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New high order symplectic integrators via generating functions with its application in many-body problem

Xiongbiao Tu[1,2] · **Ander Murua**[3] · **Yifa Tