - 0.18517818207556687181\, i, \end{aligned} \tag{3.2}$$

previously considered in [8]. This integrator is intended for Eq. (1.1) when f can be decomposed as $f(x) = f_a(x) + f_b(x)$ in such a way that each sub-problem

$$\dot{x} = f_a(x), \qquad \dot{x} = f_b(x),$$

with $x(0) = x_0$, has solution $x(t) = \varphi_t^{[a]}(x_0)$, and $x(t) = \varphi_t^{[b]}(x_0)$, respectively.

The implementation of all the integrators has been done in Python 3.7 running on Debian GNU/Linux 10 and the operations with complex arithmetics have been coded using the complex class of the numpy library.

Kepler problem. The Hamiltonian function for the planar two-body problem reads

$$H(q,p) = T(p) + V(q) = \frac{1}{2} p^T p - \mu \frac{1}{r}. \tag{3.3}$$

Here $q = (q_1, q_2)$, $p = (p_1, p_2)$, $r = \|q\|$, $\mu = GM$, G is the gravitational constant and M is the sum of the masses of the two bodies. The corresponding equations of motion are then

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = p_i, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} = -\mu \frac{q_i}{r^3}, \qquad i = 1, 2.$$

Taking $\mu = 1$ and initial conditions

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \tag{3.4}$$

the resulting trajectory is an ellipse of eccentricity $0 \le e < 1$. In this case $\varphi_h^{[a]}$ (respectively, $\varphi_h^{[b]}$) corresponds to the exact solution obtained by integrating the kinetic energy $T(p)$ (resp., potential energy $V(q)$) in (3.3).

We take $e = 0.6$, integrate until the final time $t_f = 20\pi$ with the basic splitting method $\mathcal{S}_h^{[4]}$ given by (3.1) and schemes $T_h^{(k)}$, with $k = 1, 2, 3$ for several time steps and then we compute the average error in energy along the integration interval. Figure 1 (left) shows this error as a function of the number of evaluations of the basic scheme $\mathcal{S}_h^{[4]}$. The diagram clearly exhibits the order of convergence of each method: order 4 for $\mathcal{S}_h^{[4]}$, and orders 6, 8 and 10 for $T_h^{(1)}$, $T_h^{(2)}$ and $T_h^{(3)}$, respectively.

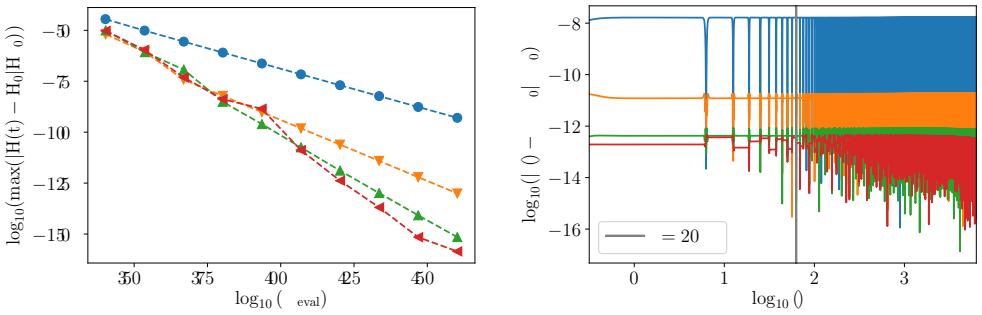

Figure 1: Left: Relative error in energy vs. number of evaluations of the basic scheme $\mathcal{S}^{[4]}$ (blue) for the different T-methods: $T^{(1)}$ (orange), $T^{(2)}$ (green) and $T^{(3)}$ (red), in the interval $t \in [0, 20\pi]$. Right: Evolution of this error along the integration when $t \in [0, 2000\pi]$. In this case the step size is chosen so that all schemes involve the same number of evaluations of the basic method.

In the right panel we show the long-time behavior of the error in energy for each method when the step size is chosen so that all of them involve the same computational cost. We see that the error in energy is almost constant for $t \le 2000\pi$, as is the case for symplectic integrators. In other words, the lack of symplecticity at order h^{12} has no effect in this integration interval. In addition, the scheme $T_h^{(3)}$ provides the smaller error.

A linear parabolic equation. Our second example concerns the linear equation in one-dimension

$$\frac{\partial}{\partial t} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) + V(x) u(x,t), \qquad u(x,0) = \sin(2\pi x), \tag{3.5}$$

with periodic boundary conditions in the space domain $[0,1]$. We take $V(x) = 8 + 4\sin(2\pi x)$ and partition the interval $[0,1]$ into N parts of length $\Delta x = 1/N$, so that the vector $U = (U_0, \ldots, U_{N-1})^T \in \mathbb{R}^N$ is formed, with $U_j = u(x_j, t)$ and $x_j = j/N$, $j = 0, 1, \ldots, N-1$. If a Fourier spectral collocation method is used, we end up with the N-dimensional linear ODE

$$\frac{dU}{dt} = A\,U + B\,U, \tag{3.6}$$

where $B = \mathrm{diag}(V(x_0), \ldots, V(x_{N-1}))$ and A is a (full) differentiation matrix related with the second derivative ∂_{xx}. The splitting here corresponds to solving separately the systems $\dot{U} = A\,U$ and $\dot{U} = B\,U$. Notice that, since B is diagonal, then

$$(\mathrm{e}^{hB}U)_j = \mathrm{e}^{hV(x_j)}U_j$$

and only requires the computation of N multiplications. On the other hand, $A\,U = \mathcal{F}^{-1}D_A\mathcal{F}\,U$, where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are the forward and backward discrete Fourier transform, and D_A is again diagonal [23]. In consequence,

$$\mathrm{e}^{hA}\,U = \mathcal{F}^{-1}\mathrm{e}^{hD_A}\mathcal{F}\,U,$$

requiring $\mathcal{O}(N \log N)$ operations when the transformation $\mathcal{F}$ (and its inverse) is computed with the fast Fourier transform (FFT) algorithm.

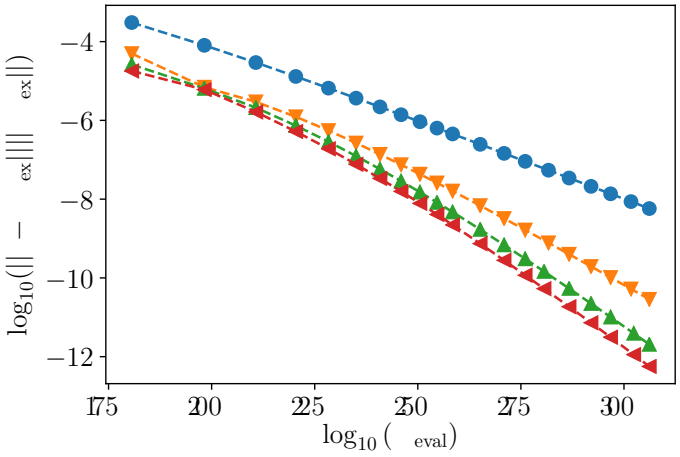

Figure 2: Error vs. number of evaluations of the basic method (3.1) obtained by schemes $T_h^{(1)}$ (orange), $T_h^{(2)}$ (green) and $T_h^{(3)}$ (red). The blue line corresponds to $\mathcal{S}_h^{[4]}$.

We take $N = 128$ and integrate until $t_f = 1$, where we compute the relative error $\|U - U_{ex}\|/\|U_{ex}\|$ with each method $T_h^{(k)}$, $k = 1, 2, 3$, in addition to the basic scheme (3.1). The 'exact' solution U_{ex} is taken as the

output of the 8th-order composition method **P8S15** of [8]. The corresponding efficiency diagram is shown in Figure 2, where the same notation is used for the curves depicted. Here also the higher degree integrators provide the best efficiency.

4 Discussion

4.1 T-methods and R-methods

Methods $T_h^{(k)}$ have indeed close similarities with the compositions $R_h^{(k)}$ (1.9) previously analyzed in [11]: not only their starting point is the same (the basic time-symmetric method $\mathcal{S}_h^{[2n]}$), but one has in addition $T_h^{(1)} = R_h^{(1)}$ and also the same coefficients $\gamma^{[2m]}$ defined in (1.7) enter into their formulation. Finally, they have the same preservation properties. There is, however, a fundamental difference: whereas T-methods are linear combinations of symmetric-conjugate compositions only, this is not the case of R-methods, and in fact schemes $R_h^{(k)}$ involve a much larger number of compositions. This can be clearly seen by writing explicitly the expression of $R_h^{(2)}$:

$$\begin{aligned} R_h^{(2)} \;=\; \frac{1}{8}\Big(& (\gamma^{[2n+2]}\gamma^{[2n]}, \gamma^{[2n+2]}\bar\gamma^{[2n]}, \bar\gamma^{[2n+2]}\gamma^{[2n]}, \bar\gamma^{[2n+2]}\bar\gamma^{[2n]}) \\ & +(\gamma^{[2n+2]}\bar\gamma^{[2n]}, \gamma^{[2n+2]}\gamma^{[2n]}, \bar\gamma^{[2n+2]}\bar\gamma^{[2n]}, \bar\gamma^{[2n+2]}\gamma^{[2n]}) \\ & +(\gamma^{[2n+2]}\gamma^{[2n]}, \gamma^{[2n+2]}\bar\gamma^{[2n]}, \bar\gamma^{[2n+2]}\bar\gamma^{[2n]}, \bar\gamma^{[2n+2]}\gamma^{[2n]}) \\ & +(\gamma^{[2n+2]}\bar\gamma^{[2n]}, \gamma^{[2n+2]}\gamma^{[2n]}, \bar\gamma^{[2n+2]}\gamma^{[2n]}, \bar\gamma^{[2n+2]}\bar\gamma^{[2n]}) \\ & +\text{c.c.}\Big), \end{aligned} \tag{4.1}$$

whereas $R_h^{(3)}$ is the sum of 64 compositions containing 8 basic schemes with weights $\gamma^{[2n+4]}\gamma^{[2n+2]}\gamma^{[2n]}$, $\bar\gamma^{[2n+4]}\gamma^{[2n+2]}\gamma^{[2n]}$, etc. plus their complex conjugate divided by 128. In general, $R_h^{(k)}$ involves the sum of 2^{2^k-2} compositions of 2^k appropriately weighted basic schemes:

$$R_h^{(k)} = \frac{1}{2^{2^k-1}} \sum_{j=1}^{2^{2^k-2}} \Big((\alpha_{j_{2^k}}, \ldots, \alpha_{j_1}) + \text{c.c.} \Big),$$

where α_{j_i} are products of the k coefficients $\gamma^{[2n]}, \ldots, \gamma^{[2(n+k-1)]}$ and their complex conjugate. This should be compared with the T-methods: in general, $T_h^{(k)}$ involves the sum of 2^{k-1} compositions of 2^k basic schemes. In either case, the computation of the complex conjugate part can be avoided just by taking the real part, with no extra evaluations of $\mathcal{S}_h^{[2n]}$.

These numbers are collected in Table 1, when schemes $R_h^{(k)}$ (second column) and $T_h^{(k)}$ (last column) are formulated explicitly. Of course, a recursive implementation of R-methods by applying the procedure (1.9) turns out to be more efficient. In that case the required computational effort, measured as the number of basic schemes, is shown in the third column of the table. Again, in this case we only have to compute the real part in the last iteration.

In view of the number of basic maps required by the recursive implementation of R-methods and the explicit formulation (1.11) of T-methods, it is natural to ask what are the advantages (if any) of the later

k	R (explicit)	R (recursive)	T (explicit)
1	2	2	2
2	16	8	8
3	512	32	32
$\vdots$	$\vdots$	$\vdots$	$\vdots$
m	$2^m \cdot 2^{2^m-2}$	$2^m \cdot 2^{m-1}$	$2^m \cdot 2^{m-1}$

Table 1: Number of basic maps $\mathcal{S}_h^{[2n]}$ necessary to compute when formulating R- and T-methods explicitly or recursively (in the case of R-methods).

schemes with respect to the former ones. In this respect, one should take into account that both explicit formulations (1.11) and (4.1) are directly amenable to parallelization, whereas this is less obvious for the recursion (1.9).

If one has a computer with, say, 2ℓ threads, it is easy to estimate the effective number of evaluations of $\mathcal{S}_h^{[2n]}$ both for R- and T-methods. Thus, for $R_h^{(k)}$ one has:

- if $\ell \leq 2^k - 2$ then the number of evaluations is 2^k;
- if $\ell > 2^k - 2$ then the number of evaluations is $2^k \cdot 2^{2^k-2-\ell}$,

whereas this number is considerably reduced for schemes $T_h^{(k)}$:

- if $\ell \leq k - 1$ then the number of evaluations is 2^k;
- if $\ell > k - 1$ then the number of evaluations is $2^k \cdot 2^{k-1-\ell}$.

In Table 2 we collect these numbers for the first values of k in the particular case of $2^2 = 4$ and $2^5 = 32$ threads. We see that the implementation of the explicit expression of the R-methods is more advantageous than the recursive procedure already with a relatively small number of threads, and that, in any case, T-methods require less computational effort.

	4 threads		32 threads	
k	R	T	R	T
1	2	2	2	2
2	4	4	4	4
3	128	8	16	8

Table 2: Effective number of evaluations of the basic map $\mathcal{S}_h^{[2n]}$ when the corresponding R- and T-method is implemented in parallel with 4 and 32 threads.

To better illustrate this issue, we next compare the efficiency of the different methods when implemented on a computer able to execute 4 threads without loss of performance. The corresponding results are displayed

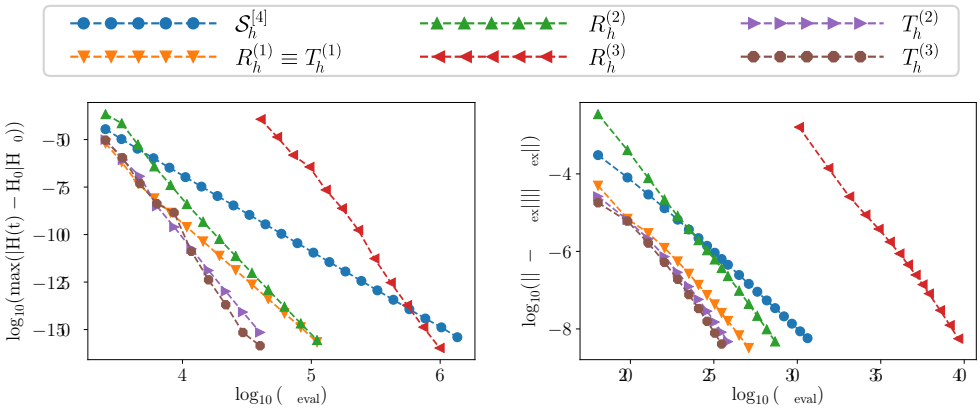

Figure 3: Efficiency diagram for R- and T-methods in a computer accepting 4 threads without loss of performance. Left: Kepler problem. Right: linear parabolic equation.

in Figure 3 for the Kepler problem (left) and the linear parabolic equation (3.5) (right). The gain in efficiency of the new schemes is clearly visible.

Even in the case when one could run the schemes on a machine such that the effective number of evaluations of both $R_h^{(k)}$ and $T_h^{(k)}$ is the same, i.e., 2^k in both cases, the latter turn out to be more efficient. This is clearly visible in Figure 4, obtained again by applying the previous schemes to the Kepler problem (left) and the linear parabolic equation (right).

Finally, it is also illustrative to compare the efficiency of the new T-methods with the standard triple-jump procedure, Eqs. (1.3)-(1.4), both applied to the same basic scheme (3.1). Thus, in Figure 5 we depict the results achieved by projecting $\mathcal{S}_h^{[6]}$, $\mathcal{S}_h^{[8]}$, and $\mathcal{S}_h^{[10]}$ at each step, together with $T_h^{(k)}$, $k = 1, 2, 3$ for the Kepler problem with the same parameters and final time $t_f = 20\pi$. Here the effective number of evaluations of the basic scheme has been taken as 2^k for T-methods and 3^k for triple-jump. Not surprisingly, the new schemes turn out to be much more efficient.

4.2 Concluding remarks

The standard triple-jump procedure is a popular technique that allows one to construct numerical integrators for differential equations of arbitrarily high order by composition of a basic integrator of low order. It has nevertheless certain limitations: the number of basic maps grows rapidly with the order, and the main error terms are quite large in comparison with other specially built integrators. Moreover, they involve some negative coefficients when the order $r \geq 3$, so that the resulting schemes cannot be used in particular when the initial value problem (1.1) results from the space discretization of a parabolic partial differential equation involving the Laplace operator. In this context it is quite natural to explore whether it is still possible using the triple-jump technique (1.3), but with the complex coefficients furnished by (1.5) as long as their real part is positive. It has been established that this is indeed the case, although once again they require an exceedingly

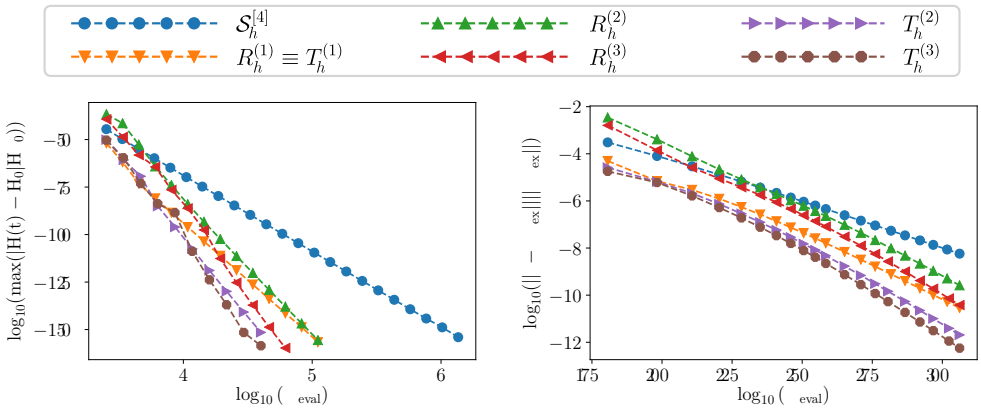

Figure 4: Efficiency diagram for R- and T-methods when the effective number of evaluations of the basic scheme is the same (2^k in both cases). Left: Kepler problem. Right: linear parabolic equation.

large number of basic methods. For this reason, other alternatives for constructing high-order composition methods have also been proposed [8, 12, 17]. Among them, the class of schemes (1.8) possess some special features: starting from a time-symmetric basic scheme $\mathcal{S}_h^{[2n]}$ of order $2n$, it is possible to construct recursively methods of order $2n + 2k$, $k = 1, 2, \ldots$ that are still time-symmetric up to order $4n + 3$. Moreover, if the differential equation in (1.1) has some qualitative properties (such as symplecticity or volume preservation) then these properties are still shared by the numerical solution up to order $4n + 3$ [11].

Methods (1.9) are based on the simple symmetric-conjugate composition (1.6). As shown in [7], symmetric-conjugate composition methods still possess remarkable preservation properties when projected on the real axis at each integration step, and so it makes sense to consider more general linear combinations of methods within this class. The corresponding analysis has been carried out here, and as a result we have built a new class of schemes that essentially have the same preservation properties as methods (1.9), but requiring a much reduced computational cost. In addition, these methods are particularly well suited for their parallel implementation. The examples included show a significant improvement in efficiency with respect to schemes (1.9) and those obtained by applying the triple-jump procedure.

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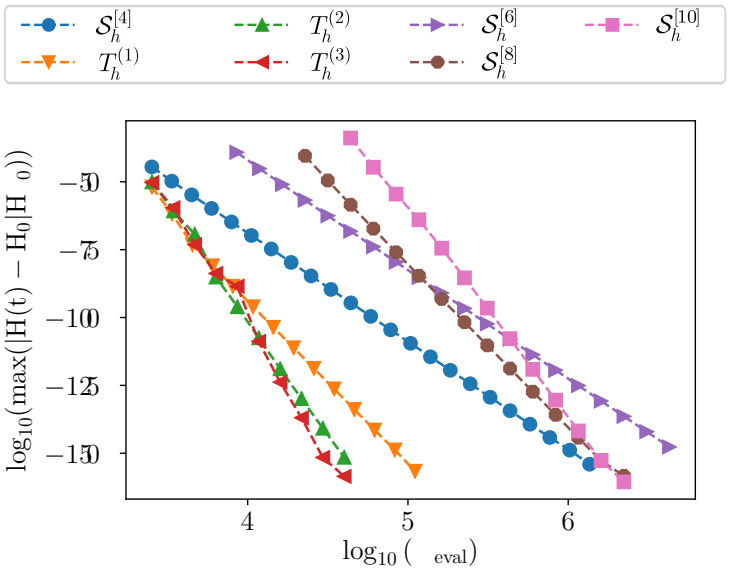

Figure 5: Error in energy vs. number of basic maps $\mathcal{S}_h^{[4]}$ for T-methods in comparison with schemes obtained by triple-jump for the Kepler problem.

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Capítulo 7

On symmetric–conjugate composition methods in the numerical integration of differential equations

On symmetric-conjugate composition methods in the numerical integration of differential equations

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Abstract

We analyze composition methods with complex coefficients exhibiting the so-called "symmetry-conjugate" pattern in their distribution. In particular, we study their behavior with respect to preservation of qualitative properties when projected on the real axis and we compare them with the usual left-right palindromic compositions. New schemes within this family up to order 8 are proposed and their efficiency is tested on several examples. Our analysis shows that higher-order schemes are more efficient even when time step sizes are relatively large.

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1 Introduction

We are concerned in this work with compositions of a time-symmetric 2nd-order integrator, denoted by $S_h^{[2]}$. To be more specific, given the initial value problem

$$x' = f(x), \qquad x(t_0) = x_0 \in \mathbb{R}^d \tag{1}$$

with solution $x(t) = \varphi_t(x_0)$, method $S_h^{[2]}$ verifies that $S_h^{[2]}(x_0) = \varphi_h(x_0) + \mathcal{O}(h^3)$ for a time step h and moreover $S_h^{[2]} \circ S_{-h}^{[2]} = \mathrm{id}$, the identity map, for any h. Then, the s-stage composition methods we are considering here are of the form

$$\psi_h^{[r]} = S_{\alpha_s h}^{[2]} \circ S_{\alpha_{s-1} h}^{[2]} \circ \cdots \circ S_{\alpha_2 h}^{[2]} \circ S_{\alpha_1 h}^{[2]}, \tag{2}$$

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where the coefficients α_j are certain numbers chosen in such a way that the order of approximation of $\psi_h^{[r]}$ is $r \geq 2$.

Methods (2) constitute a very efficient class of numerical integrators for (1), especially when f has some geometric properties that is advantageous to preserve under discretization. In fact, composition methods preserve any group properties shared by the basic scheme $S_h^{[2]}$: symplecticity, phase space volume, first integrals, symmetries, etc., and therefore they provide a general and flexible class of geometric numerical integrators [13].

If in addition the sequence of coefficients in (2) is *left-right palindromic*, i.e., $\alpha_{s+1-j} = \alpha_j$, $j = 1, 2, \ldots$, then $\psi_h^{[r]}$ is also time-symmetric, i.e., it verifies for small h

$$\psi_h^{[r]} \circ \psi_{-h}^{[r]} = \mathrm{id}, \tag{3}$$

and are of even order, $r = 2n$ [13]. Methods of this class are called symmetric compositions of symmetric schemes [15] and constitute an efficient way to construct high-order approximations, due to the reduction in the number of order conditions to be satisfied.

Nevertheless, the fact that composition methods of order greater than 2 require some negative coefficients α_j typically imposes severe stability restrictions on the time step, especially when dealing with semidiscretized PDEs [4]. To try to remedy this situation, *complex* coefficients with positive real part have been considered in the literature for this class of problems [6, 11, 14]. In fact, methods with complex coefficients have also been used even for problems when the presence of negative fractional time steps is not problematic [3, 12].

If composition methods with complex coefficients are applied to a real vector field f in (1), then the approximation x_1 at the end of the first time step $t_1 = t_0 + h$ will be of course complex, whereas the exact solution is real. A relevant issue is then how to proceed with the computation of the trajectory. Two possibilities exist: either one pursues the determination of the solution for $t > t_1$ with the previously computed value of $x_1 \in \mathbb{C}$ and project on the real axis only when output is desired (after, say, N integration steps) or one just discards the imaginary part of x_1 and initiates the next step only with $\Re(x_1)$. In both cases, however, the favourable properties the composition inherits from the basic scheme $S_h^{[2]}$ (such as symplecticity) are most often lost. Previous (heuristic) analyses show that, generally speaking, the later approach provides a better description of the problem [6, 8, 12].

One purpose of this work is to provide a rigorous justification of this observation and determine up to what degree symplecticity, say, is still preserved when using complex coefficients. We show, in particular, that a $2n$-th order left-right palindromic composition with complex coefficients, when projected on the real axis after each step, still preserves the time-symmetry and other relevant geometric properties up to order $4n+1$. Moreover, we also show that it is possible to preserve the time-symmetry up to a higher order by considering another family of compositions, namely methods of the form (2) with the special symmetry

$$\alpha_{s+1-j} = \bar{\alpha}_j, \qquad j = 1, 2, \ldots, \tag{4}$$

where $\bar{\alpha}_j$ denotes the complex conjugate of α_j. For obvious reasons, we call the resulting scheme

$$\psi_h^{[r]} = S_{\bar{\alpha}_1 h}^{[2]} \circ S_{\bar{\alpha}_2 h}^{[2]} \circ \cdots \circ S_{\alpha_2 h}^{[2]} \circ S_{\alpha_1 h}^{[2]}, \tag{5}$$

a *symmetric-conjugate* composition. The simplest method within this family is of course

$$\psi_h^{[3]} = S_{\alpha h}^{[2]} \circ S_{\bar{\alpha} h}^{[2]}. \tag{6}$$

If

$$\alpha = \frac{1}{2} \pm i \frac{\sqrt{3}}{6},$$

then $\psi_h^{[3]}$ is of order 3, but if one considers instead only its real part,

$$\Re(\psi_h^{[3]}) = \frac{1}{2}\left(\psi_h^{[3]} + \overline{\psi}_h^{[3]}\right) = \hat{R}_h^{[4]}, \tag{7}$$

or equivalently, if one projects $\psi_h^{[3]}$ at each time step on the real axis, then the resulting scheme $\hat{R}_h^{[4]}$ is an integration method of order 4. This fact has been previously recognized by several authors [3, 12]. Although $\hat{R}_h^{[4]}$ is no longer time-symmetric, it nevertheless verifies

$$\hat{R}_{-h}^{[4]} \circ \hat{R}_h^{[4]} = \mathrm{id} + \mathcal{O}(h^8)$$

when the vector field f in (1) is real [10]. Moreover, if f is a (real) Hamiltonian vector field and S_h is a 2nd-order symplectic integrator, then $\hat{R}_h^{[4]}$ is also symplectic with an error $\mathcal{O}(h^8)$.

Motivated by this feature of scheme $\hat{R}_h^{[4]}$ and the excellent preservation properties of methods (5) reported in particular in [8], we shall analyze in detail this class of integrators. In doing so, we will pay special attention to their preservation properties, and eventually we will propose new schemes requiring less number of stages for achieving a given order than left-right palindromic compositions when projected on the real axis after each integration step.

2 Compositions of a second-order symmetric scheme

2.1 Integrators and series of operators

If φ_h is the exact flow of the equation (1), then for each infinitely differentiable map g, the function $g(\varphi_h(x))$ admits an expansion of the form [1, 19]

$$g(\varphi_h(x)) = \exp(hF)[g](x) = g(x) + \sum_{k\geq 1} \frac{h^k}{k!} F^k[g](x),$$

where F is the Lie derivative associated with f,

$$F = \sum_{i\geq 1} f_i(x) \frac{\partial}{\partial x_i}. \tag{8}$$

Analogously, for the class of integrators ψ_h we are considering, one can associate a series of linear operators so that

$$g(\psi_h(x)) = \exp(Y(h))[g](x), \qquad \text{with} \qquad Y(h) = \sum_{j\geq 1} h^j Y_j$$

for all functions g [7]. Here Y_j are operators depending on the particular method considered. The integrator ψ_h is of order r if

$$Y_1 = F \qquad \text{and} \qquad Y_j = 0 \quad \text{for} \quad 2 \le j \le r.$$

For the adjoint integrator, defined as $\psi_h^* := \psi_{-h}^{-1}$, one clearly has

$$g(\psi_h^*(x)) = \exp\big(-Y(-h)\big)[g](x).$$

Notice that ψ_h is time-symmetric, i.e., it verifies (3), if and only if $\psi_h^* = \psi_h$, and therefore $Y(h)$ only contains odd powers of h. In particular, time-symmetric methods are of even order.

According with these comments, the time-symmetric 2nd-order scheme $S_h^{[2]}$ can be associated with the series

$$\Phi^{[2]}(h) = \exp(hF + h^3 Y_3 + h^5 Y_5 + \cdots + h^{2k+1} Y_{2k+1} + \cdots). \tag{9}$$

Then, the series of operators associated with the integrator (2) can be determined by applying the Baker–Campbell–Hausdorff formula, thus resulting in

$$\Psi^{[r]}(h) = \exp(V(h)), \tag{10}$$

where $V(h)$ is formally given by

$$V(h) = hw_1 F + h^3 w_{3,1} Y_3 + h^4 w_{4,1}[F, Y_3] + h^5\big(w_{5,1} Y_5 + w_{5,2}[F,[F,Y_3]]\big) + \mathcal{O}(h^6).$$

Here $[F, Y_3]$ stands for the Lie bracket of the operators F and Y_3, etc. and

$$\begin{aligned}
w_1 &= \sum_{j=1}^{s} \alpha_j, \qquad w_{3,1} = \sum_{j=1}^{s} \alpha_j^3, \qquad w_{5,1} = \sum_{j=1}^{s} \alpha_j^5, \\
w_{4,1} &= \frac{1}{2} \sum_{j=1}^{s-1} \left(\alpha_j^3 \left(\sum_{k=j+1}^{s} \alpha_k \right) - \alpha_j \left(\sum_{k=j+1}^{s} \alpha_k^3 \right) \right) \\
w_{5,2} &= \frac{1}{12} \sum_{j=1}^{s} \alpha_j^3 \left(\left(\sum_{k=1}^{j-1} \alpha_k \right)^2 + \left(\sum_{k=j+1}^{s} \alpha_k \right)^2 - 4 \sum_{k=1}^{j-1} \alpha_k \sum_{\ell=j+1}^{s} \alpha_\ell \right) \\
&\quad - \frac{1}{12} \sum_{j=1}^{s} \alpha_j^4 \left(\sum_{k=1}^{j-1} \alpha_k + \sum_{k=j+1}^{s} \alpha_k \right).
\end{aligned} \tag{11}$$

(In the expression of $w_{5,2}$ above the sum is zero when the upper index is smaller than the lower index). In general, $V(h)$ is an element of the free Lie algebra $\mathcal{L}$ generated by $\{F, Y_3, Y_5, \ldots\}$ [18], i.e., $V(h)$ is a linear combination of $F, Y_3, Y_5, \ldots$, and all their nested Lie brackets,

$$V(h) = hw_1 F + \sum_{n \ge 3} h^n \sum_{k=1}^{c(n)} w_{n,k} E_{n,k}. \tag{12}$$

Here $w_{n,k}$ are polynomials in the coefficients of the method, $E_{2n+1,1} = Y_{2n+1}$ and $E_{n,k}$, $k > 1$, are independent nested Lie brackets of $\{F, Y_3, Y_5, \ldots\}$ forming a basis of the

Order r	1	2	3	4	5	6	7	8
$N^{[r]}$ (General)	1	0	2	3	5	7	11	16
$N_P^{[r=2n]}$ (Palindromic)		1		2		4		8
$N^{[r]} - c(2n)$ (Sym-Conjugate)		1		2		5		11(9)

Table 1: Total number of order conditions to achieve order r for the method resulting from projecting after each step (i) the general composition (2) of time-symmetric 2nd-order methods (second row), a left-right palindromic composition (third row) and a symmetric-conjugate composition (fourth row). It turns out that by solving only 9 order conditions one can achieve order 8 with symmetric-conjugate compositions.

homogeneous component $\mathcal{L}_n$ of $\mathcal{L}$, with dimension $c(n)$ [17]. Thus, in particular, $\mathcal{L}_5$ has dimension $c(5) = 2$, and a basis is given by $\{E_{5,1} = Y_5, E_{5,2} = [F, [F, Y_3]]\}$.

Method (2) is of order r if $w_1 = 1$ and the polynomials $w_{n,k}$ vanish whenever $1 < n \leq r$, and $k = 1, \ldots, c(n)$. The number of the resulting equations (the order conditions) $N^{[r]}$ agrees of course with the sum of the dimensions $c(n)$, i.e.,

$$N^{[r]} = \sum_{n=1}^{r} c(n)$$

and is collected in Table 1 (second row) for the first values of r. A composition without any special symmetry would involve then at least $s = N^{[r]}$ stages so as to have enough parameters to solve the equations.

2.2 Left-right palindromic compositions

Before establishing general results about preservation of properties of composition methods with complex coefficients after projection on the real axis, it is worth to introduce the following definitions, as in [10]:

Definition 1 *Let ψ_h be a smooth and consistent integrator. Then*

1. *ψ_h is said to be* pseudo-symmetric *of* pseudo-symmetry order *q if for all sufficiently small h, it is true that*

$$\psi_h^* = \psi_h + \mathcal{O}(h^{q+1}), \tag{13}$$

where the constant in the $\mathcal{O}$-term depends on bounds of derivatives of ψ_h.

2. *ψ_h is said to be* pseudo-symplectic *of* pseudo-symplecticity order *p if for all sufficiently small h, the following relation holds true when it is applied to a Hamiltonian system:*

$$(\psi_h')^T \, J \, \psi_h' = J + \mathcal{O}(h^{p+1}), \tag{14}$$

where J denotes the canonical symplectic matrix and the constant in the $\mathcal{O}$-term depends on bounds of derivatives of ψ_h.

Remark 1 *A symmetric method is pseudo-symmetric of any order $q \in \mathbb{N}$, whereas a method of order r is pseudo-symmetric of order $q \geq r$. A similar statement holds for symplectic methods.*

We first proceed with left-right palindromic compositions. According to the considerations in the previous section, the series of operators associated with such a method of order $2n$ is $\Psi^{[2n]}(h) = \exp(V(h))$, with

$$V(h) = hw_1 F + \sum_{j\geq n} h^{2j+1} \sum_{k=1}^{c(2j+1)} w_{2j+1,k} E_{2j+1,k} \tag{15}$$

and $w_{2j+1,k}$ have in general real and imaginary parts when $\alpha_j \in \mathbb{C}$. Then one has the following

Proposition 1 *Given $S_h^{[2]}$ a time-symmetric 2nd-order method, consider the left-right palindromic composition*

$$\mathcal{S}_h^{[r]} = \mathcal{S}^{[2]}_{\alpha_1 h} \circ \mathcal{S}^{[2]}_{\alpha_2 h} \circ \cdots \circ \mathcal{S}^{[2]}_{\alpha_2 h} \circ \mathcal{S}^{[2]}_{\alpha_1 h} \tag{16}$$

of order $r = 2n$, $n = 2, 3, \ldots$, when the coefficients α_j are complex numbers satisfying $2(\alpha_1 + \alpha_2 + \cdots) = 1$. Then the method obtained by taking its real part,

$$\phi_h^{[2n]} \equiv \frac{1}{2}(\mathcal{S}_h^{[2n]} + \bar{\mathcal{S}}_h^{[2n]}),$$

is of the same order $r = 2n$ and pseudo-symmetric of order $q = 4n + 1$ when the vector field f in (1) is real. If in addition f is a (real) Hamiltonian vector field and $S_h^{[2]}$ is a symplectic integrator, then $\phi_h^{[2n]}$ is pseudo-symplectic of order $p = 4n + 1$.

Proof: In this and the remaining proofs we apply a similar approach as in [9] for determining the pseudo-symplectic character of methods obtained by polynomial extrapolation. An important ingredient is the symmetric BCH formula [5]: given X and Y two non-commuting operators, then

$$\exp(\frac{1}{2}X)\, \exp(Y)\, \exp(\frac{1}{2}X) = \exp(Z),$$

where $Z = \sum_{n\geq 0} Z_{2n+1}$ and Z_{2n+1}, $n \geq 1$, is a linear combination of nested brackets involving $2n + 1$ operators X and Y. The first terms read

$$Z_1 = X + Y, \qquad Z_3 = -\frac{1}{24}[X,[X,Y]] - \frac{1}{12}[Y,[X,Y]].$$

To begin with, we write the expression (15) associated with (16) as

$$V(h) = hF + h^{2n+1} V_{2n+1} + h^{2n+3} V_{2n+3} + \cdots$$

where V_{2n+j}, $j = 1, 3, \ldots$ are *complex* operators in the free Lie algebra generated by $\{F, Y_3, Y_5, \ldots\}$. In consequence, the series corresponding to $\phi_h^{[2n]}$ is

$$\Phi^{[2n]}(h) = \frac{1}{2}\exp((V(h)) + \frac{1}{2}\exp(\overline{V}(h)),$$

which can be written in fact as

$$\Phi^{[2n]}(h) = \exp\left(\frac{h}{2}F\right)\left(\frac{1}{2}\exp((W(h)) + \frac{1}{2}\exp(\overline{W}(h))\right)\exp\left(\frac{h}{2}F\right), \qquad (17)$$

where $W(h)$ is determined by applying the symmetric BCH formula to $\exp(W(h)) = \exp(-hF/2)\exp(V(h))\exp(-hF/2)$, thus leading to

$$W(h) = h^{2n+1}V_{2n+1} + h^{2n+3}\left(V_{2n+3} + \frac{1}{24}[F,[F,V_{2n+1}]]\right) + \mathcal{O}(h^{2n+5}).$$

Now the idea is to write $\Phi^{[2n]}(h)$ in (17) as $\mathrm{e}^{hF/2}\,\mathrm{e}^{(W+\overline{W})/2}\,\mathrm{e}^{hF/2} + \mathcal{O}(h^q)$, for some q. Therefore, we have to analyze $\frac{1}{2}(\mathrm{e}^{W} + \mathrm{e}^{\overline{W}}) - \mathrm{e}^{(W+\overline{W})/2}$. To this end, first we note that

$$W(h)+\overline{W}(h) = 2h^{2n+1}\Re(V_{2n+1})+2h^{2n+3}\left(\Re(V_{2n+3}) + \frac{1}{24}[F,[F,\Re(V_{2n+1})]]\right)+\mathcal{O}(h^{2n+5}),$$

i.e., only contains odd powers of h and

$$\frac{1}{8}\big(W(h) + \overline{W}(h)\big)^2 = \frac{1}{2}h^{4n+2}\,\Re(V_{2n+1})^2 + \mathcal{O}(h^{4n+4}),$$

whereas

$$\frac{1}{4}\big(W(h)^2 + \overline{W}(h)^2\big) = \frac{1}{2}h^{4n+2}\left(\Re(V_{2n+1})^2 - \Im(V_{2n+1})^2\right) + \mathcal{O}(h^{4n+4}).$$

In consequence,

$$\begin{aligned}\frac{1}{2}\left(\mathrm{e}^{W(h)} + \mathrm{e}^{\overline{W}(h)}\right) - \mathrm{e}^{\frac{1}{2}\left(W(h)+\overline{W}(h)\right)} &= \frac{1}{4}\big(W(h)^2 + \overline{W}(h)^2\big) - \frac{1}{8}\big(W(h) + \overline{W}(h)\big)^2 + \mathcal{O}(h^{4n+4})\\ &= -\frac{1}{2}h^{4n+2}\Im(V_{2n+1})^2 + \mathcal{O}(h^{4n+4})\end{aligned}$$

so that

$$\Phi^{[2n]}(h) = \exp\left(\frac{h}{2}F\right)\exp\left(\frac{1}{2}\big(W(h) + \overline{W}(h)\big)\right)\exp\left(\frac{h}{2}F\right) + \mathcal{O}(h^{4n+2})$$

whence the following statements follow at once:

- Method (16) is of order $2n$, since $\Phi^{[2n]}(h) = \exp(hF) + \mathcal{O}(h^{2n+1})$.
- Since $Z = (W(h) + \overline{W}(h))/2$ only contains odd powers of h, then $\mathrm{e}^{\frac{h}{2}F}\mathrm{e}^{Z}\mathrm{e}^{\frac{h}{2}F}$ is a time-symmetric composition and $\phi_h^{[2n]}$ is pseudo-symmetric of order $4n+1$.
- Let us suppose that scheme (16) is applied to a Hamiltonian system and that $S_h^{[2]}$ is symplectic. Since Z is an operator in the free Lie algebra generated by $\{F, Y_3, Y_5, \ldots\}$, clearly the composition $\mathrm{e}^{\frac{h}{2}F}\mathrm{e}^{Z}\mathrm{e}^{\frac{h}{2}F}$ is symplectic. As a matter of fact, this can be extended to any geometric property the differential equation (1) has: volume-preserving, unitary, etc., as long as the basic scheme $S_h^{[2]}$ preserves this property.

□

As an example, let us consider the well known 4th-order palindromic scheme used in the triple jump procedure [20],

$$S_h^{[4]} = S_{\alpha_1 h}^{[2]} \circ S_{\alpha_2 h}^{[2]} \circ S_{\alpha_1 h}^{[2]}, \tag{18}$$

with

$$\alpha_1 = \frac{1}{2 - 2^{1/3} \mathrm{e}^{2ik\pi/3}}, \qquad \alpha_2 = 1 - 2\alpha_1, \qquad k = 1, 2.$$

(Note that with $k = 0$ one gets the usual real solution). Then $\phi_h^{[4]} = \Re(S_h^{[4]})$ is still a method of order 4, but pseudo-symmetric and pseudo-symplectic of order 9.

As is well known, the number of order conditions required by left-right palindromic compositions to achieve order $r = 2n$ is [17]

$$N_P^{[2n]} = \sum_{j=1}^{n} c(2j-1).$$

In consequence, a palindromic composition requires at least $2N_P^{[2n]} - 1$ stages so as to have the same number of (complex) coefficients as order conditions. The values of $N_P^{[2n]}$ to achieve orders $2n = 2, 4, 6, 8$ are collected in the third row of Table 1.

2.3 Symmetric-conjugate compositions

In contrast with left-right palindromic compositions, even and odd order methods of the form (5) exist, but their behavior with respect to structure preservation is different when they are projected on the real axis at each step. The reason lies in the special structure of the associated series of differential operators. More specifically, we have the following

Lemma 1 *Let $S_h^{[2]}$ be a time-symmetric 2nd-order method for (1), with f real, and consider the composition method*

$$\psi_h^{[r]} = S_{\alpha_s h}^{[2]} \circ S_{\alpha_{s-1} h}^{[2]} \circ \cdots \circ S_{\alpha_2 h}^{[2]} \circ S_{\alpha_1 h}^{[2]},$$

verifying

$$\alpha_{s+1-j} = \bar{\alpha}_j, \qquad j = 1, 2, \ldots .$$

Then $\psi_h^{[r]}$ has an associated series of operators $\Psi^{[r]}(h) = \exp(V(h))$, with

$$V(h) = hw_1 F + \sum_{j\geq 1} h^{2j+1} \sum_{k=1}^{c(2j+1)} \mu_{2j+1,k} E_{2j+1,k} + i \sum_{j\geq 2} h^{2j} \sum_{k=1}^{c(2j)} \sigma_{2j,k} E_{2j,k}. \tag{19}$$

Here $w_1, \mu_{2j+1,k}, \sigma_{2j,k}$ are real *polynomials depending on the real and imaginary parts of the parameters α_i. In other words, the terms of even powers in h in $V(h)$ are pure imaginary, whereas terms of odd powers in h are real.*

Proof: We start by noticing that, since $S_h^{[2]}$ is a time-symmetric integrator, the adjoint $(\psi_h^{[r]})^*$ is precisely the *complex conjugate* of $\psi_h^{[r]}$, i.e., $(\psi_h^{[r]})^* = \overline{\psi}_h^{[r]}$. In consequence, the corresponding series of operators are also identical,

$$\overline{\Psi}^{[r]}(h) = (\Psi^{[r]})^*(h)$$

and therefore $\overline{V}(h) = -V(-h)$. From (12), these series are respectively

$$\begin{aligned}
\overline{V}(h) &= h\overline{w}_1 F + \sum_{j\geq 1} h^{2j+1} \sum_{k\geq 1} \overline{w}_{2j+1,k} E_{2j+1,k} + \sum_{j\geq 1} h^{2j} \sum_{k\geq 1} \overline{w}_{2j,k} E_{2j,k} \\
-V(-h) &= hw_1 F + \sum_{j\geq 1} h^{2j+1} \sum_{k\geq 1} w_{2j+1,k} E_{2j+1,k} - \sum_{j\geq 1} h^{2j} \sum_{k\geq 1} w_{2j,k} E_{2j,k},
\end{aligned}$$

so that

$$\overline{w}_1 = w_1, \qquad \overline{w}_{2j+1,k} = w_{2j+1,k}, \qquad \overline{w}_{2j,k} = -w_{2j,k},$$

and (19) is obtained with $\mu_{2j+1,k} = w_{2j+1,k} \in \mathbb{R}$, $\sigma_{2j,k} = \Im(w_{2j,k}) \in \mathbb{R}$. □

From this lemma one has the following general result concerning the preservation of properties of symmetric-conjugate compositions.

Proposition 2 *Given $S_h^{[2]}$ a time-symmetric 2nd-order method, let us consider the symmetric-conjugate composition*

$$\psi_h^{[r]} = S^{[2]}_{\tilde{\alpha}_1 h} \circ S^{[2]}_{\tilde{\alpha}_2 h} \circ \cdots \circ S^{[2]}_{\alpha_2 h} \circ S^{[2]}_{\alpha_1 h}$$

of order $r \geq 3$ and its real part, i.e.,

$$\hat{R}_h^{[2n]} = \frac{1}{2}\left(\psi_h^{[r]} + \overline{\psi}_h^{[r]}\right), \tag{20}$$

applied to the differential equation (1) with a real vector field f. Then the following statements concerning the pseudo-symmetry and pseudo-symplecticity of $\hat{R}_h^{[2n]}$ hold:

(a) If $\psi_h^{[r]}$ is of odd order, $r = 2n-1$, $n = 2, 3, \ldots$, then $\hat{R}_h^{[2n]}$ is a method of order $2n$ and pseudo-symmetric of order $q = 4n-1$. If in addition f is a (real) Hamiltonian vector field and $S_h^{[2]}$ is a symplectic integrator, then $\hat{R}_h^{[2n]}$ is pseudo-symplectic of order $p = 4n-1$.

(b) If $\psi_h^{[r]}$ is of even order, $r = 2n$, $n = 2, 3, \ldots$, then $\hat{R}_h^{[2n]}$ is a method of order $2n$ and pseudo-symmetric of order $q = 4n+3$. If in addition f is a (real) Hamiltonian vector field and $S_h^{[2]}$ is a symplectic integrator, then $\hat{R}_h^{[2n]}$ is pseudo-symplectic of order $p = 4n+3$.

Proof: We apply the same strategy as in the proof of Proposition 1.
(a) Since $r = 2n-1$, then the series of operators associated with $\psi_h^{[r]}$ is $\Psi^{[r]}(h) = \exp(V(h))$, with

$$V(h) = hF + ih^{2n}V_{2n} + h^{2n+1}V_{2n+1} + ih^{2n+2}V_{2n+2} + \cdots \tag{21}$$

where V_{2n+j}, $j = 0, 1, 2, \ldots$ are, according to Lemma 1, *real* operators in the free Lie algebra generated by $\{F, Y_3, Y_5, \ldots\}$. From here the series corresponding to $\hat{R}_h^{[2n]}$,

$$\mathcal{R}^{[2n]}(h) = \frac{1}{2}\left(\exp((V(h)) + \exp(\overline{V}(h))\right),$$

can be written as

$$\mathcal{R}^{[2n]}(h) = \exp\left(\frac{h}{2}F\right)\left(\frac{1}{2}\exp((W(h)) + \frac{1}{2}\exp(\overline{W}(h))\right)\exp\left(\frac{h}{2}F\right),$$

where $W(h)$ is obtained from $\exp(W(h)) = \exp(-hF/2)\,\exp(V(h))\,\exp(-hF/2)$ as

$$W(h) = ih^{2n}W_{2n} + h^{2n+1}W_{2n+1} + ih^{2n+2}W_{2n+2} + h^{2n+3}W_{2n+3} + ih^{2n+4}W_{2n+4} + \mathcal{O}(h^{2n+5})$$

with

$$W_{2n} = V_{2n}, \qquad W_{2n+1} = V_{2n+1}, \qquad W_{2n+2} = V_{2n+2} + \frac{1}{24}[F,[F,V_{2n}]]$$
$$W_{2n+3} = V_{2n+3} + \frac{1}{24}[F,[F,V_{2n+1}]],$$
$$W_{2n+4} = V_{2n+4} + \frac{1}{24}[F,[F,V_{2n+2}]] + \frac{1}{1920}[F,[F,[F,[F,V_{2n}]]]].$$

In general, terms in $W(h)$ of odd powers in h are real and terms of even powers of h are pure imaginary. Then, it is clear that

$$W(h) + \overline{W}(h) = 2h^{2n+1}V_{2n+1} + 2h^{2n+3}\left(V_{2n+3} + \frac{1}{24}[F,[F,V_{2n+1}]]\right) + \mathcal{O}(h^{2n+5})$$

and only contains odd powers of h. Furthermore,

$$\begin{aligned}\left(W(h) + \overline{W}(h)\right)^2 &= 4h^{4n+2}V_{2n+1}^2 + 4h^{4n+4}\Big(V_{2n+1}(V_{2n+3} + \frac{1}{24}[F,[F,V_{2n+1}]]) + \\ &\quad + (V_{2n+3} + \frac{1}{24}[F,[F,V_{2n+1}]])V_{2n+1}\Big) + \mathcal{O}(h^{4n+6})\end{aligned}$$

and

$$W(h)^2 + \overline{W}(h)^2 = -2h^{4n}V_{2n}^2 + \mathcal{O}(h^{4n+2}).$$

Proceeding as before,

$$\frac{1}{2}\left(\mathrm{e}^{W(h)} + \mathrm{e}^{\overline{W}(h)}\right) - \mathrm{e}^{\frac{1}{2}\left(W(h)+\overline{W}(h)\right)} = -\frac{1}{2}h^{4n}V_{2n}^2 + \mathcal{O}(h^{4n+2}),$$

so that

$$\mathcal{R}^{[2n]}(h) = \exp\left(\frac{h}{2}F\right)\exp\left(\frac{1}{2}\left(W(h) + \overline{W}(h)\right)\right)\exp\left(\frac{h}{2}F\right) + \mathcal{O}(h^{4n}),$$

whence the conclusions follow readily.
(b) We proceed along the same lines as in the preceding case for even order, $r = 2n$. Now

$$V(h) = hF + h^{2n+1}V_{2n+1} + ih^{2n+2}V_{2n+2} + h^{2n+3}V_{2n+3} + \cdots$$

and

$$W(h) = h^{2n+1}W_{2n+1}+ih^{2n+2}W_{2n+2}+h^{2n+3}W_{2n+3}+ih^{2n+4}W_{2n+4}+h^{2n+5}W_{2n+5}+\mathcal{O}(h^{2n+6})$$

with

$$W_{2n+1} = V_{2n+1}, \qquad W_{2n+2} = V_{2n+2}, \qquad W_{2n+3} = V_{2n+3} + \frac{1}{24}[F,[F,V_{2n+1}]]$$
$$W_{2n+4} = V_{2n+4} + \frac{1}{24}[F,[F,V_{2n+2}]],$$
$$W_{2n+5} = V_{2n+5} + \frac{1}{24}[F,[F,V_{2n+3}]] + \frac{1}{1920}[F,[F,[F,[F,V_{2n+1}]]]],$$

whence, as before,

$$W(h) + \overline{W}(h) = 2h^{2n+1}W_{2n+1} + 2h^{2n+3}W_{2n+3} + 2h^{2n+5}W_{2n+5} + \mathcal{O}(h^{2n+7}).$$

On the other hand,

$$\begin{aligned} W(h)^2 &= h^{4n+2}W_{2n+1}^2 + ih^{4n+3}\big(W_{2n+1}W_{2n+2} + W_{2n+2}W_{2n+1}\big) \\ &+ h^{4n+4}\big(W_{2n+1}W_{2n+3} + W_{2n+3}W_{2n+1} - W_{2n+2}^2\big) \\ &+ ih^{2n+5}\big(W_{2n+1}W_{2n+4} + W_{2n+4}W_{2n+1} + W_{2n+2}W_{2n+3} + W_{2n+3}W_{2n+2}\big) + \mathcal{O}(h^{4n+6}), \end{aligned}$$

whereas

$$\begin{aligned} \overline{W}(h)^2 &= h^{4n+2}W_{2n+1}^2 - ih^{4n+3}\big(W_{2n+1}W_{2n+2} + W_{2n+2}W_{2n+1}\big) \\ &+ h^{4n+4}\big(W_{2n+1}W_{2n+3} + W_{2n+3}W_{2n+1} - W_{2n+2}^2\big) \\ &- ih^{2n+5}\big(W_{2n+1}W_{2n+4} + W_{2n+4}W_{2n+1} + W_{2n+2}W_{2n+3} + W_{2n+3}W_{2n+2}\big) + \mathcal{O}(h^{4n+6}). \end{aligned}$$

An straightforward calculation shows that

$$\begin{aligned} \frac{1}{2}\left(\mathrm{e}^{W(h)} + \mathrm{e}^{\overline{W}(h)}\right) - \mathrm{e}^{\frac{1}{2}\left(W(h)+\overline{W}(h)\right)} &= \frac{1}{4}\big(W(h)^2 + \overline{W}(h)^2\big) - \frac{1}{8}\big(W(h) + \overline{W}(h)\big)^2 + \cdots \\ &= -\frac{1}{2}h^{4n+4}W_{2n+2}^2 + \mathcal{O}(h^{4n+6}) \end{aligned}$$

and finally

$$\mathcal{R}^{[2n]}(h) = \exp\left(\frac{h}{2}F\right)\exp\left(\frac{1}{2}\big(W(h) + \overline{W}(h)\big)\right)\exp\left(\frac{h}{2}F\right) + \mathcal{O}(h^{4n+4}). \qquad (22)$$

Now $\hat{R}_h^{[2n]}$ is of orden $2n$, but the time-symmetry (and symplecticity) holds up to order $4n+3$. □

Although apparently a symmetric-conjugate composition requires solving $N^{[r]}$ equations to achieve order r, just as general compositions, this is not the case, however, when one is interested in projecting on the real axis, since the symmetry in the coefficients introduces additional reductions. As Lemma 1 and Proposition 2 show, for a scheme of order $r = 2n$, the $c(2n)$ order conditions at order h^{2n} are pure imaginary and so it is not necessary to solve them. Therefore, the number of conditions is actually $N^{[2n]} - c(2n)$. This number is collected in the last row of Table 1. This saving in the cost comes of

course at the price of reducing the preservation of time-symmetry (or symplecticity, etc.) from order $4n+3$ to $4n-1$.

We can proceed in the same vein, since the $c(2n-2)$ order conditions at order h^{2n-2} are also pure imaginary. Now, however, the resulting schemes after projection are only pseudo-symmetric of pseudo-symmetry order $4n-5$. If $4n-5 > 2n$, or equivalently if $2n > 5$, then we still have a method of order $r = 2n$ obtained from a symmetric-conjugate composition with $N^{[2n]} - c(2n) - c(2n-2)$ stages if the corresponding order conditions have solutions.

This can be generalized as follows:

Proposition 3 *Let*

$$\psi_h^{[r]} = S^{[2]}_{\tilde{\alpha}_1 h} \circ S^{[2]}_{\tilde{\alpha}_2 h} \circ \cdots \circ S^{[2]}_{\alpha_2 h} \circ S^{[2]}_{\alpha_1 h}$$

be a symmetric-conjugate composition of order $r = 2n$ after projection on the real axis. If $4n-(4q+1) > 2n$ for some $q \geq 0$ (or equivalently if $2n > 4q+1$), then the number of order conditions to be satisfied by $\psi_h^{[r]}$ to get a pseudo-symmetric scheme of pseudo-symmetry order $4n-(4q+1)$ after projection on the real axis is

$$N^{[2n]} - \sum_{j=0}^{q} c(2n-2j).$$

The simplest example corresponds to scheme (6): Part *(a)* of Proposition 2 with $r = 3$ reproduces the result obtained in [10] and summarized in section 1: its real part renders a method of order 4 and pseudo-symmetric of order 7.

If we consider instead a composition (5) of order $r = 4$, then by taking the real part at each step we do not increase the order, but the pseudo-symmetry order is $q = 11$ (instead of 7). In view of Table 1, it is worth remarking that, although the symmetric-conjugate compositions require more order conditions to be satisfied than palindromic compositions for orders higher than four, the methods resulting from projecting on the real axis require less stages: thus, in particular, it is possible to achieve a 6th-order scheme with only 5 stages, whereas schemes based on palindromic composition require at least 7 stages.

As an additional illustration, let us take the composition

$$\psi_h^{[4]} = S^{[2]}_{\tilde{\alpha}_1 h} \circ S^{[2]}_{\alpha_2 h} \circ S^{[2]}_{\alpha_1 h}, \tag{23}$$

with $s = 3$. It is of order $r = 2n = 4$ if

$$\alpha_1 = \frac{1}{4} \pm i \frac{1}{4}\sqrt{\frac{5}{3}}, \qquad \alpha_2 = \frac{1}{2}.$$

Taking its real part, $\Re(\psi_h^{[4]})$, results in a method also of order 4, but pseudo-symmetric and pseudo-symplectic of order 11. Both schemes $\Re(\psi_h^{[3]})$, (eq. (7)), and $\Re(\psi_h^{[4]})$ are of order 4, but whereas the former requires two evaluations of $S_h^{[2]}$ (instead of three), the latter preserves qualitative properties up to a higher order.

2.4 Example: harmonic oscillator

At this point it may be illustrative to apply all the previous 4th-order methods obtained by projecting on the real axis to a simple example and check how different behaviors with respect to structure preservation manifest in practice. To this end we choose the one-dimensional harmonic oscillator,

$$q' = p, \qquad p' = -q$$

with Hamiltonian

$$H(q,p) = T(p) + V(q) = \frac{1}{2}p^2 + \frac{1}{2}q^2. \tag{24}$$

Denoting by $M_X(h)$ the exact matrix evolution associated with the Hamiltonians $X = H, T$ and V, i.e., $x(h) = (q(h), p(h))^T = M_X(h)(q(0), p(0))^T$, then

$$M_H(h) = \begin{pmatrix} \cos(h) & \sin(h) \\ -\sin(h) & \cos(h) \end{pmatrix}, \quad M_T(h) = \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix}, \quad M_V(h) = \begin{pmatrix} 1 & 0 \\ -h & 1 \end{pmatrix}.$$

As our basic time-symmetric 2nd-order scheme $S_h^{[2]}$ we take the leapfrog/Strang integrator

$$S_h^{[2]} = M_T(h/2)M_V(h)M_T(h/2) \tag{25}$$

and form the 4th-order schemes $\mathfrak{R}(\psi_h^{[3]})$ (eq. (7)), $\mathfrak{R}(\psi_h^{[4]})$ (eq. (23)), and $\mathfrak{R}(S_h^{[4]})$ (eq. (18)). In this case, it is straightforward to verify the order of the methods (by computing explicitly the difference $\psi_h - M_H(h)$ for each method ψ_h), the pseudo-symmetry order (by evaluating $\psi_h \circ \psi_{-h} - I$) and the pseudo-symplecticity order (for instance, by computing the determinant of the corresponding approximation matrix). In all cases the result agrees with Propositions 1 and 2.

We can also check the relative efficiency of the three schemes by computing the error in the energy along a time interval with different time steps. Thus, Figure 1 (top panel) shows this relative error in H as a function of the number of evaluations of the basic second order method $S_h^{[2]}$ when $q_0 = 2.5, p_0 = 0$ and the final time is $t_f = 650$. We see that the efficiency of schemes $\mathfrak{R}(S_h^{[4]})$ and $\mathfrak{R}(\psi_h^{[3]})$ is quite similar for relatively small values of h.

It is also illustrative to test the behavior of these schemes for very long time intervals. This is done in Figure 1 (bottom) for $t \in [0, 10^7]$ and constant step size $h = 1/4$ for $\mathfrak{R}(\psi_h^{[4]})$ and $\mathfrak{R}(S_h^{[4]})$, and $h = 1/6$ for $\mathfrak{R}(\psi_h^{[3]})$, so that all schemes require the same computational effort. We see that even for large values of time $\mathfrak{R}(\psi_h^{[4]})$ does not exhibit a secular component in the error in energy (one might need still larger final times), as is the case for compositions (2) involving real coefficients (see [2], where this phenomenon is explained). In any case the results are consistent with Proposition 2 and in particular with expression (22).

3 Symmetric-conjugate composition methods obtained from a 2nd-order symmetric basic scheme

In this section we propose new methods constructed from a basic time-symmetric 2nd-order basic scheme by symmetric-conjugate composition. Since the case of order 4 has

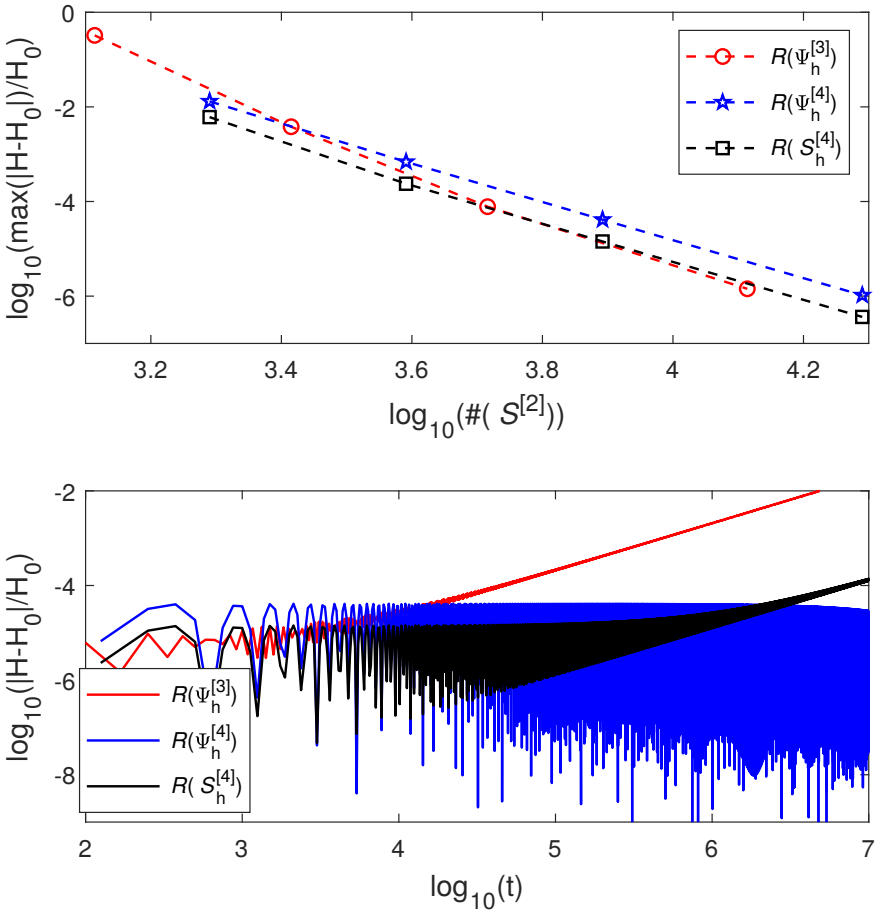

Figure 1: Top: Relative error in energy vs. the number of evaluations of the basic $S_h^{[2]}$ scheme for the harmonic oscillator for $t \in [0, 650]$. Bottom: Evolution of this error along the integration; here the same step size $h = 1/4$ is used by $\Re(\psi_h^{[4]})$ and $\Re(S_h^{[4]})$, and $h = 1/6$ by $\Re(\psi_h^{[3]})$.

been already analyzed in section 2, here we study compositions with $s \geq 4$ stages. From Proposition 2 it is clearly advantageous to consider conjugate-symmetric compositions of odd order $r = 2n - 1$, since taking the real part leads automatically to a method of order $r = 2n$ (but requiring only the computational cost of a method of order $2n - 1$).

For simplicity, we denote in the sequel the general composition (2) by its sequence of coefficients:

$$(\alpha_s, \alpha_{s-1}, \ldots, \alpha_2, \alpha_1).$$

As a general rule for selecting a particular method, we follow the same criterion as in [6], namely we first choose a subset of solutions with small 1-norm of the coefficient vector $(\alpha_s, \ldots, \alpha_1)$ and, among them, choose the one that minimizes the norm of the

main term in the corresponding truncation error.

Order 6. According to the previous treatment, one could consider in principle a symmetric-conjugate composition verifying the order conditions

$$w_1 = 1, \qquad w_{3,1} = 0, \qquad w_{5,1} = w_{5,2} = 0$$

in (11), since $w_{4,1}$ is pure imaginary, so that when taking the real part of the composition, it does not contribute to the error. Four stages would then be necessary to construct a 6th-order method. It turns out, however, that these equations do not admit solutions with the required symmetry $\alpha_4 = \bar{\alpha}_1$, $\alpha_3 = \bar{\alpha}_2$, and thus at least $s = 5$ stages are necessary. The additional parameter can be used to solve the condition $w_{4,1} = 0$ so as to achieve order 5. These equations admit 5 solutions (plus the corresponding complex conjugate) for the sequence (5), i.e., for

$$\psi_h^{[5]} = S^{[2]}_{\tilde{\alpha}_1 h} \circ S^{[2]}_{\tilde{\alpha}_2 h} \circ S^{[2]}_{\alpha_3 h} \circ S^{[2]}_{\alpha_2 h} \circ S^{[2]}_{\alpha_1 h}. \tag{26}$$

Among them, we select

$$\begin{aligned}
\alpha_1 &= 0.17526840907207411405835 63 + 0.05761474413053870201304364\, i \\
\alpha_2 &= 0.18487368019298416042888 98 - 0.19412192275724958850677 58\, i \\
\alpha_3 &= 0.27971582146988345102550 77
\end{aligned}$$

so that the real part

$$\hat{R}_h^{[6]} = \frac{1}{2}\left(\psi_h^{[5]} + \overline{\psi}_h^{[5]}\right)$$

leads to a method of order 6 which, according with Part *(a)* of Proposition 2, is pseudo-symmetric and pseudo-symplectic of order 11, although it only has 5 stages (one of them being real). Notice that, according to Table 1, $s = 7$ stages are required to construct a conjugate-symmetric composition of order 6. Such a method was indeed proposed and tested on several numerical examples in [8], exhibiting a good long time behavior. This behavior can be explained by Proposition 2, since the corresponding method $\hat{R}_h^{[6]}$ constructed by taking its real part is pseudo-symmetric and pseudo-symplectic of order 15.

The same number of stages ($s = 7$) is also required by a palindromic composition to solve the 4 order conditions necessary to achieve order 6. As shown in [6], the best solution within this class is the composition $S_7 6$ previously found in [12]. By taking the real part, the corresponding scheme $\phi_h^{[6]}$ is pseudo-symmetric of order 13 and involves 2 more stages than $\hat{R}_h^{[6]}$.

Order 8. In view of the structure of the series of operators $\exp(V(h))$ associated with a symmetric-conjugate composition, eq. (19), it is clear that if the order conditions

$$\begin{aligned}
&w_1 = 1, \qquad w_{3,1} = 0, \qquad w_{4,1} = 0, \qquad w_{5,1} = w_{5,2} = 0, \\
&w_{7,1} = w_{7,2} = w_{7,3} = w_{7,4} = 0
\end{aligned} \tag{27}$$

are satisfied by $\psi_h^{[r]}$, then we get a 5th-order composition whose projection on the real axis is an 8th-order approximation. Here the condition $w_{4,1} = 0$ has to be included,

since otherwise there appears a contribution in h^8. In consequence, at least $s = 9$ stages are necessary to solve equations (27). We have in fact found 7 solutions (+ c.c.) with the required symmetry and positive real part. Among them, we propose, according with the previous criteria,

$$\begin{aligned}
\alpha_1 &= \bar{\alpha}_9 = 0.088484578241299884956668 30 - 0.074271853091521247182760 00\, i \\
\alpha_2 &= \bar{\alpha}_8 = 0.159568705018801741982910 33 + 0.023225652810097209134544 62\, i \\
\alpha_3 &= \bar{\alpha}_7 = 0.093594614608494519042511 62 + 0.137963569244965498196190 86\, i \\
\alpha_4 &= \bar{\alpha}_6 = 0.157692249551218577741443 15 - 0.071669601078922955499409 96\, i \\
\alpha_5 &= 0.001319705160370552552933 18
\end{aligned} \tag{28}$$

We thus have an 8th-order scheme obtained from a symmetric-conjugate composition of a basic 2nd-order time symmetric scheme requiring only 9 stages. This is the reason for the last entry in Table 1. Since the composition is of order 5, the final scheme will be pseudo-symmetric of order 11. In case one is interested in preserving properties up to a higher order, then two more stages are necessary to solve the order conditions at order 6. In that case, we have a symmetric-conjugate composition of order 7 involving $s = 11$ stages which is pseudo-symmetric of order 15.

By contrast, $s = 15$ stages are required to solve the 8 order conditions of an 8-th order left-right palindromic composition. In [6], an optimized method of this class is proposed. Notice that, when one takes its real part, the final method is pseudo-symmetric of order 17. In any case, this different behavior with respect to time-symmetry will be hardly visible in most practical situations.

We have carried out a numerical search of solutions such an 11-stage symmetric-conjugate composition, finding 29 sets of coefficients with positive real part. Among them, we recommend the following:

$$\begin{aligned}
\alpha_1 &= \bar{\alpha}_{11} = 0.076832925977387362055 03 - 0.059658050846138607577 35\, i \\
\alpha_2 &= \bar{\alpha}_{10} = 0.128444820703686506129 73 + 0.024798126975725316686 68\, i \\
\alpha_3 &= \bar{\alpha}_9 = 0.068557239041684503891 58 + 0.112761293253394826179 90\, i \\
\alpha_4 &= \bar{\alpha}_8 = 0.118794148101288912570 46 - 0.040557657315345720310 90\, i \\
\alpha_5 &= \bar{\alpha}_7 = 0.102794690761693068325 15 + 0.067359173413537379636 38\, i \\
\alpha_6 &= 0.009152350828519294056 116
\end{aligned} \tag{29}$$

A method of order 10 within this family would require at least 17 stages, since one has to construct a symmetric-conjugate composition of order 5 (5 order conditions) also verifying the 4 conditions at order 7 and the 8 conditions corresponding to order 9. This method would be pseudo-symmetric of order 11. The pseudo-symmetry can be raised up to order 15 by adding the 2 conditions at order 6 for a total of 19 stages. By contrast, a palindromic composition requires a minimum of 31 stages.

4 Numerical examples

4.1 Kepler problem

As a first example we take the two-dimensional Kepler problem with Hamiltonian

$$H(q,p) = T(p) + V(q) = \frac{1}{2}p^T p - \mu\frac{1}{r}.$$

Here $q = (q_1, q_2)$, $p = (p_1, p_2)$, $\mu = GM$, G is the gravitational constant and M is the sum of the masses of the two bodies. We take $\mu = 1$ and initial conditions

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}},$$

so that the trajectory corresponds to an ellipse of eccentricity $e = 0.6$, and integrate with the 6th- and 8th-order methods resulting from symmetric-conjugate and palindromic compositions after projecting on the real axis at each step. We denote them by $\mathcal{S}_p^{r(*)}$ and $\mathcal{S}_p^r$, respectively, where r is the order of the method and p is the number of stages (basic 2n-order integrators) involved in the composition. Thus,

- $\mathcal{S}_5^{6(*)}$ refers to scheme (26);
- $\mathcal{S}_7^{6(*)}$ is method S_7^{*6} of [8];
- $\mathcal{S}_7^6$ corresponds to composition $\mathrm{S}_7 6$ found in [12];
- $\mathcal{S}_9^{8(*)}$ refers to method (28);
- $\mathcal{S}_{11}^{8(*)}$ denotes method (29);
- $\mathcal{S}_{15}^8$ corresponds to composition $\mathrm{S}_{15}8$ obtained in [6].

In our fist experiment we fix the final time $t_f = 650$ and compute the maximum of the relative error in the energy along the trajectory for different step sizes. Thus, we end up with Figure 2 (top), which shows this relative error in energy vs. the number of basic 2nd-order methods necessary for each scheme.

Notice that the new 8th-order schemes obtained from symmetric-conjugate compositions are almost one order of magnitude more efficient than $\mathcal{S}_{15}8$ coming from a palindromic composition, due to the reduced number of basic 2nd-order integrators they require. In addition, it is also worth remarking that these 8th-order methods work better than 6th-order methods even for large time steps, in contrast with what usually happens with compositions with real coefficients.

In Figure 2 (bottom) we illustrate the long-time behavior of the previous 6th-order schemes. To this end, for the same initial conditions, we integrate until the final time $t_f = 10^6$ with a constant step size in such a way that all methods involve the same number of evaluations of the basic integrator. Specifically, $h = 2/5$ for both $\mathcal{S}_7^{6(*)}$ and $\mathcal{S}_7^6$, whereas $h = 2/7$ for $\mathcal{S}_5^{6(*)}$. We see that the latter behaves as a symplectic integrator for the whole integration interval.

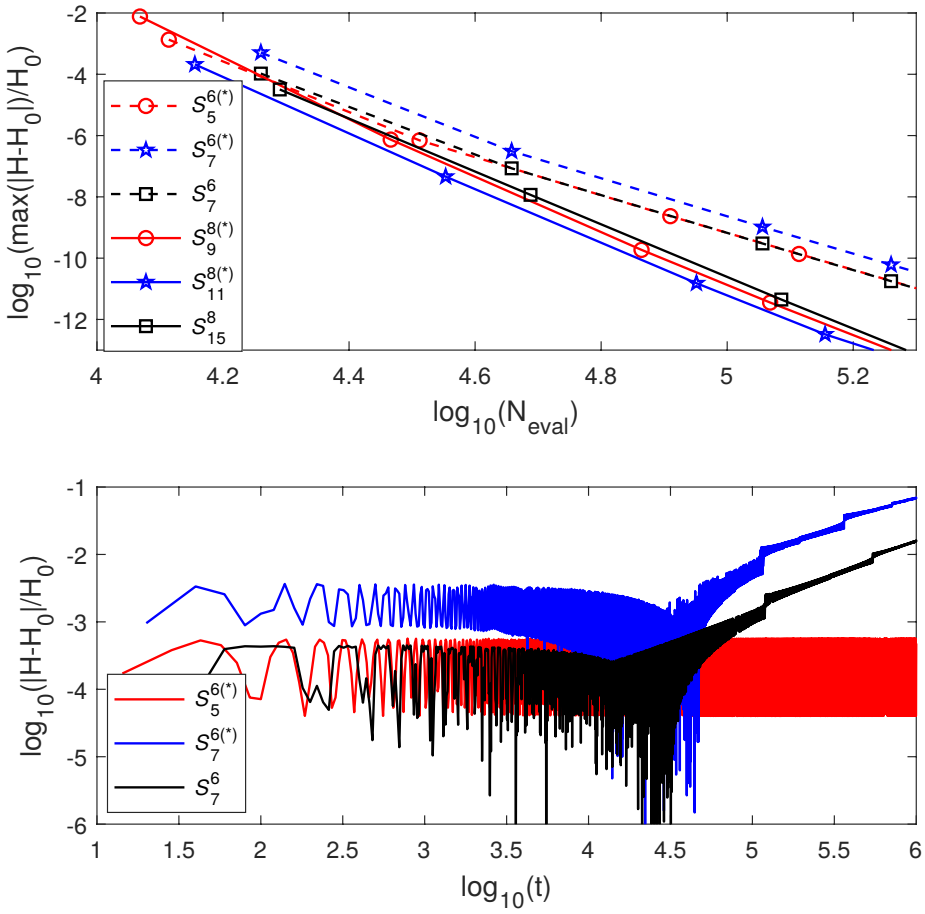

Figure 2: Top: Relative error in energy vs. the number of evaluations of the basic $S_h^{[2]}$ scheme for the Kepler problem. Bottom: Evolution of this error along the integration of 6th-order methods.

4.2 The pendulum

We consider next the one-dimensional pendulum with Hamiltonian

$$H(q,p) = T(p) + V(q) = \frac{1}{2}p^2 + (1 - \cos(q)).$$

We take as initial conditions $q_0 = 0, p_0 = \alpha$, such that for small values of α this is close to a harmonic oscillator, whereas for $\alpha > 2$ the pendulum gives full turns. We take $\alpha = \frac{1}{2}$ (small oscillations) and $\alpha = 5$ (full turns), integrate until $t_f = 200\pi$ and measure the average error in energy as well as the average two-norm error in q, p at times $t = k \cdot 2\pi,\ k = 1, 2, \ldots, 100$ versus the number of stages. The results are shown in Figure 3. We also observe the superiority of the higher order methods for nearly all

accuracies and, among the eighth-order schemes, $\mathcal{S}_{11}^{8(*)}$ shows the best performance in all cases we have considered.

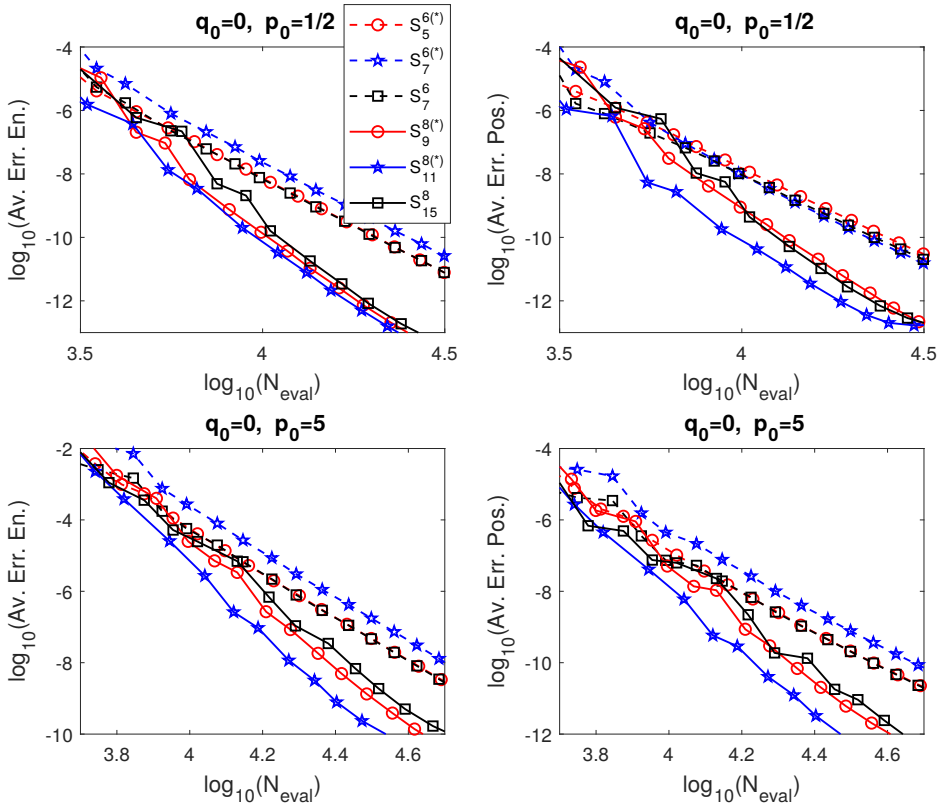

Figure 3: Average relative error in energy (left figures) and average error in positions (right) vs. the number of evaluations of the basic $\mathcal{S}_h^{[2]}$ scheme for the pendulum.

5 Stability

Efficiency diagrams of Figures 2 and 3 show a distinctive pattern: methods of order 8 are more efficient than schemes of order 6 not only for small values of h, but in fact for the whole region of h where errors are of practical interest. This comes in contrast with what happens for methods with real coefficients: in that case the error (in a log-log plot) of a given integrator typically exhibits a corner where higher error terms contribute by the same amount as the main error term. In this way, the errors of the different schemes form an envelope and one is interested in selecting those particular methods lying close to this envelope.

In reference [16] McLachlan presents a simple model to determine in first approximation this corner by defining the *elbow* of a given method as a crude estimate for the envelope and for the nonlinear stability of the method. The idea is as follows: if one

assumes that all vector fields Y_j in (9) have the same order of magnitude, and considers only a single error term e_j at each order for a given palindromic composition (16) of order r, then this effective error scales as

$$\mathcal{E} := h^r e_{r+1} + h^{r+2} e_{r+3} + \cdots .$$

Here e_j includes a factor s^r multiplying the error coefficient of the s-stage composition, so that it can be compared to the reference value 1 for the basic method $\mathcal{S}_h^{[2]}$. Then the elbow is defined as

$$h^* := \sqrt{\frac{e_{r+1}}{e_{r+3}}}$$

thus indicating the value of h below which the asymptotic error $\mathcal{O}(h^r)$ is observed, so that no method should be used with time steps larger than h^*. What is remarkable about this model is that both $\mathcal{E}$ and h^* provide a good qualitative picture of palindromic compositions of different orders [16].

We have carried out a similar treatment for the compositions (both palindromic and symmetric-conjugate) with complex coefficients of this work and the corresponding results are collected in Table 2. Symmetric-conjugate compositions are denoted by SC, whereas PR and PC stand for palindromic compositions with real and complex coefficients, respectively. We also collect in the last column the effective stability limit, i.e the supremum of the step sizes h for which the approximate solution matrix for the harmonic oscillator furnished by each scheme may be bounded independently of the iteration n so that the error does not grow exponentially as n increases. The reference values of h^* and h_t/s for the basic integrator $\mathcal{S}_h^{[2]}$ are respectively 1 and 2.

We also depict in Figure 4 the effective error $\mathcal{E}$ vs. $1/h$ for the basic scheme $\mathcal{S}_h^{[2]}$ and several compositions with complex coefficients of order 4 (dash-dotted lines), 6 (dashed) and 8 (solid lines) whose errors terms are collected in Table 2. For comparison we also include the curve corresponding to the triple-jump of order 4 with real coefficients (dotted line).

In view of Table 2 and Figure 4 some comments are in order. First, the size of the scaled error terms are much smaller for compositions with complex coefficients than for schemes with real coefficients. Second, these error terms grow only moderately with the order for a given method, in contrast with compositions involving real coefficients. In some cases (e.g., for symmetric-conjugate compositions of order 8) they even decrease in size. Third, as a result, the elbow h^* is typically much larger for schemes with complex coefficients, attaining values for which the error is quite considerable. As a consequence, the asymptotic behavior of the error for this class of methods is already visible for all practical values of the step size in a given integration. This can be clearly seen in Figure 4, which qualitatively reproduces quite well the behavior observed for the Kepler and pendulum problems (Figures 2, 3): we notice that the curves corresponding to the 8th-order symmetric-conjugate compositions are placed below the one given by the basic scheme $\mathcal{S}_h^{[2]}$ for all relevant errors.

6 Concluding remarks

Although compositions of basic second-order time-symmetric integrators $\mathcal{S}_h^{[2]}$ involving complex coefficients have been proposed in the past for overcoming the difficulties

Order 4					
Method	s	e_5	e_7	h^*	h_t/s
SC	2	1.7778	2.3704	0.8660	1.7320
SC	3	2.2500	8.4375	0.5164	0.8622
PR	3	428.60	18222	0.1534	0.5245
PC	3	1.9562	3.0189	0.8050	1.3771

Order 6					
Method	s	e_7	e_9	h^*	h_t/s
SC	5	4.4951	44.651	0.3173	0.6172
SC	7	4.5667	147.577	0.1759	0.4457
PR	7	104518	9.7×10^6	0.1038	0.3242
PC	7	4.3876	92.115	0.2182	0.4482

Order 8					
Method	s	e_9	e_{11}	h^*	h_t/s
SC	9	14.060	5.996	1.5312	0.8638
SC	11	7.4082	2.4572	1.7363	0.9353
PC	15	2.0506	10.429	0.4434	0.7896

Table 2: Scaled error coefficients for different compositions of order 4, 6 and 8 with complex and real coefficients. s is the number of stages, h^* is the elbow of the method and h_t/s corresponds to the effective linear stability limit. SC refers to symmetric-conjugate compositions, whereas PR and PC stand for palindromic compositions with real and complex coefficients, respectively.

associated with the presence of negative real coefficients when the order $r \geq 3$, this is, we believe, the first systematic analysis of such composition methods.

When the vector field defining the differential equation is real, the goal is of course to get accurate *real* approximations to the exact solution, whereas the direct application of a composition method with complex coefficients leads in general to a *complex* approximation at each step. Two approaches present themselves in a natural way: either one projects the solution on the real axis at the end of each integration step or the numerical solution is only projected at the end of the integration interval (or more generally only when output is required). In either case, however, the favorable preservation properties the composition inherits from the basic scheme (such as time-symmetry, symplecticity, volume preservation, etc.) are generally lost and the question is characterizing this loss in a precise way.

We have seen that, in general, projecting at each time step preserves these qualitative properties up to an order much higher than the order of accuracy of the composition itself, and provides a good description of the system. In addition to the usual palindromic sequence of coefficients in a composition, we have also explored symmetric-conjugate sequences, showing that it is indeed possible to construct numerical integrators of high order requiring a smaller number of basic schemes. Thus, in particular, we have present a 6th-order method requiring 5 $\mathcal{S}_h^{[2]}$ evaluations, and an 8th-order scheme involving only 9 $\mathcal{S}_h^{[2]}$ evaluations. These numbers have to be compared with 7 and 15, respectively, for palindromic compositions. The numerical tests carried out clearly

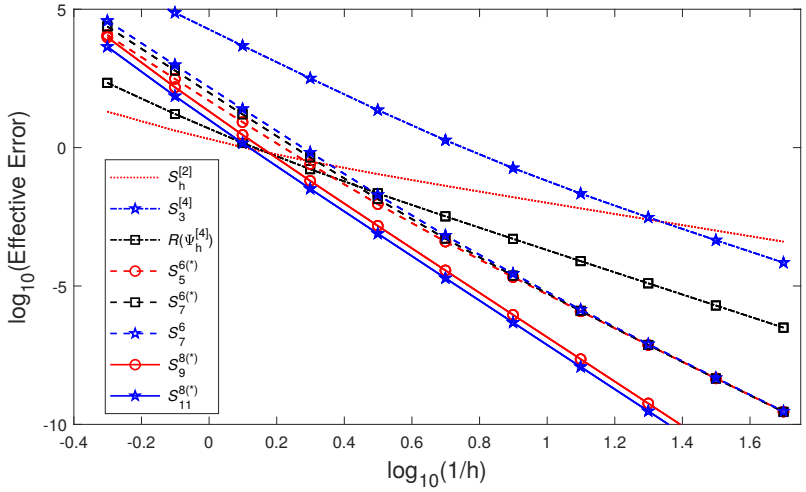

Figure 4: Nominal effective error $\mathcal{E}$ vs. $1/h$ for different compositions with complex coefficients of order 4, 6 and 8. Triple-jump of order 4 with real coefficients (dash-dotted line with stars) is included for comparison. The order of the methods is clearly visible.

illustrate how this reduction in the computational complexity translates into a better performance whereas still sharing with the exact solution its main qualitative properties up to a higher order. Moreover, the efficiency diagrams show that higher order methods involving complex coefficients are more efficient than lower order schemes, not only for small values of the step size h as occurs typically with real coefficients, but in the whole region of h where errors are reasonably small. This remarkable property has been traced back to the structure and size of the successive terms in the asymptotic expansion of the error of these compositions.

Since high order methods obtained from compositions with complex coefficients provide good accuracy and behave in practice as geometric numerical integrators, one might consider comparing them with composition methods with real coefficients on practical applications. Take, for instance, the 8th-order method $S_9^{8(*)}$, involving 9 basic schemes $S_h^{[2]}$. The minimum number for a composition method of the same order with real coefficients is 15, and more are required to have efficient schemes. It might be the case that for certain problems this reduction in the number of evaluations compensates the extra cost due to using complex arithmetic, although this of course is highly dependent of the particular structure of the processor and the implementation. In any case, this will be the subject of future research.

When dealing with this class of schemes, one might contemplate the possibility of projecting at the end of the whole integration interval or alternatively after N time steps, with $t = Nh$, instead of projecting after each step. In that case, however, the approximate numerical solution explores along the evolution regions in the complex plane not necessarily in the proximity of the real axis, so that a rigorous analysis is more involved. Preliminary results show that even in such a situation one might still

have preservation of structures depending on the particular system, the step size and the initial conditions one is considering. This issue deserves further analysis and will be explored in a forthcoming paper.

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Capítulo 8

Applying splitting methods with complex coefficients to the numerical integration of unitary problems

Applying splitting methods with complex coefficients to the numerical integration of unitary problems

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Abstract

We explore the applicability of splitting methods involving complex coefficients to solve numerically the time-dependent Schrödinger equation. We prove that a particular class of integrators are conjugate to unitary methods for sufficiently small step sizes when applied to problems defined in the group $\mathrm{SU}(2)$. In the general case, the error in both the energy and the norm of the numerical approximation provided by these methods does not possess a secular component over long time intervals, when combined with pseudo-spectral discretization techniques in space.

1 Introduction

Splitting methods constitute a natural choice for the numerical time integration of differential equations of the form

$$\frac{du}{dt} = A(u) + B(u), \qquad u(0) = u_0, \tag{1.1}$$

when each subproblem

$$\frac{du}{dt} = A(u), \qquad \frac{du}{dt} = B(u)$$

with $u(0) = u_0$ can be solved explicitly [3, 15, 19]. Then, by composing the solution of each part with appropriately chosen coefficients, it is possible to construct an integrator of a given order $r \geq 1$ for (1.1). In the particular case of a linear problem,

$$\frac{du}{dt} = Au + Bu, \tag{1.2}$$

a splitting method is a composition of the form

$$\Psi^{[r]}(h) = \mathrm{e}^{b_{s+1}hB}\mathrm{e}^{a_s hA}\mathrm{e}^{b_s hB}\cdots\mathrm{e}^{a_1 hA}\,\mathrm{e}^{b_1 hB}, \tag{1.3}$$

where $h := \Delta t$ is the time step and the coefficients a_j , b_j are chosen as solutions of the order conditions, a set of polynomial equations that must be satisfied to achieve an order of accuracy r , i.e., so that $\exp(h(A+B))u_0 - \Psi^{[r]}(h)u_0 = \mathcal{O}(h^{r+1})$.

The simplest example within this class is the Lie–Trotter splitting,

$$\mathrm{e}^{hA}\,\mathrm{e}^{hB} \qquad \text{or} \qquad \mathrm{e}^{hB}\,\mathrm{e}^{hA}, \tag{1.4}$$

providing a first order approximation ($r = 1$), whereas the palindromic versions

$$\mathcal{S}(h) = \mathrm{e}^{h/2A}\,\mathrm{e}^{hB}\,\mathrm{e}^{h/2A} \qquad \text{or} \qquad \mathcal{S}(h) = \mathrm{e}^{h/2B}\,\mathrm{e}^{hA}\,\mathrm{e}^{h/2B}, \tag{1.5}$$

known as Strang splittings, are methods of order $r = 2$.

Although very efficient high order splitting methods can be found in the literature for the numerical integration of Eq. (1.1), it is important to remark that if the order $r \geq 3$, then necessarily some of the coefficient a_j and b_j have to be negative [2, 21, 22]. This, while does not constitute a particular problem when the differential equation is reversible, makes unfeasible their application in parabolic differential equations of evolutionary type, when the operators A and B are only assumed to generate C^0 semi-groups (and not groups): in that case the flows e^{tA} and/or e^{tB} may not be defined for $t < 0$ [10, 16, 17]. Notice that this is the case, in particular, if A is the Laplacian operator.

Moreover, even in problems where splitting methods of order $r \geq 3$ can be safely applied, the presence of negative coefficients usually leads to large truncation errors, so that more stages than strictly necessary to achieve a given order have to be included in the composition to reduce these errors and improve the overall efficiency [6].

It is with the aim of circumventing these drawbacks that splitting methods with complex coefficients (with positive real part) have entered into the literature, mainly in the context of the integration of parabolic differential equations [10, 17, 5], but also for ordinary differential equations (ODEs) when structure-preserving (symplecticity, energy conservation, reversibility) is at stake [11].

Splitting and composition methods with complex coefficients, although computationally between 2 and 4 times more costly than their real counterparts when applied to ODEs involving real vector fields, possess however some remarkable properties: their truncation errors with the minimum number of stages are typically very small, and their stability threshold is comparatively large. Moreover, when the numerical solution is projected at each time step, they lead to approximations that still preserve important qualitative features (such as symplecticity and time-symmetry) up to an order much higher than the order of the method itself [7, 9, 4].

To better illustrate these points, let us consider a time-symmetric second order method $\mathcal{S}(h)$ (such as one of the compositions (1.5). Then, a fourth-order method can be obtained by composition. More specifically, since the coefficients of such a scheme have to satisfy three order conditions, it makes sense to take three maps,

$$\mathcal{S}(\gamma_3 h)\,\mathcal{S}(\gamma_2 h)\,\mathcal{S}(\gamma_1 h).$$

In that case, the order conditions read [6, 15]

$$\sum_{j=1}^{3} \gamma_j = 1, \qquad \sum_{j=1}^{3} \gamma_j^3 = 0, \qquad \sum_{j=1}^{2} \left(\gamma_j^3 \left(\sum_{k=j+1}^{3} \gamma_k \right) - \gamma_j \left(\sum_{k=j+1}^{3} \gamma_k^3 \right) \right) = 0. \tag{1.6}$$

and admit only one real solution, namely

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{1/3}}, \qquad \gamma_2 = 1 - 2\gamma_1$$

leading to a time-symmetric composition scheme, usually referred to as Yoshida's method, here denoted as $\mathcal{S}^{[4]}(h)$. Notice, however, that there are four more complex solutions. The first pair,

$$\gamma_1 = \gamma_3 \equiv \gamma = \frac{1}{2 - 2^{1/3} \mathrm{e}^{2ik\pi/3}}, \qquad \gamma_2 = 1 - 2\gamma, \qquad k = 1, 2 \tag{1.7}$$

leads again to two time-symmetric methods, denoted as $\Psi^{[4]}_{P,c}(h)$, whereas the second one, denoted as $\Psi^{[4]}_{SC,c}(h)$,

$$\gamma_1 = \bar{\gamma}_3 = \frac{1}{4} \pm i \, \frac{1}{4} \sqrt{\frac{5}{3}}, \qquad \gamma_2 = \frac{1}{2} \tag{1.8}$$

(here the bar indicates the complex conjugate), corresponds to a so–called *symmetric-conjugate* composition method [4]: it is symmetric in the real part of the coefficients and skew-symmetric in the imaginary part. Here and in the sequel, the first sub-index in a method (either P or SC) refers to its type (either palindromic or symmetric-conjugate, respectively), whereas the second sub-index (either r or c) indicates that the a_i coefficients in the splitting are real or complex, respectively.

At order five there are two additional order conditions. One of them, $\omega_{5,1} = \sum_{j=1}^{3} \gamma_j^5$, has been typically used to measure the relative error of methods of the same class. If one defines the error as $\mathcal{E} = |\omega_{5,1}|$, then one has for the previous methods the following values of $\mathcal{E}$:

$$\begin{array}{ll} \mathcal{S}^{[4]}(h) & \mathcal{E} = 5.29\ldots, \\ \Psi^{[4]}_{P,c}(h) & \mathcal{E} = 0.024\ldots, \\ \Psi^{[4]}_{SC,c}(h) & \mathcal{E} = 0.027\ldots \end{array}$$

Notice that the error of methods with complex coefficients is about 200 smaller than in the real case.

In the particular case in which $\mathcal{S}(h)$ is given by (1.5), the previous methods can also be written as

$$\mathrm{e}^{b_4 hB} \, \mathrm{e}^{a_3 hA} \, \mathrm{e}^{b_3 hB} \, \mathrm{e}^{a_2 hA} \, \mathrm{e}^{b_2 hB} \, \mathrm{e}^{a_1 hA} \, \mathrm{e}^{b_1 hB}, \tag{1.9}$$

with

$$b_1 = \frac{1}{2}\gamma_1, \quad a_1 = \gamma_1, \quad b_2 = \frac{1}{2}(\gamma_1 + \gamma_2), \quad a_2 = \gamma_2, \quad b_3 = \frac{1}{2}(\gamma_2 + \gamma_3), \quad a_3 = \gamma_3, \quad b_4 = \frac{1}{2}\gamma_3.$$

As a matter of fact, the simplest symmetric-conjugate composition corresponds to the third order scheme

$$\Psi^{[3]}_{SC,c}(h) = \mathcal{S}^{[2]}_{\alpha_2 h} \circ \mathcal{S}^{[2]}_{\alpha_1 h}, \tag{1.10}$$

with

$$\alpha_1 = \bar{\alpha}_2 \equiv \alpha = \frac{1}{2} + i \frac{\sqrt{3}}{6}.$$

For equation (1.2), method (1.10) can be written as

$$\Psi^{[3]}_{SC,c}(h) = \mathrm{e}^{\bar{b}_1 hB} \, \mathrm{e}^{\bar{a}_1 hA} \, \mathrm{e}^{b_2 hB} \, \mathrm{e}^{a_1 hA} \, \mathrm{e}^{b_1 hB}, \tag{1.11}$$

with $a_1 = \alpha\,,\ b_1 = \alpha/2\,,\ b_2 = 1/2\,.$

Although (1.11) is of order 3, if A and B are real, then it renders a scheme of order 4 when it is projected on the real axis after each time step. In addition, it verifies $\Psi^{[3]}_{SC,c}(-h) \circ \Psi^{[3]}_{SC,c}(h) = I + \mathcal{O}(h^8)\,.$ It is said that the scheme is pseudo-symmetric of order 7, since it preserves the time-symmetry property up to terms of order h^7 [9].

Schemes with complex coefficients have been proposed before for the treatment of quantum problems, mainly in the context of imaginary time propagation, with the purpose of computing ground state energies [1] and in quantum Monte Carlo simulations [23, 14], but also in the decomposition of unitary operators [20]. In the later case it is shown, both for unitary 2×2 matrices and empirically for exponentials of Gaussian random Hermitian matrices, that a splitting method does indeed possess a maximal time step for which the scheme is numerically stable. We generalize the treatment to differential equations defined in $\mathrm{SU}(2)$ for methods possessing a particular symmetry and eventually examine their behavior when they are applied to the time dependent Schrödinger equation.

2 Splitting methods in $\mathrm{SU}(2)$

In the study of the evolution of two-level quantum systems one has to deal with the Schrödinger equation, which in this context reads ($\hbar = 1$)

$$i\frac{dU}{dt} = H\,U, \qquad U(0) = I, \tag{2.1}$$

where $U(t)$ is a 2×2 unitary matrix with unit determinant and the skew-Hermitian Hamiltonian H can be expressed as a linear combination of Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.2}$$

Since our purpose is to analyze splitting methods in this context, we assume that H can be written as

$$H = \mathbf{a} \cdot \sigma + \mathbf{b} \cdot \sigma \tag{2.3}$$

for given vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$ and $\sigma = (\sigma_1, \sigma_2, \sigma_3)$, so that, by comparing with (1.2), one has $A \equiv -i\,\mathbf{a} \cdot \sigma$ and $B \equiv -i\,\mathbf{b} \cdot \sigma$. The exact solution of Eq. (2.1) after one time step h is

$$U_{\mathrm{ex}}(h) = \mathrm{e}^{-ihH} = \mathrm{e}^{-ih(\mathbf{a}\cdot\sigma + \mathbf{b}\cdot\sigma)}.$$

On the other hand, if a splitting method of the form (1.3) of order r with *real* coefficients is applied to solve this very simple problem, it is clear that the corresponding approximation can be written as

$$U_{\mathrm{app}}(h) = \mathrm{e}^{-i\,h\,\mathbf{d}(h)\cdot\sigma}, \qquad \text{where} \qquad \mathbf{d}(h) = \mathbf{a} + \mathbf{b} + \mathcal{O}(h^r) \in \mathbb{R}^3,$$

and thus the method still renders an approximation in $\mathrm{SU}(2)$. The situation is different, however, when the splitting method (1.3) involves *complex* coefficients, since in that case $\mathbf{d}(h) \in \mathbb{C}^3$ and the approximation is no longer unitary. In general, the scheme will be unstable and the errors will grow exponentially along the integration.

Example. At this point it is worth testing the previous third- and fourth-order schemes obtained by composing the Strang splitting and involving complex coefficients, namely $\Psi^{[3]}_{SC,c}(h)$, $\Psi^{[4]}_{SC,c}(h)$, and $\Psi^{[4]}_{P,c}(h)$. To do that, we consider the following simple Hamiltonian in $\mathrm{SU}(2)$: $H = \sigma_1 + \sigma_2$, or alternatively, $\mathbf{a} = (1,0,0)$, $\mathbf{b} = (0,1,0)$ in (3.5).

In our experiment, we take as initial condition $U(t_0 = 0) = I$, integrate Eq. (2.1) with different values of the time step h and compute the error of the approximation (in the 2-norm) at the final time $t_f = 10$ as a function of the computational cost (estimated as the number of exponentials involved in the whole integration). The results obtained with each method are displayed in Figure 1 (left panel). We notice that all schemes involving complex coefficients provide considerably more accurate results than $\mathcal{S}^{[4]}(h)$ (black solid line), the fourth-order methods being also more efficient than $\Psi^{[3]}_{SC,c}(h)$ for high accuracy.

In order to check how each scheme with complex coefficients behaves with respect to unitarity, we take as a final time $t_f = 1000$, and adjust h (and therefore the number of iterations N) so that they require the same computational cost. Specifically, $N = 6000$ ($h = 1/6$) for scheme $\Psi^{[3]}_{SC,c}(h)$ and $N = 4000$ ($h = 1/4$) for all methods of order 4. Finally we compute $|\|U_{\rm app}(nh)\| - 1|$, $n = 1, 2, \ldots, N = (t_f - t_0)/h$, where $U_{\rm app}(nh)$ denotes the approximate solution after n steps. The outcome is depicted in Figure 1 (right panel). Notice how the error in unitarity grows for $\Psi^{[4]}_{P,c}(h)$, whereas it is bounded, even for large intervals, for the symmetric-conjugate methods $\Psi^{[3]}_{SC,c}(h)$ and $\Psi^{[4]}_{SC,c}(h)$. Among them, the later clearly provides more accurate results.

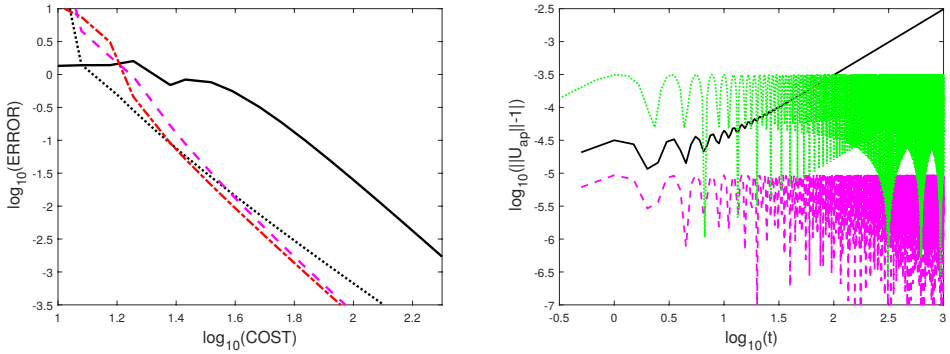

Figure 1: Left: 2-norm error vs. computational cost (number of exponentials) for $\Psi^{[3]}_{SC,c}$ (dotted line), $\mathcal{S}^{[4]}$ (real coefficients, solid line), $\Psi^{[4]}_{P,c}$ (complex coefficients, dash-dotted line) and $\Psi^{[4]}_{SC,c}$ (dashed line). Right: Error in unitarity for $\Psi^{[4]}_{P,c}$ (solid line) and the symmetric-conjugate methods $\Psi^{[3]}_{SC,c}$ (dotted line) and $\Psi^{[4]}_{SC,c}$ (dashed line).

This marked difference of both types of integrators can also be illustrated by computing the eigenvalues λ_1, λ_2 of the approximate solution after one step size, i.e., of the corresponding matrix $U_{\rm app}(h)$. In the exact case, of course, both evolve on the unit circle in the complex plane, whereas here one has still $\lambda_1\lambda_2 = 1$, since the determinant is one. In Figure 2 we depict $|\lambda_j|$, $j = 1, 2$, as a function of h for the palindromic scheme $\Psi^{[4]}_{P,c}$ with $k = 1$ (black, dashed lines) and the symmetric-conjugate splittings $\Psi^{[3]}_{SC,c}$ (blue, dotted line) and $\Psi^{[4]}_{SC,c}$ (red, solid line) in the range $1 \leq h \leq 3$. It is worth remarking that for the

symmetric-conjugate methods both $|\lambda_j|$ are exactly 1 for $0 \leq h \leq h^*$, with $h^* = 1.7570473$ for $\Psi^{[3]}_{SC,c}$ and $h^* = 2.9139468357$ for $\Psi^{[4]}_{SC,c}$. In other words, they behave as unitary maps when $h \leq h^*$. On the other hand, it can be checked that $|\lambda_1| > 1$ for any $h > 0$ for $\Psi^{[4]}_{P,c}$. □

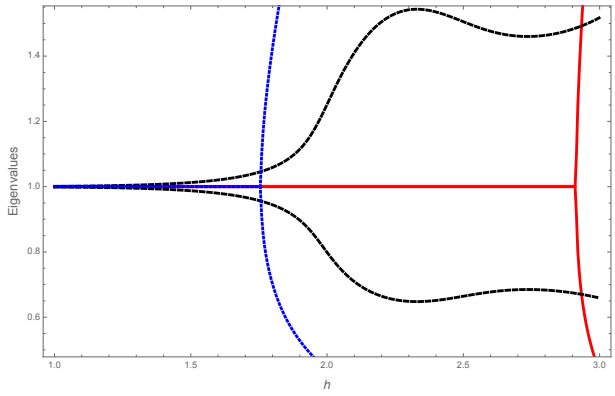

Figure 2: Absolute value of the eigenvalues of the approximate solution matrix obtained with $\Psi^{[4]}_{P,c}$ with complex coefficients ($k = 1$, black dashed line), $\Psi^{[3]}_{SC,c}$ (blue dotted line) and $\Psi^{[4]}_{SC,c}$ (red, solid line).

The previous example illustrates in fact a general pattern exhibited by symmetric-conjugate methods for this problem, as we next prove.

Proposition 2.1 *Suppose a symmetric-conjugate splitting method of the form (1.3), with* $a_{s+1-j} = \bar{a}_j$, $b_{s+2-j} = \bar{b}_j$, *is applied to the numerical integration of the Schrödinger equation (2.1) with the Hamiltonian given by (3.5). In that case, the following statements hold:*

(a) The eigenvalues of the matrix approximating the solution after on time step h *lie on the unit circle in the complex plane for sufficiently small* h.

(b) The symmetric-conjugate splitting method is itself conjugate to a unitary method for sufficiently small h.

Proof. When a splitting method of the form (1.3) is applied to solve Eq. (2.1), the corresponding approximation after one step can be written as $U_{\rm app}(h) = \exp(V(h))$, where $V(h)$ is a linear combination of A, B and all their nested commutators,

$$V(h) = h(w_{1,1}A + w_{1,2}B) + h^2 w_{2,1}[A,B] + h^3(w_{3,1}[A,[A,B]] + w_{3,2}[B,[A,B]]) + \mathcal{O}(h^4), \qquad (2.4)$$

and $w_{n,k}$ are polynomials in the coefficients a_j, b_j. Method (1.3) is of order r if $w_{1,1} = w_{1,2} = 1$ and the polynomials $w_{n,k}$ vanish for $1 < n < r$. In our case, since

$$[-i\,\mathbf{a}\cdot\sigma, -i\,\mathbf{b}\cdot\sigma] = -i\,2\,(\mathbf{a}\times\mathbf{b})\cdot\sigma,$$

it is clear that the vector fields associated with all commutators in (2.4) containing an even number of operators are perpendicular to the plane generated by the vectors $\mathbf{a}$ and $\mathbf{b}$, whereas those containing an odd number of operators A and B are in such a plane. If in addition the method is symmetric-conjugate, then a straightforward computation shows that $V^\dagger(h) = V(-h)$, and so all polynomials $w_{2j+1,k}$ are real whereas all polynomials $w_{2j,k}$ are pure imaginary. Therefore, $V(h)$ can be written as

$$V(h) = -i\,h\tilde{H}(h), \qquad \text{with} \qquad \tilde{H}(h) = \mathbf{d}(h)\cdot\sigma + i\,\mathbf{c}(h)\cdot\sigma, \tag{2.5}$$

for two vectors $\mathbf{c}, \mathbf{d} \in \mathbb{R}^3$ verifying $\mathbf{c}\cdot\mathbf{d} = 0$ and

$$\mathbf{d}(h) = \mathbf{a} + \mathbf{b} + \mathcal{O}(h^{r+1}), \qquad \mathbf{c}(h) = \mathcal{O}(h^r). \tag{2.6}$$

This special structure of $\tilde{H}(h)$ allows one to obtain statements (a) and (b) above. First, if we write

$$\mathrm{e}^{-i\,h\tilde{H}(h)} = \mathrm{e}^{h\,\mathbf{u}\cdot\sigma}, \qquad \text{with} \qquad \mathbf{u} = \mathbf{c} - i\,\mathbf{d},$$

then

$$U_{\mathrm{app}}(h) = \mathrm{e}^{h\,\mathbf{u}\cdot\sigma} = \cosh(hu)I + \frac{\sinh(hu)}{u}\,\mathbf{u}\cdot\sigma,$$

with $u = \sqrt{\mathbf{u}\cdot\mathbf{u}} = (\|\mathbf{c}\|^2 - \|\mathbf{d}\|^2)^{1/2}$. Of course, if $\|\mathbf{c}\| < \|\mathbf{d}\|$, then $\cosh(u) = \cos\alpha$, $\sinh(u) = i\sin\alpha$, with $\alpha = (\|\mathbf{d}\|^2 - \|\mathbf{c}\|^2)^{1/2}$, and the eigenvalues of $U_{\mathrm{app}}(h)$ are $\lambda_{1,2} = \exp(\pm ih\alpha(h))$. But, in virtue of (2.6), this always holds for sufficiently small values of h.
Statement (b) can demonstrated as follows. Let us introduce the unitary vector

$$\mathbf{C} = \frac{\mathbf{d}\times\mathbf{c}}{\|\mathbf{d}\times\mathbf{c}\|}.$$

A trivial computation shows that

$$\mathbf{d}\times\mathbf{C} = -\frac{\|\mathbf{d}\|}{\|\mathbf{c}\|}\,\mathbf{c}, \qquad \mathbf{c}\times\mathbf{C} = \frac{\|\mathbf{c}\|}{\|\mathbf{d}\|}\,\mathbf{d},$$

and furthermore, for a given parameter $s \in \mathbb{R}$,

$$\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}\,\mathrm{e}^{h\mathbf{u}\cdot\sigma}\,\mathrm{e}^{-s\,\mathbf{C}\cdot\sigma} = \exp\left(\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}\,(h\,\mathbf{u}\cdot\sigma)\,\mathrm{e}^{-s\,\mathbf{C}\cdot\sigma}\right).$$

From the definition of $\mathbf{C}$ and the properties of the Pauli matrices [13], one has

$$\begin{aligned}
\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}\,(\mathbf{c}\cdot\sigma)\,\mathrm{e}^{-s\,\mathbf{C}\cdot\sigma} &= \cosh(2s)(\mathbf{c}\cdot\sigma) - i\,\sinh(2s)\frac{\|\mathbf{c}\|}{\|\mathbf{d}\|}\,\mathbf{d}\cdot\sigma \\
\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}\,(\mathbf{d}\cdot\sigma)\,\mathrm{e}^{-s\,\mathbf{C}\cdot\sigma} &= \cosh(2s)(\mathbf{d}\cdot\sigma) + i\,\sinh(2s)\frac{\|\mathbf{d}\|}{\|\mathbf{c}\|}\,\mathbf{c}\cdot\sigma,
\end{aligned}$$

and thus

$$\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}\,(\mathbf{u}\cdot\sigma)\,\mathrm{e}^{-s\,\mathbf{C}\cdot\sigma} = \left(\sinh(2s)\frac{\|\mathbf{d}\|}{\|\mathbf{c}\|} + \cosh(2s)\right)\mathbf{c}\cdot\sigma - i\left(\sinh(2s)\frac{\|\mathbf{c}\|}{\|\mathbf{d}\|} + \cosh(2s)\right)\mathbf{d}\cdot\sigma.$$

If we now take s such that

$$\sinh(2s)\frac{\|\mathbf{d}\|}{\|\mathbf{c}\|} + \cosh(2s) = 0, \qquad \text{i.e.,} \qquad \tanh(2s) = -\frac{\|\mathbf{c}\|}{\|\mathbf{d}\|}, \tag{2.7}$$

then, clearly

$$\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}\,(-ih\tilde{H})\,\mathrm{e}^{-s\,\mathbf{C}\cdot\sigma} = -i\,h\,\mathbf{D}(h)\cdot\sigma,$$

with

$$\mathbf{D}(h) = \sinh(2s)\left(\frac{\|\mathbf{c}\|}{\|\mathbf{d}\|} - \frac{\|\mathbf{d}\|}{\|\mathbf{c}\|}\right)\mathbf{d} \in \mathbb{R}^3.$$

In consequence,

$$\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}\,\mathrm{e}^{-ih\tilde{H}}\,\mathrm{e}^{-s\,\mathbf{C}\cdot\sigma} = \mathrm{e}^{-ih\mathbf{D}(h)\cdot\sigma}. \tag{2.8}$$

In other words, if s is such that Eq. (2.7) holds, then the map obtained by applying a symmetric-conjugate splitting method is conjugate to a unitary matrix. Notice that if $\|\mathbf{c}\| < \|\mathbf{d}\|$ this is always possible, in agreement with statement (a) for the eigenvalues of the approximate solution matrix. ■

Proposition 2.1 thus provides a rigorous justification of the results shown in Figures 1 and 2: since a symmetric-conjugate splitting method is ultimately conjugate to a unitary map in the sense of eq. (2.8) for sufficiently small values of h, then the error in the unitarity of the numerical solution is bounded, whereas the eigenvalues remain on the unit circle in the complex plane.

Methods of the form (2.8) are called *processed* or *corrected* in the literature (see, e.g. [3, 6, 15, 19]). In that context, method $\mathrm{e}^{-ih\tilde{H}}$ is called the kernel, and $\mathrm{e}^{s\,\mathbf{C}\cdot\sigma}$ the processor. For integrators of this class, only the error terms in the kernel that cannot be removed by a processor are relevant in the long run. In the case of unitary problems in $\mathrm{SU}(2)$ we have shown that any symmetric-conjugate splitting method is indeed the kernel of a processed unitary scheme.

3 Application to the time-dependent Schrödinger equation

In view of the previous results in $\mathrm{SU}(2)$, it is natural to examine the situation when splitting methods with complex coefficients, and in particular symmetric-conjugate schemes, are applied in a more general setting. To this end, we next consider the numerical integration of the general time dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{1}{2\mu}\Delta\psi(x,t) + V(x)\psi(x,t), \tag{3.1}$$

where now $\psi : \mathbb{R}^d \times \mathbb{R} \longrightarrow \mathbb{C}$ is the wave function representing the state of the system and the initial state is $\psi(x,0) = \psi_0(x)$. We take again $\hbar = 1$ and a reduced mass μ. Equation (3.1) can be written as

$$i\frac{\partial}{\partial t}\psi = (\hat{T}(P) + \hat{V}(X))\psi, \tag{3.2}$$

with $\hat{T}(P) = P^2/(2\mu)$, and the operators X and P are defined by their actions on $\psi(x,t)$ as

$$X\psi(x,t) = x\,\psi(x,t), \qquad P\,\psi(x,t) = -i\,\nabla\psi(x,t). \tag{3.3}$$

The usual procedure for applying splitting methods in this setting consists first in discretizing the space variables x, so as to get a system of ordinary differential equations (ODEs) which is subsequently integrated in time by the splitting scheme. If, for simplicity, we consider the one-dimensional problem, $d = 1$, and suppose that it is defined in $x \in [x_0, x_N]$, first this interval is partitioned into N parts of length $\Delta x = (x_N - x_0)/N$ and the vector $u = (u_0, \ldots, u_{N-1})^T \in \mathbb{C}^N$ is formed, with $u_n = \psi(x_n, t)$ and $x_n = x_0 + n\Delta x$, $n = 0, 1, \ldots, N-1$. The partial differential equation (3.1) is then replaced by the N-dimensional linear ODE

$$i\frac{d}{dt}u(t) = H\,u(t), \qquad u(0) = u_0 \in \mathbb{C}^N, \tag{3.4}$$

where now H represents the (real symmetric) $N \times N$ matrix associated with the Hamiltonian.

When a Fourier spectral collocation method is used, then the matrix H in (3.4) is

$$H = T + V, \tag{3.5}$$

where V is a diagonal matrix associated with the potential $\hat{V}$ and T is a (full) differentiation matrix related with the kinetic energy $\hat{T}$. Their action on the wave function vector u is trivial: on the one hand, $(Vu)_n = V(x_n)u_n$ and thus the product Vu requires to compute N complex multiplications. On the other hand, $Tu = \mathcal{F}^{-1} D_T \mathcal{F} u$, where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are the forward and backward discrete Fourier transform, and D_T is again diagonal. The transformation $\mathcal{F}$ from the discrete coordinate representation to the discrete momentum representation (and back) is done via the fast Fourier transform (FFT) algorithm, requiring $\mathcal{O}(N \log N)$ operations.

Notice that, since

$$\left(\mathrm{e}^{\tau V} u\right)_i = \mathrm{e}^{\tau V(x_i)} u_i, \qquad \mathrm{e}^{\tau T} u = \mathcal{F}^{-1} \mathrm{e}^{\tau D_T} \mathcal{F}\, u,$$

splitting methods constitute a valid alternative to approximate the solution $u(t) = \mathrm{e}^{\tau(T+V)} u_0$ for a time step Δt, with $\tau = -i\Delta t$. Thus, with the Lie–Trotter scheme (1.4) one has

$$\mathrm{e}^{\tau(T+V)} = \mathrm{e}^{\tau T}\, \mathrm{e}^{\tau V} + \mathcal{O}(\tau^2),$$

whereas the 2nd-order Strang splitting (1.5) constructs the numerical approximation u_{n+1} at time $t_{n+1} = t_n + \Delta t$ by

$$u_{n+1} = \mathrm{e}^{\tau/2V}\, \mathrm{e}^{\tau T}\, \mathrm{e}^{\tau/2V}\, u_n \equiv \mathcal{S}(\tau) u_n.$$

The resulting scheme is called split-step Fourier method in the chemical literature, and has some remarkable properties. In particular, it is both unitary and symplectic [18], as well as time-reversible. In addition, for suitable regularity assumptions on the potential and on the norm of the commutators $[\hat{T}, \hat{V}] = \hat{T}\hat{V} - \hat{V}\hat{T}$ and $[\hat{T}, [\hat{T}, \hat{V}]]$, the error at t_n is bounded by

$$\|u_n - u(t)\| \le C\, \Delta t^2\, t \max_{0 \le s \le t} \|u(s)\|_2.$$

Higher order methods can be obtained of course by considering compositions (1.3), which in this setting read

$$\Psi^{[r]}(\tau) = \mathrm{e}^{b_{s+1}\tau V} \mathrm{e}^{a_s \tau T} \mathrm{e}^{b_s \tau V} \cdots \mathrm{e}^{a_1 \tau T}\, \mathrm{e}^{b_1 \tau V}, \tag{3.6}$$

and in fact, a large collection of practical schemes of different orders exist for carrying out the numerical integration (see e.g. [6, 15, 19] and references therein). In addition, from (3.3), it is clear that $[\hat{X}, \hat{P}]\, \psi(x,t) = i\, \psi(x,t)$, and so

$$[\hat{V}, [\hat{V}, [\hat{V}, \hat{T}]]]\, \psi(x,t) = 0. \tag{3.7}$$

This property leads to a reduction in the number of order conditions necessary to achieve a given order r and allows one to construct highly efficient schemes.

4 Splitting methods with complex coefficients

When exploring the applicability of splitting methods with complex coefficients to the general time-dependent Schrödinger equation, several aspects must be addressed. First, since the computational cost of method (3.6) is dominated by the number of FFTs per step, the presence of complex a_j, b_j does not contribute significantly to increase this cost. In addition, it has been shown in other problems that splitting methods with complex coefficients involving the minimum number of flows to achieve a given order already provide good efficiency, in contrast with their real counterparts. On the other hand, however, since $\sum_j a_j = 1$ for a consistent method, if $a_j \in \mathbb{C}$, then imaginary parts positive *and* negative enter into the game, with the result that severe instabilities may arise in practice due to the unboundedness of the Laplace operator. With respect to the potential, since in regions where it takes large values the wave function typically is close to zero, we can introduce an artificial cut-off bound in the computation if necessary, so that complex b_j can in principle be used, at least for a sufficiently small Δt. It makes sense therefore to construct and examine in detail methods with real a_j and complex b_j coefficients.

In the following, and for simplicity, we restrict ourselves to splitting methods (3.6) of order $r \leq 4$, which we denote by their sequence of coefficients as

$$(b_{s+1}, a_s, b_s, \ldots, a_2, b_2, a_1, b_1).$$

The order conditions are then

$$\begin{aligned}
&\text{Order 1:} && \sum_{i=1}^{s} a_i = 1, && \sum_{i=1}^{s} b_i = 1, \\
&\text{Order 2:} && \sum_{i=1}^{s} b_i \left(\sum_{j=1}^{i} a_j \right) = \frac{1}{2}, \\
&\text{Order 3:} && \sum_{i=1}^{s} b_i \left(\sum_{j=1}^{i} a_j \right)^2 = \frac{1}{3}, && \sum_{i=1}^{s} a_i \left(\sum_{j=i}^{s} b_j \right)^2 = \frac{1}{3}, \\
&\text{Order 4:} && \sum_{i=1}^{s} b_i \left(\sum_{j=1}^{i} a_j \right)^3 = \frac{1}{4}, && \sum_{i=1}^{s} a_i \left(\sum_{j=i}^{s} b_j \right)^3 = \frac{1}{4}, \\
& && \sum_{i=1}^{s} a_i^2 \left(\sum_{j=i}^{s} b_j \right)^2 + 2 \sum_{i=2}^{s} a_i \left(\sum_{j=1}^{i-1} a_j \right) \left(\sum_{k=i}^{s} b_k \right)^2 = \frac{1}{6}.
\end{aligned} \tag{4.1}$$

In typical applications of splitting methods with real coefficients, only palindromic sequences of coefficients, i.e., methods (3.6) with $b_{s+2-j} = b_j$, $a_{s+1-j} = a_j$ for all j are used. In that case, all the conditions at even order are automatically satisfied and the resulting schemes are time-symmetric, $\Psi^{[r]}(\tau)\,\Psi^{[r]}(-\tau) = I$, and of even order. Here, however, since we are dealing with complex coefficients, we also analyze the case $r = 3$ for completeness.

Order 3. The first five order conditions in (4.1) admit solutions with all a_j real and positive and $b_j \in \mathbb{C}$ with positive real part if one considers a composition of the form

$$\Psi^{[3]}_{SC,r}(\tau) = (\bar{b}_1, a_1, \bar{b}_2, a_2, b_2, a_1, b_1) \tag{4.2}$$

involving 6 parameters. Then one gets a 1-parametric family of solutions (+c.c.) with the required properties. Among them, we choose

$$a_1 = \frac{3}{10}, \qquad a_2 = \frac{2}{5}, \qquad b_1 = \frac{13}{126} - i\frac{\sqrt{59/2}}{63}, \qquad b_2 = \frac{25}{63} + i\frac{5\sqrt{59/2}}{126}.$$

Composition (1.11) constitutes of course another symmetric-conjugate method of order 3, denoted here by

$$\Psi^{[3]}_{SC,c}(\tau) = (\bar{b}_1, \bar{a}_1, b_2, a_1, b_1) \tag{4.3}$$

and involving less maps, although in this case $a_1 \in \mathbb{C}$.

Order 4. The simplest approach to construct a palindromic scheme with $a_j \in \mathbb{R}$ and $b_j \in \mathbb{C}$ consists in taking all the a_j equal. In that case, with $s = 4$, one has enough parameters to solve the required four order conditions (at odd orders). Only two solutions (complex conjugate to each other) are obtained, as shown in [10], thus resulting in the scheme

$$\Psi^{[4]}_{P,r}(\tau) = (b_1, a_1, b_2, a_2, b_3, a_2, b_2, a_1, b_1) \tag{4.4}$$

with

$$a_1 = a_2 = \frac{1}{4}, \qquad b_1 = \frac{1}{10} - i\frac{1}{30}, \qquad b_2 = \frac{4}{15} + i\frac{2}{15}, \qquad b_3 = \frac{4}{15} - i\frac{1}{5}.$$

Although more efficient schemes can be obtained if one allows for different a_j 's [5], since we are interested here mainly in the qualitative behavior of the different methods, we limit ourselves to (4.4) as representative of palindromic splitting methods with real a_j 's and complex b_j 's, whereas we can take scheme (1.9)

$$\Psi^{[4]}_{P,c}(\tau) = (b_1, a_1, b_2, a_2, b_2, a_1, b_1), \tag{4.5}$$

as representative of palindromic methods with both $a_j \in \mathbb{C}$ and $b_j \in \mathbb{C}$.

Symmetric-conjugate splitting methods with real a_j 's require at least $s = 5$ stages, in which case one has a free parameter. If we fix this as $a_1 = 1/8$, we get the scheme

$$\Psi^{[4]}_{SC,r}(\tau) = (\bar{b}_1, a_1, \bar{b}_2, a_2, \bar{b}_3, a_3, b_3, a_2, b_2, a_1, b_1) \tag{4.6}$$

with

$$\begin{aligned}
a_2 &= 0.23670501659941197298,\\
a_3 &= 0.27658996680117605403,\\
b_1 &= 0.03881396214419327198 - 0.045572109263923104872\, i,\\
b_2 &= 0.19047619047619047619 + 0.11546207230040874 1306\, i,\\
b_3 &= 0.27070984737961625182 - 0.14832224550962640 3888\, i
\end{aligned}$$

It is worth noticing that one can obtain symmetric-conjugate methods from palindromic schemes and vice versa. Thus, in particular, by composing the palindromic scheme (4.4) with its complex conjugate we can form a symmetric-conjugate splitting method with 8 stages and $a_j \in \mathbb{R}$, $b_j \in \mathbb{C}$:

$$\Xi^{[4]}_{SC,r}(\tau) = \Psi^{[4]}_{P,r}(\tau/2)\,\overline{\Psi}^{[4]}_{P,r}(\tau/2), \tag{4.7}$$

whereas doing the same with the 3rd-order symmetric-conjugate method (4.2) results in the 4th-order palindromic scheme with 6 stages and $a_j \in \mathbb{R}$, $b_j \in \mathbb{C}$:

$$\Xi^{[4]}_{P,r}(\tau) = \Psi^{[3]}_{SC,r}(\tau/2)\,\overline{\Psi}^{[3]}_{SC,r}(\tau/2). \tag{4.8}$$

This is possible because the adjoint of $(\Psi^{[3]}_{SC,r}(\tau))^*$ verifies

$$(\Psi^{[3]}_{SC,r}(\tau))^* = \overline{\Psi}^{[3]}_{SC,r}(\tau).$$

In our numerical experiments we shall also use for comparison one of the best 4th-order splitting methods with real coefficients designed specifically for systems verifying (3.7). It reads

$$\Psi^{[4]}_{RKN}(\tau) = (b_1, a_1, b_2, a_2, b_3, a_3, b_4, a_3, b_3, a_2, b_2, a_1, b_1) \tag{4.9}$$

and the coefficients can be found in [8]. The scheme has three additional parameters that are used to minimize error terms at higher orders, and provides by construction unitary approximations.

5 Numerical experiments

We next report on some numerical tests we have carried out with the splitting methods presented in section 4 applied to the Scrödinger equation in one dimension. Since many different schemes are tested and compared, it is convenient to classify them into the following categories:

- symmetric-conjugate methods with $a_j \in \mathbb{R}$, $b_j \in \mathbb{C}$
  - Order 3: $\Psi^{[3]}_{SC,r}$, Eq. (4.2);
  - Order 4: $\Psi^{[4]}_{SC,r}$, Eq. (4.6);
- symmetric-conjugate with $a_j \in \mathbb{C}$, $b_j \in \mathbb{C}$: method $\Psi^{[3]}_{SC,c}$, Eq. (4.3), order 3;
- palindromic with $a_j \in \mathbb{R}$, $b_j \in \mathbb{C}$: method $\Psi^{[4]}_{P,r}$, Eq. (4.4), order 4;
- palindromic with $a_j \in \mathbb{C}$, $b_j \in \mathbb{C}$: method $\Psi^{[4]}_{P,c}$, Eq. (4.5), order 4;

For completeness, we also consider the following schemes of order 4 with $a_j \in \mathbb{R}$, $b_j \in \mathbb{C}$:

- symmetric-conjugate obtained from a palindromic method: $\Xi^{[4]}_{SC,r}$, Eq. (4.7);
- palindromic obtained from a symmetric-conjugate method: $\Xi^{[4]}_{P,r}$, Eq. (4.8).

Quartic potential. As the first example we take the quartic oscillator

$$V(x) = -\frac{1}{2}x^2 + \frac{1}{20}x^4 \tag{5.1}$$

and the initial condition $\psi_0(x) = \sigma\, \mathrm{e}^{-x^2/2}$, where σ is a normalization constant. As usual, and since the exact solution decays rapidly, we truncate the infinite spatial domain to the periodic domain $[-L, L]$, provided L is sufficiently large and use Fourier spectral methods. We take $L = 8$ and set up a uniform grid on the interval with $N = 128$ subdivisions. Finally, we apply the different schemes to integrate in time the resulting equation (3.4) in the interval $t \in [0, t_f]$, with $t_f = 8000$. As in the case of the example in $\mathrm{SU}(2)$, we check the behavior of each scheme with respect to unitarity by computing $|\|u_{\mathrm{app}}(t)\| - 1|$ along the integration, where $u_{\mathrm{app}}(t)$ denotes the numerical approximation obtained by each method.

In addition, we also compute the expected value of the energy, $u^*_{\mathrm{app}}(t) \cdot H u_{\mathrm{app}}(t)$ and measure the error as the difference with respect to the exact value:

$$\text{energy error:} \quad |u^*_{\mathrm{app}}(t) \cdot (H u_{\mathrm{app}}(t)) - u_0^* \cdot (H u_0)|. \tag{5.2}$$

In each case, the time step is adjusted so that the number of FFTs (and their inverses) are the same for all methods (specifically, 1572864), so that the computational cost of all schemes is similar.

Figure 3 shows the corresponding results obtained by palindromic schemes with the coefficients a_j real, $\Psi^{[4]}_{P,r}$, and a_j complex, $\Psi^{[4]}_{P,c}$, together with the symmetric-conjugate method $\Psi^{[3]}_{SC,c}$ with $a_j \in \mathbb{C}$. We notice that the qualitative behavior of all of them is similar: after some point, depending on the particular step size, the unitarity is lost and the error in energy grows rapidly.

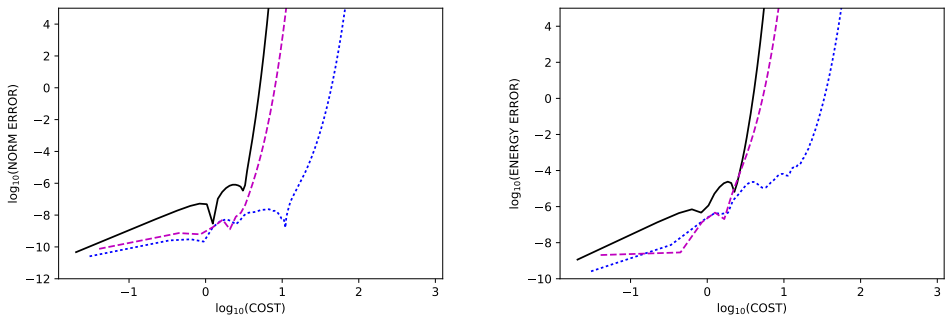

Figure 3: Error in norm of the approximate solution (left) and error in energy (5.2) (right) for the quartic potential (5.1) obtained by the palindromic schemes $\Psi^{[4]}_{P,r}$ (magenta, dashed line), $\Psi^{[4]}_{P,c}$ (blue dotted line) and the symmetric-conjugate method $\Psi^{[3]}_{SC,c}$ (black solid line) along the integration interval. The step size is chosen so that all methods have the same computational cost.

We notice here the same type of behavior observed in the case of the group $\mathrm{SU}(2)$: palindromic schemes with both real and complex coefficients a_j are unable to preserve unitarity. On the other hand, symmetric-conjugate schemes with $a_j \in \mathbb{C}$ lead also to unbounded errors, according with the comments formulated at the beginning of section 4.

We collect in Figure 4 the corresponding results achieved by the palindromic method $\Xi^{[4]}_{P,r}$ (blue dotted line), and the symmetric-conjugate schemes $\Psi^{[3]}_{SC,r}$ (black solid line) and $\Xi^{[4]}_{SC,r}$ (magenta dashed line), all of them with real parameters a_j. It is worth noticing that both the norm of the solution and the expected value of the energy are preserved for very long times by symmetric-conjugate methods with $a_j \in \mathbb{R}$, and this happens even if the method is obtained by composing a palindromic scheme (with a poor behavior) with its complex conjugate. By contrast, a symmetric-conjugate method looses its good preservation properties when composed to form a palindromic scheme, even if all a_j are real.

We have carried out the same experiment, but with the roles of T and V interchanged. In other words, the complex coefficients b_j are now multiplying the discretized Laplacian. In that case, the errors obtained by all the previous schemes grow unbounded. This indicates that, at least for this example, one needs both symmetric-conjugate schemes and real coefficients multiplying the Laplacian to get bounded errors in the preservation of unitarity and energy.

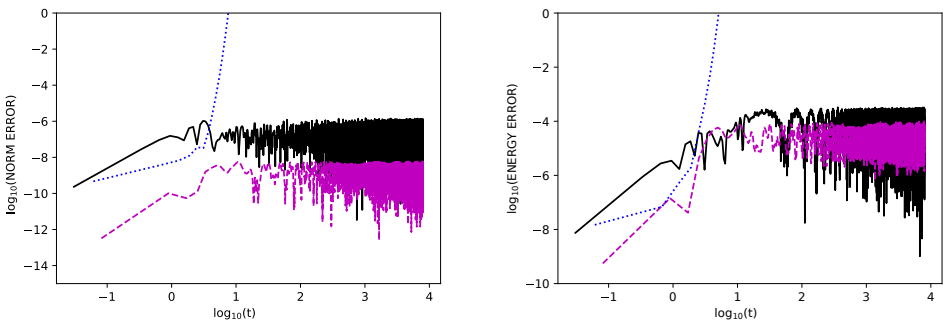

Figure 4: Error in norm of the approximate solution (left) and error in energy (5.2) (right) for the quartic potential (5.1) obtained by the palindromic scheme $\Xi^{[4]}_{P,r}$ (blue dotted line), and the symmetric-conjugate schemes $\Psi^{[3]}_{SC,r}$ (black solid line) and $\Xi^{[4]}_{SC,r}$ (magenta dashed line) along the integration interval. The step size is chosen so that all methods have the same computational cost.

Pöschl–Teller potential. The next set of simulations is carried out with the well known one-dimensional Pöschl–Teller potential,

$$V(x) = -\frac{\lambda(\lambda+1)}{2}\mathrm{sech}^2(x), \tag{5.3}$$

with $\lambda(\lambda+1) = 10$. It has been used in polyatomic molecular simulations and admits an analytic treatment [12]. We take again as initial condition $\psi_0(x) = \sigma\, \mathrm{e}^{-x^2/2}$, with σ a normalizing constant, then apply Fourier spectral methods on the interval $x \in [-8, 8]$ and integrate until the final time $t_f = 8000$ with the previous numerical splitting methods. For this potential we take $N = 512$ subdivisions of the space interval to better visualize the behavior of the different methods. Figure 5 is the analogous of Fig. 3), and only displays the results obtained by $\Psi^{[3]}_{SC,c}$ (black solid line) and $\Psi^{[4]}_{P,c}$ (blue dotted line), since the output corresponding to $\Psi^{[4]}_{P,r}$ is out of the scale (the errors are greater than 10^{87}). On the other hand, Figure 6

shows the same pattern as Figure 4: only symmetric-conjugate schemes with $a_j \in \mathbb{R}$ provide bounded errors in the norm and in the energy of the solution.

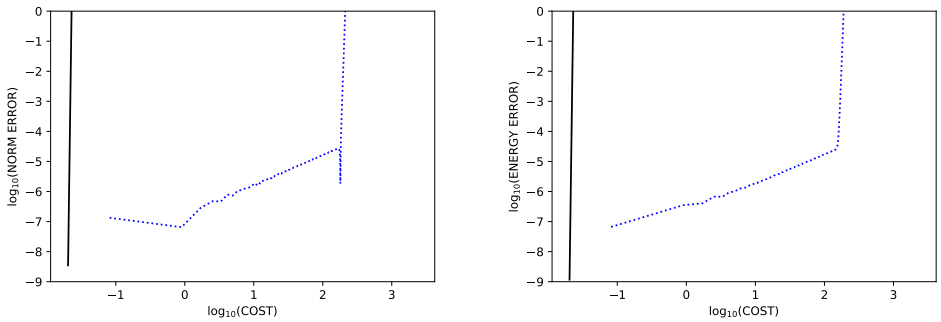

Figure 5: Error in norm of the approximate solution (left) and error in energy (5.2) (right) for the Pöschl–Teller potential (5.3) obtained by the palindromic scheme $\Psi^{[4]}_{P,c}$ (blue dotted line) and the symmetric-conjugate method $\Psi^{[3]}_{SC,c}$ (black solid line) along the integration interval. The result achieved by $\Psi^{[4]}_{P,r}$ is out of the scale.

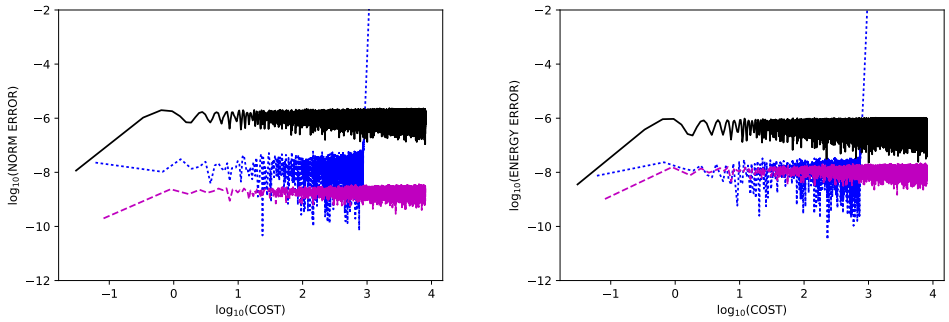

Figure 6: Error in norm of the approximate solution (left) and error in energy(5.2) (right) for the Pöschl–Teller potential (5.3) obtained by the palindromic scheme $\Xi^{[4]}_{P,r}$ (blue dotted line), and the symmetric-conjugate schemes $\Psi^{[3]}_{SC,r}$ (black solid line) and $\Xi^{[4]}_{SC,r}$ (magenta dashed line) along the integration interval.

Next, we take a shorter final time $t_f = 100$ and compute the maximum error in the energy along the time interval for several step sizes $h = \Delta t$ and integration schemes. The corresponding results are displayed in a log-log diagrama in Figure 7 (left). The order of each method is clearly visible, as well as the values of h where instabilities take place. Finally, in Figure 7 (right) we depict the same results but in terms of the computational cost as measured by the number of FFTs necessary to carry out the calculations. Notice that, for this range of times, the efficiency of the 4th-order symmetric-conjugate methods is not far away from the

optimized scheme (4.9) that takes into account the special property (3.7).

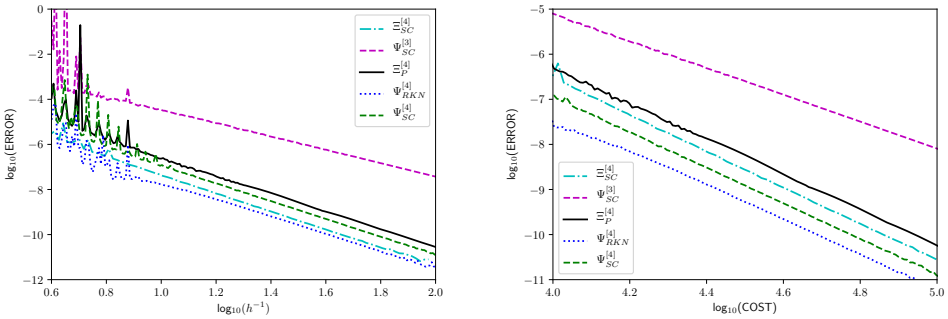

Figure 7: Maximum of error in the expected value of the energy in the interval $t \in [0, 100]$ as a function of the time step (left) and the computational cost (number of FFTs, right) for several splitting schemes. Pöschl–Teller potential.

6 Concluding remarks

Splitting and composition methods with complex coefficients have shown to be an appropriate tool in the numerical time integration of differential equations of parabolic type, when one or more pieces of the equations are only defined in semi-groups and the aim is to get high accuracy. Since it is possible to design methods of this class with positive real part, one is thus able to circumvent the existing order barrier for methods with real coefficients. In addition, these methods involve smaller truncation errors than their real counterparts and also exhibit relatively large stability thresholds. On the other hand, their computational cost notably increases, due to the use of complex arithmetic.

More recently, it has been shown that the particular class of symmetric-conjugate methods still exhibits remarkable preservation properties when applied to differential equations defined by real vector fields and the solution is projected on the real axis at each integration step. Here we have extended the analysis to problems evolving in the $\mathrm{SU}(2)$ and more generally to the numerical integration of the Schrödinger equation, where preservation of unitarity is a physical requirement. In the former case we have shown explicitly that symmetric-conjugate splitting methods are indeed conjugate to unitary methods for sufficiently small time step sizes, and thus there is not a secular component in the unitarity error propagation.

With respect to the Schrödinger equation, the examples we collect here indicate that methods of this class (with real coefficients a_j) could safely be applied just as other schemes involving only real coefficients for sufficiently small step sizes, although a general theoretical analysis similar to the one developed here for problems defined in $\mathrm{SU}(2)$ is lacking at present. Such analysis is clearly more involved, since one has to take into account the effect of the space discretization, the possible introduction of artificial cut-off bounds for unbounded potentials, etc. In this sense, this paper should be considered as a preliminary step for such analysis. In any case, we should remark that the use of methods with complex coefficients in this setting does not imply any extra computational cost, since the problem has to be treated in the complex domain anyway. Our results show that even some of the simplest methods within this class provide efficiencies close to the best

standard splitting schemes specifically designed for the integration of the Schrödinger equation. Although we have limited ourselves here to methods of order 3 and 4, it is clear that higher order integrators can also be designed, just by solving the corresponding order conditions [6, 15], and more efficient schemes can be obtained by taking into account property (3.7) and the processing technique. It is also worth noticing that, in contrast with the time integration of parabolic differential equations, here schemes with real and *negative* coefficients a_j still provide unitary approximations, and so more efficient schemes with $a_j < 0$ and $b_j \in \mathbb{C}$ might be possible. All these issues will be treated in a forthcoming paper.

Acknowledgements

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Capítulo 9

Conclusiones y trabajo futuro

En los dos primeros artículos de la presente tesis se han desarrollado nuevos integradores geométricos con coeficientes reales. Para problemas separables en tres o más partes, en el capítulo 3, se ha utilizado una técnica de construcción más eficiente que en el caso de escisión, logrando así, integradores geométricos de orden 4, los cuales llegan a ser más eficientes que los mejores métodos de escisión en dos partes aplicados a estos problemas.

En el capítulo 4, se han construido métodos de escisión RKN de orden 8 que han resultado ser más eficientes que las composiciones simétricas que existen a día de hoy del mismo orden e, incluso, más eficientes que algunos métodos de extrapolación; contestando de forma afirmativa a la pregunta planteada por McLachlan y Scovel [93] en 1996:

> *Is there a symmetric eighth-order Runge–Kutta–Nyström method which is better than general methods of type $\mathcal{SS}$?*

Y cerrando así una cuestión abierta en el campo de la integración numérica geométrica.

Por otra parte, en lo que respecta al resto de artículos presentados en esta tesis, se han desarrollado integradores numéricos haciendo uso de coeficientes complejos. La técnica del *triple–jump* es un procedimiento muy utilizado para construir integradores de orden alto partiendo de un método básico de orden bajo. Esta técnica tiene su versión con coeficientes complejos con las partes reales positivas y se puede utilizar para problemas donde los tamaños de paso negativos no son recomendables. Aun así, el problema que presenta esta técnica es que el número de etapas crece considerablemente rápido. En los capítulos 5 y 6 hemos presentado dos técnicas diferentes para construir integradores de orden alto partiendo de integradores de orden bajo. Estas nuevas técnicas tienen positivas las partes reales de los coeficientes y nos permiten integrar preservando hasta cierto orden el comportamiento

cualitativo de las soluciones. Las nuevas técnicas están pensadas para ser fácilmente paralelizables y requieren un número menor de métodos básicos en comparación con la técnica del *triple–jump*. Además, la técnica presentada en el capítulo 6 sólo contiene métodos simétrico–conjugados. Este hecho hace que el número total de métodos a ejecutar en paralelo sea menor y que presenten mejores propiedades de conservación en comparación con la técnica del *triple–jump* y con la presentada en el capítulo 5.

A causa de los buenos resultados conservativos observados en el capítulo anterior, en el capítulo 7, se ha realizado un primer analisis sistemático sobre métodos de composición simétrico–conjugados cuando son aplicados a problemas donde $f(x) \in \mathbb{R}$. Para ello, se han comparado las composiciones palindrómicas y las simétrico–conjugadas observando cómo, con coeficientes complejos, las simétrico–conjugadas son más beneficiosas que las palindrómicas. Además, los diagramas de eficiencia muestran que los métodos de orden alto con coeficientes complejos son más eficientes que los de orden más bajo, no solamente para valores de pequeños h, sino también para toda la región de valores de h.

Por último, en el capítulo 8 se hace una extensión de los métodos simétrico–conjugados a problemas donde $f(x)$ ya no es real, llegando a conclusiones muy esperanzadoras sobre este tipo de métodos en problemas unitarios. Pues, se ha probado cómo los métodos simétrico–conjugados son conjugados a métodos unitarios en el caso de matrices de $SU(2)$.

A continuación detallamos las futuras lineas de investigación previstas para los proximos meses:

- Crear métodos eficientes para problemas separables en tres o más partes siguiendo el trabajo empezado en el capítulo 3 pero utilizando la técnica de procesado.

- Continuar con la idea de llenar los huecos que quedan en [20] utilizando las técnicas ya desarrolladas para la construcción de métodos. Así pues, podríamos construir métodos de escisión RKN de orden 10 con y sin procesado para ver si son más eficientes que las composiciones simétricas de orden 10. Los óptimos resultados obtenidos en el capítulo 4 nos hacen pensar que se trata de un buen camino a seguir. Además, con las mismas técnicas se podrían conseguir métodos de escisión general de orden 8 y composiciones simétricas de métodos simétricos de orden 12.

- En el artículo [18] se presenta, entre otros, un método de orden generalizado $(10, 6, 4)$ para problemas cuasi–integrables. Como futuro trabajo se puede explorar la posibilidad de construir métodos de orden generalizado más alto con la idea de superar en eficiencia al método citado.

- En el caso concreto del Sistema Solar el error predominante es el asociado a Mercurio. Así, se podría construir un procesador para el método de orden generalizado $(10, 6, 4)$ de [18] que minimizará este error. Para construir este procesador se utilizarían las técnicas de minimización que se utilizan en Inteligencia Artificial, con la idea de ir entrenando este procesador.

- En el artículo [60] se presenta un patrón de coeficientes que es muy eficiente para la construcción de métodos para el caso del oscilador armónico:

$$\psi_h = \varphi_{c_1 h}^{[A]} \circ \varphi_{c_2 h}^{[B]} \circ \varphi_{c_3 h}^{[A]} \circ \cdots \circ \varphi_{c_3 h}^{[B]} \circ \varphi_{c_2 h}^{[A]} \circ \varphi_{c_1 h}^{[B]}.$$

  Este patrón puede servir en el caso más general para construir métodos de orden impar que al simetrizarlos aumenten un orden. Con esta idea se pueden explorar las soluciones para métodos de orden 5 que se conviertan en orden 6 al simetrizarlos, para ver si se obtienen métodos eficientes de orden 6 con más etapas de las habituales.

- En el artículo [73] se presentan métodos RK para ecuaciones cuadráticas. Este tipo de EDO en el caso hamiltoniano se pueden reexpresar como un potencial cúbico, siendo un caso concreto de este tipo de problema el potencial de Hénon–Heiles [70]. El hecho de que el potencial sea cúbico comporta una reducción de las condiciones de orden a resolver. Si a este hecho le sumamos que el sistema es RKN, la reducción es aún mayor. De este hecho se dieron cuenta McLachlan y Ryland en [92]. Hemos construido un método de orden 8 con 12 etapas muy eficiente para este caso y se pueden construir métodos de orden 10 y 12 con 22 y 41 etapas respectivamente.

- En el capítulo 7 se han diseñado métodos simétrico–conjugados hasta orden ocho. Pero, el hecho de que para los órdenes mayores son más eficientes incluso para tamaños de paso grandes hace pensar que construir métodos de orden más alto puede ser una buena opción como futuro trabajo. Así, se podrian construir métodos de orden 10 y 12.

- En este mismo capítulo, nos hemos ceñido al hecho de proyectar sobre el eje real después de cada iteración del método. Sin embargo, nos queda pendiente sacar una conclusión fundamentada a la siguiente cuestión: bajo qué circunstancias es mejor proyectar sobre el eje real en cada paso y seguir con la parte real en el siguiente paso y bajo qué circunstancias es mejor continuar la evolución sin proyectar.

- Aunque el uso de coeficientes complejos puede suponer un aumento del coste computacional, por ejemplo, el hecho de que con 9 etapas podamos construir un método simétrico–conjugado de orden 8 y que

con coeficientes reales necesitemos 15 etapas puede contrarestar este aumento del coste. Aún más, cuando en el caso de coeficientes reales el mínimo número de etapas no suele ser el más eficiente. Esto, aunque sea un problema altamente dependiente de la implementación y del tipo de máquina, es una futura vía de estudio.

- En el capítulo 8 se ha probado cómo los métodos simétrico–conjugados son conjugados a métodos unitarios para el caso de $SU(2)$. Queda pendiente ver si este resultado se puede generalizar, ya que los experimentos numéricos muestran un comportamiento de este tipo.

- Construir métodos de escisión con $a_i \in \mathbb{R}$, $b_i \in \mathbb{C}$ y con las partes reales positivas de orden más alto que los presentados en el capítulo 8. Estudiar también la construcción teniendo en cuenta la condición RKN por las posibles mejoras que puede ocasionar.

- Volviendo a los problemas cuasi–integrables, puede llegar a ser una buena técnica la construcción de métodos simétrico–conjugados para este caso. Se debería estudiar el comportamiento pseudo–simétrico y pseudo–simpléctico para integraciones largas en el tiempo. Aun así, el hecho de poder contruir métodos con coeficientes con partes reales positivas puede llegar a presentar mejoras en la eficiencia. Por ejemplo, en el caso de querer construir un método de orden generalizado $(10, 6, 4)$ con $a_i, b_i \in \mathbb{C}$ se necesitarían únicamente 8 etapas. La cuestión radicaría en ver si se puede contrarestar el uso de artimética compleja construyendo métodos con coeficientes con las partes reales positivas.

Apéndice A

Álgebras de Lie y Mecánica Hamiltoniana

A.1. Álgebras de Lie

Un álgebra de Lie es un espacio vectorial $\mathfrak{g}$ sobre un cierto cuerpo junto con una operación $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ llamada corchete de Lie, que cumple las siguientes propiedades:

a) Bilinearidad

$$[aX + bY, Z] = a[X, Z] + b[Y, Z], \quad \forall a, b \in \mathbb{C}, \quad \forall X, Y, Z \in \mathfrak{g},$$

b) Antisimetría

$$[X, Y] = -[Y, X], \quad \forall X, Y \in \mathfrak{g},$$

c) Identidad de Jacobi

$$[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0, \quad \forall X, Y, Z \in \mathfrak{g}.$$

Un ejemplo particular es el espacio de matrices $d \times d$ con el corchete de Lie definido como el conmutador $[X, Y] = XY - YX$.

Álgebras de Lie libres Un concepto importante en el análisis de los métodos de escisión y composición es el de álgebra de Lie libre (FLA de sus siglas en inglés). Un álgebra de Lie libre se puede visualizar como aquella álgebra de Lie que es común a todas las álgebras de Lie, es decir, que no tiene ninguna restricción, y por tanto será aquella generada por todos los corchetes posibles independientes teniendo en cuenta solamente las propiedades del álgebra de Lie. Esta idea se puede expresar más rigurosamente de la siguiente forma [96, 13]: dado un conjunto índice arbitrario I (finito o infinito contable), un álgebra de Lie $\mathfrak{g}$ es libre sobre el conjunto I si

a) A $i \in I$ le corresponde un elemento $G_i \in \mathfrak{g}$;

b) Para cualquier álgebra de Lie $\mathfrak{h}$ y cualquier función $i \mapsto H_i \in \mathfrak{h}$, existe un único homeomorfismo $\pi : \mathfrak{g} \to \mathfrak{h}$ entre álgebras de Lie que verifica $\pi(G_i) = H_i$ para todo $i \in I$.

Álgebras de Lie libres graduadas Definimos la función grado ω [96, 13, 55] sobre un álgebra de Lie $\mathfrak{g}$ como:

- sobre el conjunto generador $S = \{G_i : i \in I\}$:

$$\omega(G_i) = \omega_i, \qquad \omega_i \in \mathbb{Z},$$

- sobre elementos $[u, v] \in \mathfrak{g}$:

$$\omega([u, v]) = \omega(u) + \omega(v).$$

Esto permite escribir $\mathfrak{g}$ como una suma directa de subálgebras $\mathfrak{g}_n$:

$$\mathfrak{g} = \bigoplus_{n=1}^{\infty} \mathfrak{g}_n, \qquad \text{donde } \mathfrak{g}_n = \{P \in \mathfrak{g} : \omega(P) = n\},$$

que cumplen:

$$[\mathfrak{g}_n, \mathfrak{g}_m] \in \mathfrak{g}_{n+m}.$$

Así, con la función grado, $\mathfrak{g}$ se convierte en un álgebra graduada. La dimensión de la subálgebra $\mathfrak{g}_n$ viene determinada por la fórmula de Witt [90]:

$$\dim(\mathfrak{g}_n) = \frac{1}{n} \sum_{d|n} \mu(d) \nu^{\frac{n}{d}},$$

donde el sumatorio es sobre todos los enteros d que dividen a n, ν es el número de elementos generadores de S y la función μ es la función de Möbius, donde $\mu(1) = 1$, $\mu(d) = (-1)^q$ si d es el producto de q factores primos distintos y $\mu(d) = 0$ en cualquier otro caso. Los primeros valores $\dim(\mathfrak{g}_n)$ se muestran en la tabla A.1 para los tres tipos de métodos de escisión y composición que hemos utilizado.

Las álgebras de Lie en los métodos de escisión y composición

- Métodos de escisión. Los elementos generadores serán las derivadas de Lie A y B asociadas a la escisión $f(x) = f^{[A]}(x) + f^{[B]}(x)$. Llamamos $\mathfrak{g} = \mathcal{L}(A, B)$ al álgebra generada, graduada mediante la función:

$$\omega(A) = \omega(B) = 1.$$

Orden n	1	2	3	4	5	6	7	8	9	10
$\mathfrak{g}_n = \mathcal{L}^n(A,B)$	2	1	2	3	6	9	18	30	56	99
$\mathfrak{g}_n = \mathcal{L}^n(F,Y_2,Y_3,Y_4,\dots)$	1	1	2	3	6	9	18	30	56	99
$\mathfrak{g}_n = \mathcal{L}^n(F,S_3,S_5,S_7,\dots)$	1	0	1	1	2	2	4	5	8	11

Tabla A.1: Dimensión de las subálgebras asociadas a los métodos de escisión y composición: escisión en dos partes en la segunda línea, composición de método de primer orden y adjunto en la tercera línea, y composición simétrica de métodos simétricos de segundo orden en la cuarta línea.

Los elementos de una base para las primeras subálgebras son:

$$\begin{aligned}
\mathfrak{g}_1 &= \mathcal{L}^1(A,B): \quad \{A,B\};\\
\mathfrak{g}_2 &= \mathcal{L}^2(A,B): \quad \{[A,B]\};\\
\mathfrak{g}_3 &= \mathcal{L}^3(A,B): \quad \{[A,A,B],[B,A,B]\};\\
\mathfrak{g}_4 &= \mathcal{L}^4(A,B): \quad \{[A,A,A,B],[B,A,A,B],[B,B,A,B]\},
\end{aligned}$$

renombrados durante el capítulo 1 como $N_{i,j}$ y que cumplen $N_{i,j} \in \mathfrak{g}_i = \mathcal{L}^i(A,B)$.

- Composición de método y adjunto. Los elementos generadores, en este caso, serán los operadores diferenciales $\{Y_i\}_{i=1}^{\infty}$, asociados al desarrollo en serie del integrador de primer orden χ_h. El álgebra la denotaremos por $\mathfrak{g} = \mathcal{L}(Y_1,Y_2,Y_3\dots)$ y se gradúa mediante la función:

$$\omega(Y_i) = i.$$

Los elementos de una posible base para las primeras subálgebras son:

$$\begin{aligned}
\mathfrak{g}_1 &= \mathcal{L}^1(Y_1,Y_2,Y_3\dots): \quad \{Y_1\};\\
\mathfrak{g}_2 &= \mathcal{L}^2(Y_1,Y_2,Y_3\dots): \quad \{Y_2\};\\
\mathfrak{g}_3 &= \mathcal{L}^3(Y_1,Y_2,Y_3\dots): \quad \{Y_3,[Y_1,Y_2]\};\\
\mathfrak{g}_4 &= \mathcal{L}^4(Y_1,Y_2,Y_3\dots): \quad \{Y_4,[Y_1,Y_3],[Y_1,Y_1,Y_2]\},
\end{aligned}$$

renombrados durante el capítulo 1 como $C_{i,j}$ y que cumplen $C_{i,j} \in \mathfrak{g}_i = \mathcal{L}^i(Y_1,Y_2,Y_3\dots)$.

- Composición simétrica de métodos simétricos de segundo orden. En este caso los elementos generadores serán los operadores diferenciales $\{S_{2i-1}\}_{i=1}^{\infty}$, asociados al desarrollo del integrador de segundo orden $\mathcal{S}_h^{[2]}$, el álgebra generada la escribimos como $\mathfrak{g} = \mathcal{L}(S_1,S_3,S_5,\dots)$ y se gradúa mediante la función:

$$\omega(S_i) = i.$$

Los elementos de una posible base para las primeras subálgebras son:

$$\begin{aligned}\mathfrak{g}_1 &= \mathcal{L}^1(S_1, S_3, S_5, \dots): \quad \{S_1\};\\ \mathfrak{g}_3 &= \mathcal{L}^3(S_1, S_3, S_5, \dots): \quad \{S_3\};\\ \mathfrak{g}_4 &= \mathcal{L}^4(S_1, S_3, S_5, \dots): \quad \{[S_1, S_3]\},\end{aligned}$$

renombrados durante el capítulo 1 como $M_{i,j}$ y que cumplen $M_{i,j} \in \mathfrak{g}_i = \mathcal{L}^i(S_1, S_3, S_5, \dots)$.

A.1.1. La fórmula de Baker–Campbell–Hausdorff

Dado X un cierto operador, definimos la exponencial de éste como:

$$e^X = \sum_{n=0}^{\infty} \frac{1}{n!} X^n,$$

donde $X^0 \equiv \mathrm{Id}$ es el operador identidad. El producto de dos exponenciales de operadores se puede expresar como una nueva exponencial de un operador que viene determinado por la fórmula de Baker–Campbell–Hausdorff (BCH) [119]:

Sean X e Y dos operadores no conmutativos. Entonces

$$e^X e^Y = e^Z,$$

donde Z tiene la siguiente forma como desarrollo en serie:

$$Z = \sum_{m=1}^{\infty} Z_m(X, Y) \tag{A.1}$$

siendo $Z_m(X, Y)$ polinomios homogéneos de grado m que pueden ser expresados como combinaciones lineales de corchetes de Lie anidados de X e Y con coeficientes racionales. Los primeros elementos de esta serie [13] son:

$$\begin{aligned}Z_1 &= X + Y, \quad Z_2 = \frac{1}{2}[X, Y], \quad Z_3 = \frac{1}{12}[X, X, Y] - \frac{1}{12}[Y, X, Y],\\ Z_4 &= -\frac{1}{24}[Y, X, X, Y],\\ Z_5 &= -\frac{1}{720}[X, X, X, X, Y] - \frac{1}{120}[X, Y, X, X, Y] - \frac{1}{360}[X, Y, Y, X, Y]\\ &\quad + \frac{1}{360}[Y, X, X, X, Y] + \frac{1}{120}[Y, Y, X, X, Y] + \frac{1}{720}[Y, Y, Y, X, Y],\end{aligned}$$

donde los corchetes se entienden anidados a la derecha, es decir $[A, B, C] = [A, [B, C]]$. Cuando calculamos las condiciones de orden de métodos simétricos–temporales es conveniente aplicar la siguiente variación de la fórmula BCH:

$$e^{\frac{1}{2}X} e^Y e^{\frac{1}{2}X} = e^W,$$

conocida como la fórmula BCH simétrica. El operador W tiene la siguiente forma:

$$W = \sum_{m=1}^{\infty} W_{2m-1}(X, Y),$$

porque $W_{2m} = 0$. Los primeros elementos de la serie [13] son:

$$W_1 = X + Y, \quad W_3 = -\frac{1}{24}[X, X, Y] - \frac{1}{12}[Y, X, Y],$$
$$W_5 = \frac{7}{5760}[X, X, X, X, Y] + \frac{1}{480}[X, Y, X, X, Y] - \frac{1}{360}[X, Y, Y, X, Y]$$
$$+ \frac{1}{360}[Y, X, X, X, Y] + \frac{1}{120}[Y, Y, X, X, Y] + \frac{1}{720}[Y, Y, Y, X, Y].$$

A.1.2. Derivadas de Lie y transformaciones de Lie

Al campo de vectores f de $\dot{x} = f(x)$ se le puede asociar un operador [4] llamado derivada de Lie actuando sobre una función diferenciable $G : \mathbb{R}^d \to \mathbb{R}$, de la siguiente manera:

$$(L_f G)(x) = \sum_{i=1}^{n} f_i(x) \frac{\partial G}{\partial x_i}. \tag{A.2}$$

Llamamos transformación de Lie a la exponencial del operador derivada de Lie:

$$e^{L_f}[G](x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(L_f^n G\right)(x).$$

A.2. Flujos exactos como transformaciones de Lie

En este apartado utilizamos el argumento de [13] para establecer la relación entre un flujo exacto y su transformación de Lie. Cuando una ecuación diferencial $\dot{x} = f(x)$ posee una condición inicial $x(t_0) = x_0$, se tiene un problema de valores inicial o problema de Cauchy:

$$\dot{x} = \frac{dx}{dt} = f(x) \qquad x(t_0) = x_0 \in \mathbb{R}^d, \tag{A.3}$$

con $x \in \mathbb{R}^d$ y $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$. Entonces existe una única solución $\varphi_t(x_0)$ y podemos expresar la derivada de una función $G(x)$ sobre las soluciones como

$$\frac{d}{dt} G\left(\varphi_t(x_0)\right) = \sum_{i=1} \frac{\partial G}{\partial x_i} \frac{dx_i}{dt} = \sum_{i=1} f_i(t, x_i) \frac{\partial G}{\partial x_i} = \left(L_f G\right)\left(\varphi_t(x_0)\right).$$

Entonces la derivada k–ésima de $G(\varphi_t(x_0))$ será

$$\frac{d^k}{dt^k} G\left(\varphi_t(x_0)\right) = \left(L_f^k G\right)\left(\varphi_t(x_0)\right).$$

Con este resultado podemos expresar el desarrollo en serie de Taylor de $G(\varphi_t(x_0))$ alrededor de $t = 0$:

$$G(\varphi_t(x_0)) = \sum_{k=0} \frac{t^k}{k!}(L_f^k G)(x_0) = e^{tL_f}[G](x_0). \tag{A.4}$$

Si en la última expresión consideramos que G es la función identidad, $\mathrm{Id}(x) = x$, obtenemos:

$$\varphi_t(x_0) = \mathrm{Id}(\varphi_t(x_0)) = e^{tL_f}[I](x_0). \tag{A.5}$$

Así pues, si φ_t corresponde a la solución única del problema de valor inicial (A.3) esta puede expresarse como una transformación de Lie. Este resultado puede ser usado para ver que la ordenación de flujos es en sentido contrario a la ordenación de transformaciones de Lie. Utilizando (A.4) para obtener una expresión para la composición de flujos se obtiene [13]:

$$\varphi_{t_2} \circ \varphi_{t_1}(x_0) = \varphi_{t_2}\left(\varphi_{t_1}(x_0)\right) = e^{t_1 L_f}[\varphi_{t_2}](x_0) \overset{(A.5)}{=} e^{t_1 L_f} e^{t_2 L_f}[I](x_0),$$

resultado que puede generalizarse a m flujos:

$$\varphi_{t_m} \circ \cdots \circ \varphi_{t_2} \circ \varphi_{t_1}(x_0) = e^{t_1 L_f} e^{t_2 L_f} \cdots e^{t_m L_f}[I](x_0).$$

Con estos resultados, se puede reescribir las propiedades de los flujos exactos (1.4), (1.2) y (1.5) presentadas en el capítulo 1 utilizando transformaciones de Lie:

$$\begin{aligned}
&(e^{\delta L_{f_i}})^{-1} = e^{-\delta L_{f_i}}, \\
&e^{\delta_2 L_{f_i}} e^{\delta_1 L_{f_i}} = e^{(\delta_1+\delta_2) L_{f_i}}, \\
&\left(e^{\delta_2 L_{f_j}} \cdot e^{\delta_1 L_{f_i}}\right)^{-1} = \left(e^{\delta_1 L_{f_i}}\right)^{-1} \cdot \left(e^{\delta_2 L_{f_j}}\right)^{-1}.
\end{aligned}$$

A.3. Integradores numéricos y exponenciales de operadores diferenciales

Podemos asociar un operador $X(h)$ a cada integrador numérico $\chi_h : \mathbb{R}^d \to \mathbb{R}^d$ de los que utilizamos en esta tesis, tal como hemos hecho en el caso de los flujos exactos [13, 20]. La forma de este operador es:

$$X(h) = \mathrm{Id} + \sum_{n\geq 1} h^n X_n,$$

donde Id es el operador identidad y cada operador lineal X_n actúa sobre una función G como:

$$X_n[G](x) = \frac{1}{n}\frac{d^n}{dh^n}\bigg|_{h=0} G(\chi_h(x)).$$

Esto no es más que la formalización de un desarrollo en serie de Taylor del integrador χ_h. Así pues, $G(\chi_h(x)) = X(h)[G](x)$, de la misma manera que en el caso del flujo exacto (A.4). Podemos escribir este operador $X(h)$ como la exponencial de un nuevo operador $Y(h)$. Para conseguir este propósito usamos la serie del logaritmo:

$$Y(h) = \log(X(h)) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \left(\sum_{n\geq 1} h^n X_n \right)^k = \sum_{k=1}^{\infty} h^n Y_n,$$

siendo Y_n:

$$Y_n = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \sum_{j_1+\cdots+j_k=n} X_{j_1} \dots X_{j_k},$$

donde por consistencia $Y_1 = \mathcal{L}_f = X_1$. Con este resultado se puede obtener una ecuación similar a (A.4), pero para integradores numéricos:

$$G(\chi_h(x)) = e^{Y(h)}[G](x).$$

Para el adjunto de un método $\chi_h^* = \chi_{-h}^{-1}$ se obtiene:

$$G(\chi_h^*(x)) = e^{-Y(-h)}[G](x),$$

así pues, si un método χ_h es simétrico–temporal, i.e $\chi_h^* = \chi_h$, entonces $Y(h) = -Y(-h)$, y esto es sólo posible si los términos Y_{2k} son cero para $k \geq 1$, $Y(h) = \sum_{i=1}^{\infty} h^{2i-1} Y_{2i-1}$.

A.4. Mecánica Hamiltoniana

En los sistemas Hamiltonianos [58] tenemos coordenadas q_i y momentos canónicos conjugados p_i con $i = 1, \dots, d$, donde d es el número de grados de libertad, y el punto (q, p) representa el estado dinámico del sistema. Dada una función llamada Hamiltoniano $H(q, p)$ y definida en $D \subset \mathbb{R}^d \times \mathbb{R}^d$, las ecuaciones del movimiento son:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{A.6}$$

Si $x = (q, p)^\top$, se puede obtener una expresión compacta de las ecuaciones del movimiento:

$$\dot{x} = f_H(x) = J\nabla_x H(x) \qquad \text{con} \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}_{2d\times 2d},$$

siendo J la matriz canónica.

A.4.1. Corchete de Poisson

El corchete de Poisson [58] de dos funciones escalares $F(q,p)$ y $G(q,p)$ se define como:

$$\{F,G\} = \sum_{i=1}^{d} \left(\frac{\partial F}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial G}{\partial q_i} \right). \tag{A.7}$$

En particular, el corchete de Poisson de las q_i y de las p_i es:

$$\{q_i, q_j\} = \{p_i, p_j\} = 0, \qquad \{q_i, p_j\} = \delta_{ij} \qquad \forall i,j,$$

donde δ_{ij} es la delta de Kronecker cuyo valor es 1 si $i = j$ y 0 en cualquier otro caso. Nótese que, el corchete de Poisson de las x es la matriz canónica $J_{i,j} = \{x_i, x_j\}$.

Las propiedades algebraicas del corchete de Poisson son: la linearidad

$$\{aF + bG, K\} = a\{F,K\} + b\{G,K\};$$

la antisimetría

$$\{F,G\} = -\{G,F\},$$

y la identidad de Jacobi

$$\{F,\{G,K\}\} + \{G,\{K,F\}\} + \{K,\{F,G\}\} = 0, \tag{A.8}$$

para todas las funciones F, G, y K, y los escalares a y b.

Las ecuaciones del movimiento (A.6) pueden ser escritas en términos de los corchetes de Poisson como:

$$\dot{q}_i = \{q_i, H\}, \qquad \dot{p}_i = \{p_i, H\}, \qquad i = 1, \ldots, d,$$

o $\dot{x}_i = \{x_i, H\}$. Para cualquier función $F(q,p,t)$ se puede expresar su derivada total respecto del tiempo utilizando el corchete de Poisson:

$$\frac{dF}{dt} = \sum_{i=1}^{d} \left(\frac{\partial F}{\partial q_i}\dot{q}_i + \frac{\partial F}{\partial p_i}\dot{p}_i \right) + \frac{\partial F}{\partial t} = \{F,H\} + \frac{\partial F}{\partial t}.$$

La primera consecuencia de este resultado es que si el Hamiltoniano H no depende explícitamente del tiempo se tiene:

$$\frac{dH}{dt} = 0,$$

y en estos casos el Hamiltoniano es una cantidad conservada a lo largo de las soluciones.

Una importante característica de los sistemas Hamiltonianos es la simplecticidad de los flujos exactos φ_t:

$$\varphi_t'^{\top}(x) J \varphi_t'(x) = J \quad \text{para } t \geq 0,$$

donde $\varphi_t'(x)$ es la matriz jacobiana de la transformación φ_t.

A.4.2. Evolución Hamiltoniana como transformación de Lie

En Mecánica Hamiltoniana la derivada de Lie del campo de vectores f_H está relacionada con el corchete de Poisson [13] siendo

$$f_H = J\nabla H(x) = (\nabla_p H, -\nabla_q H)^\top,$$

de la siguiente manera:

$$\left(L_{f_H} G\right)(x) = \sum_{j=1}^{d} \left(\frac{\partial H}{\partial p_j}\frac{\partial G}{\partial q_j} - \frac{\partial H}{\partial q_j}\frac{\partial G}{\partial p_j} \right) = -\{H, G\}.$$

De manera análoga, $\{H, G\} = -L_{f_H} G = L_{f_G} H$. Utilizando la identidad de Jacobi (A.8) se puede obtener una relación entre el corchete de Poisson y el corchete de Lie:

$$\begin{aligned} \{H, \{F, G\}\} &= -\{F, \{G, H\}\} - \{G, \{H, F\}\} \\ L_{f_{\{F,G\}}} H &= L_{f_F}\{G, H\} - L_{f_G}\{F, H\} \\ &= -L_{f_F} L_{f_G} H + L_{f_G} L_{f_F} H \\ &= -[L_{f_F}, L_{f_G}] H \end{aligned}$$

Ahora podemos escribir las ecuaciones del movimiento (A.6) como:

$$\dot{x} = -L_{f_H}[\mathrm{Id}](x).$$

y su solución formal como una transformación de Lie:

$$x(t) = e^{-tL_{f_H}}[\mathrm{Id}]x_0,$$

que se trata de un caso particular de (A.5).

Apéndice B

Condiciones de orden para una base de corchetes anidados a la derecha para $\mathcal{L}(A, B)$

En esta sección explicaremos cómo se han implementado las técnicas para calcular y resolver las condiciones de orden [48]. El software desarrollado ha sido preparado para el caso general de un álgebra de Lie libre generada por dos elementos A y B, es decir $\mathcal{L}(A, B)$.

Para calcular las condiciones de orden, $\omega_{i,j}$, en el caso de escisión (1.24) necesitamos un CAS (computer algebra system), en nuestro caso hemos hecho uso de la librería Sympy [94] para Python [117]. El punto de vista adoptado en este desarrollo está basado en el que fue llevado a cabo por S. Blanes en su tesis doctoral [10] y puede dividirse en tres pasos: primero, calculamos los elementos de la base $\mathcal{L}(A, B)$ haciendo uso de corchetes anidados; luego, el conmutador de los elementos de la base, y finalmente implementamos la fórmula BCH y calculamos las fórmulas recursivas del desarrollo en serie del operador $Z(h) = \log(\Psi(h))$ (1.22) asociado con un método de escisión general.

B.1. Generación de una base de corchetes anidados a la derecha para $\mathcal{L}(A, B)$

Hacemos uso de las clases *Operator* y *Commutator* de Sympy [94] para calcular los elementos de la base $\mathfrak{g} = \mathcal{L}(A, B)$ con conmutadores anidados a la derecha utilizando una implementación del algoritmo 1. Necesitamos usar este algoritmo porque en el caso de los conmutadores anidados no existe una fórmula general para construir una base, como sí ocurre en el caso de las

bases de Lyndon o de Hall. Además, la base de conmutadores anidados no está definida de forma única.

Data: Base de $\mathcal{L}^{i-1}(A,B)$ en N_{i-1} y su dimensión en $n(i-1)$
Result: Base de $\mathcal{L}^{i}(A,B)$ en N_{i} y su dimensión en $n(i)$
inicializar N_i como conjunto vacío;
inicializar $n(i) \leftarrow 0$;
for $j \leftarrow 1$ **to** $n(i-1)$ **do**
  if $[A, N_{i-1,j}] \neq \sum_{k=1}^{n(i)} \alpha_k N_{i,k}$ **then**
    $N_{i,n(i)+1} \leftarrow [A, N_{i-1,j}]$;
    $n(i) \leftarrow n(i)+1$;
  end
  if $[B, N_{i-1,j}] \neq \sum_{k=1}^{n(i)} \alpha_k N_{i,k}$ **then**
    $N_{i,n(i)+1} \leftarrow [B, N_{i-1,j}]$;
    $n(i) \leftarrow n(i)+1$;
  end
end

Algoritmo 1: Calcular los elementos de la base $\mathcal{L}(A,B)$ a orden i.

El algoritmo 1 necesita como información de entrada todos los elementos de $\mathcal{L}^{i-1}(A,B)$ y nos devuelve todos los elementos de $\mathcal{L}^{i}(A,B)$ $(i \geq 1)$. Así pues, podemos aplicar este algoritmo de manera iterativa, utilizando la salida de una iteración como la entrada de la siguiente para obtener la base de $\mathcal{L}(A,B)$ hasta el orden deseado. El funcionamiento del algoritmo es sencillo: se recorren todos los elementos de la base de $\mathcal{L}^{i-1}(A,B)$ y se concatenan con los elementos generadores viendo si los nuevos conmutadores son una combiación lineal de los elementos de la base de $\mathcal{L}^{i}(A,B)$. En caso de no serlo se añaden como nuevos elementos de la base de $\mathcal{L}^{i}(A,B)$. Para evaluar los dos condicionales, lo que hacemos es expandir todos los conmutadores y tratar de resolver el sistema lineal asociado [2]. Daremos más detalles de este procedimiento en la siguiente subsección.

A continuación, damos los elementos de la base hasta orden 9. Utilizando el algoritmo 1 hemos calculado la base hasta orden 11 [48].

$$
\begin{aligned}
N_{1,1} &= A \\
N_{1,2} &= B \\
N_{2,1} &= [A,B] \\
N_{3,1} &= [A,A,B] \\
N_{3,2} &= [B,A,B] \\
N_{4,1} &= [A,A,A,B] \\
N_{4,2} &= [B,A,A,B] \\
N_{4,3} &= [B,B,B,A] \\
N_{5,1} &= [A,A,A,A,B] \\
N_{5,2} &= [B,A,A,A,B] \\
N_{5,3} &= [A,A,B,B,A] \\
N_{5,4} &= [B,B,A,A,B] \\
N_{5,5} &= [A,B,B,B,A]
\end{aligned}
$$

$N_{5,6} = [B,B,B,B,A]$
$N_{6,1} = [A, N_{5,1}]$
$N_{6,2} = [B, N_{5,1}]$
$N_{6,3} = [A, N_{5,2}]$
$N_{6,4} = [A, N_{5,4}]$
$N_{6,5} = [B, N_{5,2}]$
$N_{6,6} = [A, N_{5,5}]$
$N_{6,7} = [B, N_{5,5}]$
$N_{6,8} = [A, N_{5,6}]$
$N_{6,9} = [B, N_{5,6}]$
$N_{7,2i-1} = [A, N_{6,i}] \quad i \leq 9$
$N_{7,2i} = [B, N_{6,i}] \quad i \leq 9$
$N_{8,2i-1} = [A, N_{7,i}] \quad i \leq 4$
$N_{8,2i} = [B, N_{7,i}] \quad i \leq 4$
$N_{8,2i-1} = [B, N_{7,i}] \quad 5 \leq i \leq 10$
$N_{8,2i-2} = [A, N_{7,i}] \quad 6 \leq i \leq 10$
$N_{8,20} = [B, N_{7,11}]$
$N_{8,21} = [A, N_{7,12}]$
$N_{8,22} = [B, N_{7,12}]$
$N_{8,23} = [B, N_{7,13}]$
$N_{8,24} = [A, N_{7,14}]$
$N_{8,25} = [B, N_{7,14}]$
$N_{8,26} = [B, N_{7,15}]$
$N_{8,27} = [A, N_{7,16}]$
$N_{8,28} = [B, N_{7,16}]$
$N_{8,29} = [B, N_{7,17}]$
$N_{8,30} = [B, N_{7,18}]$
$N_{9,2i-1} = [A, N_{8,i}] \quad i \leq 15$
$N_{9,2i} = [B, N_{8,i}] \quad i \leq 15$
$N_{9,2i-1} = [B, N_{8,i}] \quad 16 \leq i \leq 19$
$N_{9,2i-2} = [B, N_{8,i}] \quad 20 \leq i \leq 26$
$N_{9,2i-2} = [A, N_{8,i}] \quad 17 \leq i \leq 19$
$N_{9,2i-3} = [A, N_{8,i}] \quad 21 \leq i \leq 26$
$N_{9,51} = [B, N_{8,27}]$
$N_{9,52} = [A, N_{8,28}]$
$N_{9,53} = [B, N_{8,28}]$
$N_{9,54} = [B, N_{8,29}]$
$N_{9,55} = [A, N_{8,30}]$
$N_{9,56} = [B, N_{8,30}]$

B.2. Cálculo de las relaciones entre los elementos de la base anidada a la derecha de $\mathcal{L}(A,B)$

Para construir las condiciones de orden, $\omega_{i,j}$, para el caso de métodos de escisión necesitamos conocer todas las relaciones entre los elementos de la base. Es decir, cuál es el resultado (en elementos de la base) del conmutador de dos elementos de la base:

$$[N_{i,j}, N_{k,l}] = \sum_{m=1}^{n(i+k)} \alpha_m N_{i+k,m}, \tag{B.1}$$

donde α_m son coeficientes reales y $n(i+k)$ es la dimensión de la base de $\mathcal{L}^{i+k}(A,B)$ que viene determinada por la fórmula de Witt [90]. El procedimiento para calcular α_m es similar al procedimiento utilizado en los condicionales del algoritmo 1 y está basado en el procedimiento presentado en [2]. Para ilustrarlo, utilizamos a modo de ejemplo el conmutador $[N_{2,1}, N_{3,2}]$:

- Expandimos el lado derecho de la ecuación (B.1):

$$[N_{2,1}, N_{3,2}] = [B, [B, A, B]] = AB^3 - 3BAB^2 + 3B^2AB - B^3A.$$

- Expandimos el lado izquierdo de la ecuación (B.1):

$$\begin{aligned}\sum_{m=1}^{c(4)} \alpha_m N_{4,m} &= \alpha_1 N_{4,1} + \alpha_2 N_{4,2} + \alpha_3 N_{4,3} \\ &= 3\alpha_1 ABA^2 - 3\alpha_1 A^2 BA + \alpha_1 A^3 B - \alpha_1 BA^3 \\ &\quad + 2\alpha_2 ABAB - \alpha_2 A^2 B^2 - 2\alpha_2 BABA + \alpha_2 B^2 A^2 \\ &\quad - \alpha_3 AB^3 + 3\alpha_3 BAB^2 - 3\alpha_3 B^2 AB + \alpha_3 B^3 A.\end{aligned}$$

  Nótese que sólo necesitamos realizar este paso una vez para todos los elementos donde el valor de $i+k$ sea el mismo.

- Igualamos las dos partes y resolvemos el sistema lineal asociado. En este ejemplo, la solución es $\alpha_1 = \alpha_2 = 0$ y $\alpha_3 = -1$. Por lo tanto, $[N_{2,1}, N_{3,2}] = -N_{4,3}$.

Ahora, daremos las relaciones entre los conmutadores de nuestra base hasta orden 6, pero han sido calculados hasta orden 9 [48]:

$$\begin{aligned}
&[N_{1,1}, N_{1,2}] = N_{2,1} \\
&[N_{1,1}, N_{2,1}] = N_{3,1} \\
&[N_{1,2}, N_{2,1}] = N_{3,2} \\
&[N_{1,1}, N_{3,1}] = N_{4,1} \\
&[N_{1,1}, N_{3,2}] = N_{4,2} \\
&[N_{1,2}, N_{3,1}] = N_{4,2} \\
&[N_{1,2}, N_{3,2}] = -N_{4,3} \\
&[N_{1,1}, N_{4,1}] = N_{5,1} \\
&[N_{1,1}, N_{4,2}] = -N_{5,3} \\
&[N_{1,1}, N_{4,3}] = N_{5,5} \\
&[N_{1,2}, N_{4,1}] = N_{5,2} \\
&[N_{1,2}, N_{4,2}] = N_{5,4} \\
&[N_{1,2}, N_{4,3}] = N_{5,6} \\
&[N_{2,1}, N_{3,1}] = -N_{5,2} - N_{5,3} \\
&[N_{2,1}, N_{3,2}] = -N_{5,5} - N_{5,4} \\
&[N_{1,1}, N_{5,1}] = N_{6,1} \\
&[N_{1,1}, N_{5,2}] = N_{6,3} \\
&[N_{1,1}, N_{5,3}] = -2N_{6,3} + N_{6,2} \\
&[N_{1,1}, N_{5,4}] = N_{6,4} \\
&[N_{1,1}, N_{5,5}] = N_{6,6} \\
&[N_{1,1}, N_{5,6}] = N_{6,8} \\
&[N_{1,2}, N_{5,1}] = N_{6,2} \\
&[N_{1,2}, N_{5,2}] = N_{6,5} \\
&[N_{1,2}, N_{5,3}] = -\frac{1}{3}N_{6,6} - \frac{1}{3}N_{6,5} - N_{6,4} \\
&[N_{1,2}, N_{5,4}] = N_{6,8} - 2N_{6,7} \\
&[N_{1,2}, N_{5,5}] = N_{6,7} \\
&[N_{1,2}, N_{5,6}] = N_{6,9} \\
&[N_{2,1}, N_{4,1}] = -N_{6,2} + N_{6,3} \\
&[N_{2,1}, N_{4,2}] = -\frac{1}{3}N_{6,6} - \frac{1}{3}N_{6,5} \\
&[N_{2,1}, N_{4,3}] = N_{6,8} - N_{6,7} \\
&[N_{3,1}, N_{3,2}] = -\frac{2}{3}N_{6,6} - N_{6,4} + \frac{1}{3}N_{6,5}
\end{aligned}$$

B.3. Fórmulas recursivas

Con las relaciones que se acaban de obtener y la fórmula BCH se pueden construir las fórmulas recursivas para obtener las funciones $\omega_{i,j}$. A la hora

de implementar la fórmula BCH hemos utilizado la expresada en [2] por ser la más eficiente para nuestro caso, ya que viene expresada en función de conmutadores anidados a la derecha.

A continuación presentamos las fórmulas recursivas para cuatro casos distintos hasta orden 5 y en [48] se pueden ver hasta orden 9.

Recursión general con A. Dado $C \in \mathcal{L}(A, B)$:

$$C = \sum_{i}^{\infty} \sum_{j}^{n(i)} \alpha_{i,j} N_{i,j},$$

el producto del operador e^{xA} por e^{C} dará un nuevo operador e^{D}:

$$e^{D} = e^{xA} e^{C}, \qquad x \in \mathbb{R},$$

donde D tendrá la forma

$$D = \sum_{i}^{\infty} \sum_{j}^{n(i)} \beta_{i,j} N_{i,j}.$$

con $\beta_{i,j} = f(x, \boldsymbol{\alpha})$:

$$\begin{aligned}
\beta_{1,1} &= x + \alpha_{1,1} \\
\beta_{1,2} &= \alpha_{1,2} \\
\beta_{2,1} &= \frac{1}{2} x \alpha_{1,2} + \alpha_{2,1} \\
\beta_{3,1} &= \frac{1}{12} x^2 \alpha_{1,2} - \frac{1}{12} x \alpha_{1,1} \alpha_{1,2} + \frac{1}{2} x \alpha_{2,1} + \alpha_{3,1} \\
\beta_{3,2} &= -\frac{1}{12} x \alpha_{1,2}^2 + \alpha_{3,2} \\
\beta_{4,1} &= -\frac{1}{24} x^2 \alpha_{1,1} \alpha_{1,2} + \frac{1}{12} x^2 \alpha_{2,1} - \frac{1}{12} x \alpha_{1,1} \alpha_{2,1} + \frac{1}{2} x \alpha_{3,1} + \alpha_{4,1} \\
\beta_{4,2} &= -\frac{1}{24} x^2 \alpha_{1,2}^2 - \frac{1}{12} x \alpha_{1,2} \alpha_{2,1} + \frac{1}{2} x \alpha_{3,2} + \alpha_{4,2} \\
\beta_{4,3} &= \alpha_{4,3} \\
\beta_{5,1} &= -\frac{1}{720} x^4 \alpha_{1,2} - \frac{1}{180} x^3 \alpha_{1,1} \alpha_{1,2} + \frac{1}{180} x^2 \alpha_{1,1}^2 \alpha_{1,2} - \frac{1}{24} x^2 \alpha_{1,1} \alpha_{2,1} + \frac{1}{12} x^2 \alpha_{3,1} \\
&\quad + \frac{1}{720} x \alpha_{1,1}^3 \alpha_{1,2} - \frac{1}{12} x \alpha_{1,1} \alpha_{3,1} + \frac{1}{2} x \alpha_{4,1} + \alpha_{5,1} \\
\beta_{5,2} &= \frac{1}{360} x^3 \alpha_{1,2}^2 + \frac{1}{120} x^2 \alpha_{1,1} \alpha_{1,2}^2 + \frac{1}{720} x \alpha_{1,1}^2 \alpha_{1,2}^2 - \frac{1}{6} x \alpha_{1,2} \alpha_{3,1} + \frac{1}{12} x \alpha_{2,1}^2 + \alpha_{5,2} \\
\beta_{5,3} &= \frac{1}{120} x^3 \alpha_{1,2}^2 - \frac{1}{360} x^2 \alpha_{1,1} \alpha_{1,2}^2 + \frac{1}{24} x^2 \alpha_{1,2} \alpha_{2,1} - \frac{1}{12} x^2 \alpha_{3,2} - \frac{1}{360} x \alpha_{1,1}^2 \alpha_{1,2}^2 \\
&\quad + \frac{1}{12} x \alpha_{1,1} \alpha_{3,2} - \frac{1}{12} x \alpha_{1,2} \alpha_{3,1} + \frac{1}{12} x \alpha_{2,1}^2 - \frac{1}{2} x \alpha_{4,2} + \alpha_{5,3}
\end{aligned}$$

$$\beta_{5,4} = \frac{1}{120}x^2\alpha_{1,2}^3 + \frac{1}{360}x\alpha_{1,1}\alpha_{1,2}^3 - \frac{1}{6}x\alpha_{1,2}\alpha_{3,2} + \alpha_{5,4}$$
$$\beta_{5,5} = \frac{1}{360}x^2\alpha_{1,2}^3 - \frac{1}{720}x\alpha_{1,1}\alpha_{1,2}^3 - \frac{1}{12}x\alpha_{1,2}\alpha_{3,2} + \frac{1}{2}x\alpha_{4,3} + \alpha_{5,5}$$
$$\beta_{5,6} = -\frac{1}{720}x\alpha_{1,2}^4 + \alpha_{5,6}$$

Recursión general con B. Dado $C \in \mathcal{L}(A,B)$:

$$C = \sum_i^\infty \sum_j^{n(i)} \alpha_{i,j} N_{i,j},$$

el producto del operador e^{xB} por e^C dará un nuevo operador e^D:

$$e^D = e^{xB}e^C, \qquad x \in \mathbb{R},$$

donde D tendrá la forma

$$D = \sum_i^\infty \sum_j^{n(i)} \beta_{i,j} N_{i,j},$$

con $\beta_{i,j} = f(x, \boldsymbol{\alpha})$:

$$\beta_{1,1} = \alpha_{1,1}$$
$$\beta_{1,2} = x + \alpha_{1,2}$$
$$\beta_{2,1} = -\frac{1}{2}x\alpha_{1,1} + \alpha_{2,1}$$
$$\beta_{3,1} = \frac{1}{12}x\alpha_{1,1}^2 + \alpha_{3,1}$$
$$\beta_{3,2} = -\frac{1}{12}x^2\alpha_{1,1} + \frac{1}{12}x\alpha_{1,1}\alpha_{1,2} + \frac{1}{2}x\alpha_{2,1} + \alpha_{3,2}$$
$$\beta_{4,1} = \alpha_{4,1}$$
$$\beta_{4,2} = \frac{1}{24}x^2\alpha_{1,1}^2 - \frac{1}{12}x\alpha_{1,1}\alpha_{2,1} + \frac{1}{2}x\alpha_{3,1} + \alpha_{4,2}$$
$$\beta_{4,3} = -\frac{1}{24}x^2\alpha_{1,1}\alpha_{1,2} - \frac{1}{12}x^2\alpha_{2,1} + \frac{1}{12}x\alpha_{1,2}\alpha_{2,1} - \frac{1}{2}x\alpha_{3,2} + \alpha_{4,3}$$
$$\beta_{5,1} = -\frac{1}{720}x\alpha_{1,1}^4 + \alpha_{5,1}$$
$$\beta_{5,2} = \frac{1}{360}x^2\alpha_{1,1}^3 - \frac{1}{720}x\alpha_{1,1}^3\alpha_{1,2} + \frac{1}{12}x\alpha_{1,1}\alpha_{3,1} + \frac{1}{2}x\alpha_{4,1} + \alpha_{5,2}$$
$$\beta_{5,3} = \frac{1}{120}x^2\alpha_{1,1}^3 + \frac{1}{360}x\alpha_{1,1}^3\alpha_{1,2} + \frac{1}{6}x\alpha_{1,1}\alpha_{3,1} + \alpha_{5,3}$$
$$\beta_{5,4} = \frac{1}{120}x^3\alpha_{1,1}^2 - \frac{1}{360}x^2\alpha_{1,1}^2\alpha_{1,2} - \frac{1}{24}x^2\alpha_{1,1}\alpha_{2,1} + \frac{1}{12}x^2\alpha_{3,1} - \frac{1}{360}x\alpha_{1,1}^2\alpha_{1,2}^2$$
$$+ \frac{1}{12}x\alpha_{1,1}\alpha_{3,2} - \frac{1}{12}x\alpha_{1,2}\alpha_{3,1} + \frac{1}{12}x\alpha_{2,1}^2 + \frac{1}{2}x\alpha_{4,2} + \alpha_{5,4}$$

$$\beta_{5,5} = \frac{1}{360}x^3\alpha_{1,1}^2 + \frac{1}{120}x^2\alpha_{1,1}^2\alpha_{1,2} + \frac{1}{720}x\alpha_{1,1}^2\alpha_{1,2}^2 + \frac{1}{6}x\alpha_{1,1}\alpha_{3,2} + \frac{1}{12}x\alpha_{2,1}^2 + \alpha_{5,5}$$

$$\beta_{5,6} = -\frac{1}{720}x^4\alpha_{1,1} - \frac{1}{180}x^3\alpha_{1,1}\alpha_{1,2} + \frac{1}{180}x^2\alpha_{1,1}\alpha_{1,2}^2 + \frac{1}{24}x^2\alpha_{1,2}\alpha_{2,1} - \frac{1}{12}x^2\alpha_{3,2} + \frac{1}{720}x\alpha_{1,1}\alpha_{1,2}^3 + \frac{1}{12}x\alpha_{1,2}\alpha_{3,2} + \frac{1}{2}x\alpha_{4,3} + \alpha_{5,6}$$

Recursión simétrico–conjugada con A. Si $C \in \mathcal{L}(A,B)$, con e^C un operador asociado a un integrador simétrico–conjugado, entonces:

$$C = \sum_i^{\infty}\left(\sum_j^{n(2i-1)} \alpha_{2i-1,j}N_{2i-1,j} + i\sum_j^{n(2i)} \alpha_{2i,j}N_{2i,j}\right).$$

El producto por la izquierda por e^{zA} y por la derecha por $e^{\bar{z}A}$ dará un nuevo operador e^D, asociado a otro integrador simétrico–conjugado:

$$e^D = e^{zA}e^Ce^{\bar{z}A}, \qquad z = x + iy \in \mathbb{C},$$

donde D tendrá la forma

$$D = \sum_i^{\infty}\left(\sum_j^{n(2i-1)} \beta_{2i-1,j}N_{2i-1,j} + i\sum_j^{n(2i)} \beta_{2i,j}N_{2i,j}\right)$$

con $\beta_{i,j} = f(x,\boldsymbol{\alpha})$:

$$\beta_{1,1} = 2x + \alpha_{1,1}$$
$$\beta_{1,2} = \alpha_{1,2}$$
$$\beta_{2,1} = y\alpha_{1,2} + \alpha_{2,1}$$
$$\beta_{3,1} = -\frac{1}{6}x^2\alpha_{1,2} - \frac{1}{6}x\alpha_{1,1}\alpha_{1,2} - \frac{1}{2}y^2\alpha_{1,2} - y\alpha_{2,1} + \alpha_{3,1}$$
$$\beta_{3,2} = -\frac{1}{6}x\alpha_{1,2}^2 + \alpha_{3,2}$$
$$\beta_{4,1} = -\frac{1}{6}x^2y\alpha_{1,2} - \frac{1}{6}x^2\alpha_{2,1} - \frac{1}{6}xy\alpha_{1,1}\alpha_{1,2} - \frac{1}{6}x\alpha_{1,1}\alpha_{2,1} - \frac{1}{6}y^3\alpha_{1,2} - \frac{1}{2}y^2\alpha_{2,1} + y\alpha_{3,1} + \alpha_{4,1}$$
$$\beta_{4,2} = -\frac{1}{6}xy\alpha_{1,2}^2 - \frac{1}{6}x\alpha_{1,2}\alpha_{2,1} + y\alpha_{3,2} + \alpha_{4,2}$$
$$\beta_{4,3} = \alpha_{4,3}$$
$$\beta_{5,1} = \frac{7}{360}x^4\alpha_{1,2} + \frac{7}{180}x^3\alpha_{1,1}\alpha_{1,2} + \frac{1}{12}x^2y^2\alpha_{1,2} + \frac{1}{6}x^2y\alpha_{2,1} + \frac{1}{45}x^2\alpha_{1,1}^2\alpha_{1,2} - \frac{1}{6}x^2\alpha_{3,1} + \frac{1}{12}xy^2\alpha_{1,1}\alpha_{1,2} + \frac{1}{6}xy\alpha_{1,1}\alpha_{2,1} + \frac{1}{360}x\alpha_{1,1}^3\alpha_{1,2} - \frac{1}{6}x\alpha_{1,1}\alpha_{3,1}$$

$$+\frac{1}{24}y^4\alpha_{1,2}+\frac{1}{6}y^3\alpha_{2,1}-\frac{1}{2}y^2\alpha_{3,1}-y\alpha_{4,1}+\alpha_{5,1}$$
$$\beta_{5,2}=\frac{1}{45}x^3\alpha_{1,2}^2+\frac{1}{30}x^2\alpha_{1,1}\alpha_{1,2}^2+\frac{1}{360}x\alpha_{1,1}^2\alpha_{1,2}^2-\frac{1}{3}x\alpha_{1,2}\alpha_{3,1}-\frac{1}{6}x\alpha_{2,1}^2+\alpha_{5,2}$$
$$\beta_{5,3}=-\frac{1}{60}x^3\alpha_{1,2}^2-\frac{1}{90}x^2\alpha_{1,1}\alpha_{1,2}^2+\frac{1}{6}x^2\alpha_{3,2}-\frac{1}{12}xy^2\alpha_{1,2}^2-\frac{1}{6}xy\alpha_{1,2}\alpha_{2,1}$$
$$-\frac{1}{180}x\alpha_{1,1}^2\alpha_{1,2}^2+\frac{1}{6}x\alpha_{1,1}\alpha_{3,2}-\frac{1}{6}x\alpha_{1,2}\alpha_{3,1}-\frac{1}{6}x\alpha_{2,1}^2+\frac{1}{2}y^2\alpha_{3,2}+y\alpha_{4,2}$$
$$+\alpha_{5,3}$$
$$\beta_{5,4}=\frac{1}{30}x^2\alpha_{1,2}^3+\frac{1}{180}x\alpha_{1,1}\alpha_{1,2}^3-\frac{1}{3}x\alpha_{1,2}\alpha_{3,2}+\alpha_{5,4}$$
$$\beta_{5,5}=\frac{1}{90}x^2\alpha_{1,2}^3-\frac{1}{360}x\alpha_{1,1}\alpha_{1,2}^3-\frac{1}{6}x\alpha_{1,2}\alpha_{3,2}-y\alpha_{4,3}+\alpha_{5,5}$$
$$\beta_{5,6}=-\frac{1}{360}x\alpha_{1,2}^4+\alpha_{5,6}$$

En el caso de $y=0$ se obtienen las fórmulas recursivas para una iteración simétrica del tipo: $e^D=e^{xA}e^Ce^{xA}$.

Recursión simétrico–conjugada con B Si $C\in\mathcal{L}(A,B)$, con e^C un operador asociado a un integrador simétrico–conjugado, entonces:

$$C=\sum_i^{\infty}\left(\sum_j^{n(2i-1)}\alpha_{2i-1,j}N_{2i-1,j}+i\sum_j^{n(2i)}\alpha_{2i,j}N_{2i,j}\right).$$

El producto por la izquierda por e^{zB} y por la derecha por $e^{\bar{z}B}$ dará un nuevo operador e^D, asociado a otro integrador simétrico–conjugado:

$$e^D=e^{zB}e^Ce^{\bar{z}B},,\qquad z=x+iy\in\mathbb{C},$$

donde D tendrá la forma

$$D=\sum_i^{\infty}\left(\sum_j^{n(2i-1)}\beta_{2i-1,j}N_{2i-1,j}+i\sum_j^{n(2i)}\beta_{2i,j}N_{2i,j}\right)$$

con $\beta_{i,j}=f(x,\boldsymbol{\alpha})$:

$$\beta_{1,1}=\alpha_{1,1}$$
$$\beta_{1,2}=2x+\alpha_{1,2}$$
$$\beta_{2,1}=-y\alpha_{1,1}+\alpha_{2,1}$$
$$\beta_{3,1}=\frac{1}{6}x\alpha_{1,1}^2+\alpha_{3,1}$$
$$\beta_{3,2}=\frac{1}{6}x^2\alpha_{1,1}+\frac{1}{6}x\alpha_{1,1}\alpha_{1,2}+\frac{1}{2}y^2\alpha_{1,1}-y\alpha_{2,1}+\alpha_{3,2}$$
$$\beta_{4,1}=\alpha_{4,1}$$

$$\beta_{4,2} = \frac{1}{6}xy\alpha_{1,1}^2 - \frac{1}{6}x\alpha_{1,1}\alpha_{2,1} + y\alpha_{3,1} + \alpha_{4,2}$$

$$\beta_{4,3} = -\frac{1}{6}x^2y\alpha_{1,1} + \frac{1}{6}x^2\alpha_{2,1} - \frac{1}{6}xy\alpha_{1,1}\alpha_{1,2} + \frac{1}{6}x\alpha_{1,2}\alpha_{2,1} - \frac{1}{6}y^3\alpha_{1,1} + \frac{1}{2}y^2\alpha_{2,1} - y\alpha_{3,2} + \alpha_{4,3}$$

$$\beta_{5,1} = -\frac{1}{360}x\alpha_{1,1}^4 + \alpha_{5,1}$$

$$\beta_{5,2} = \frac{1}{90}x^2\alpha_{1,1}^3 - \frac{1}{360}x\alpha_{1,1}^3\alpha_{1,2} + \frac{1}{6}x\alpha_{1,1}\alpha_{3,1} - y\alpha_{4,1} + \alpha_{5,2}$$

$$\beta_{5,3} = \frac{1}{30}x^2\alpha_{1,1}^3 + \frac{1}{180}x\alpha_{1,1}^3\alpha_{1,2} + \frac{1}{3}x\alpha_{1,1}\alpha_{3,1} + \alpha_{5,3}$$

$$\beta_{5,4} = -\frac{1}{60}x^3\alpha_{1,1}^2 - \frac{1}{90}x^2\alpha_{1,1}^2\alpha_{1,2} - \frac{1}{6}x^2\alpha_{3,1} - \frac{1}{12}xy^2\alpha_{1,1}^2 + \frac{1}{6}xy\alpha_{1,1}\alpha_{2,1} - \frac{1}{180}x\alpha_{1,1}^2\alpha_{1,2}^2 + \frac{1}{6}x\alpha_{1,1}\alpha_{3,2} - \frac{1}{6}x\alpha_{1,2}\alpha_{3,1} - \frac{1}{6}x\alpha_{2,1}^2 - \frac{1}{2}y^2\alpha_{3,1} - y\alpha_{4,2} + \alpha_{5,4}$$

$$\beta_{5,5} = \frac{1}{45}x^3\alpha_{1,1}^2 + \frac{1}{30}x^2\alpha_{1,1}^2\alpha_{1,2} + \frac{1}{360}x\alpha_{1,1}^2\alpha_{1,2}^2 + \frac{1}{3}x\alpha_{1,1}\alpha_{3,2} - \frac{1}{6}x\alpha_{2,1}^2 + \alpha_{5,5}$$

$$\beta_{5,6} = \frac{7}{360}x^4\alpha_{1,1} + \frac{7}{180}x^3\alpha_{1,1}\alpha_{1,2} + \frac{1}{12}x^2y^2\alpha_{1,1} - \frac{1}{6}x^2y\alpha_{2,1} + \frac{1}{45}x^2\alpha_{1,1}\alpha_{1,2}^2 + \frac{1}{6}x^2\alpha_{3,2} + \frac{1}{12}xy^2\alpha_{1,1}\alpha_{1,2} - \frac{1}{6}xy\alpha_{1,2}\alpha_{2,1} + \frac{1}{360}x\alpha_{1,1}\alpha_{1,2}^3 + \frac{1}{6}x\alpha_{1,2}\alpha_{3,2} + \frac{1}{24}y^4\alpha_{1,1} - \frac{1}{6}y^3\alpha_{2,1} + \frac{1}{2}y^2\alpha_{3,2} - y\alpha_{4,3} + \alpha_{5,6}$$

En el caso de $y = 0$ se obtienen las fórmulas recursivas para una iteración simétrica del tipo: $e^D = e^{xB}e^Ce^{xB}$.

Apéndice C

Consentimientos de los coautores

Castellón,
09/02/2022

I, Fernando Casas Pérez, hereby authorise Alejandro Escorihuela-Tomàs to include the publications listed below in his doctoral thesis. In addition, I waive the right to use those articles as part of any other doctoral thesis.

List of articles:

- Composition methods for dynamical systems separable into three parts.
- Runge-Kutta-Nyström symplectic splitting methods of order 8.
- Compositions of pseudo-symmetric integrators with complex coefficients for the numerical integration of differential equations.
- High order integrators obtained by linear combinations of symmetric-conjugate compositions.
- On symmetric-conjugate composition methods in the numerical integration of differential equations.
- Applying splitting methods with complex coefficients to the numerical integration of unitary problems.

Signed,

Firmado por CASAS PEREZ FERNANDO - 22690077W el día 10/02/2022 con un certificado emitido por AC FNMT Usuarios

UNIVERSITAT JAUME I
Escola de Doctorat · ED

València, 07,
February, 2022

I, Sergio Blanes Zamora, hereby authorise Alejandro Escorihuela-Tomàs to include the publications listed below in his/her doctoral thesis. In addition, I waive the right to use those articles as part of any other doctoral thesis.

List of articles:

- Runge-Kutta-Nyström symplectic splitting methods of order 8.
- On symmetric-conjugate composition methods in the numerical integration of differential equations.
- Applying splitting methods with complex coefficients to the numerical integration of unitary problems.

Signed,

SERGIO| BLANES| ZAMORA

Firmado digitalmente por SERGIO|BLANES|ZAMORA
Fecha: 2022.02.07 09:05:36 +01'00'

In accordance with article 28 of the Regulations on doctoral studies of the Universitat Jaume I in Castelló*, regulated by RD 99/2011, at the Universitat Jaume I (*Approved by the Governing Council at its meeting no. 8/2020 held on 2 October 2020*):*
"(...)
4. In the case of joint publications, all the co-authors must explicitly state their approval that the doctoral student presented the work as part of her/his thesis and the express waiver of presenting this same work as part of another doctoral thesis. This authorisation must be attached as documentation when the evaluation of the thesis begins."

P. Chartier
Senior researcher
INRIA Rennes Bretagne Atlantique
Ravel Technologies, Paris

Paris, 10^{th} June, 2022

I, Dr. Philippe Chartier, hereby authorise Alejandro Escorihuela-Tomàs to include the publications listed below in his/her doctoral thesis. In addition, I waive the right to use those articles as part of any other doctoral thesis.

List of articles :

- Compositions of pseudo-symmetric integrators with complex coefficients for the numerical integration of differential equations.
- On symmetric-conjugate composition methods in the numerical integration of differential equations.

Yours sincerely,

Philippe Chartier

UNIVERSITAT JAUME I
Escola de Doctorat · ED

Tian Jin, 07,
February, 2022

I, Yong Zhang , hereby authorise Alejandro Escorihuela-Tomàs to include the publications listed below in his/her doctoral thesis. In addition, I waive the right to use those articles as part of any other doctoral thesis.

List of articles:

- Compositions of pseudo-symmetric integrators with complex coefficients for the numerical integration of differential equations.

Signed, Yong Zhang

In accordance with article 28 of the Regulations on doctoral studies of the Universitat Jaume I in Castelló, *regulated by RD 99/2011, at the Universitat Jaume I* (Approved by the Governing Council at its meeting no. 8/2020 held on 2 October 2020*):*
"(...)
4. In the case of joint publications, all the co-authors must explicitly state their approval that the doctoral student presented the work as part of her/his thesis and the express waiver of presenting this same work as part of another doctoral thesis. This authorisation must be attached as documentation when the evaluation of the thesis begins."

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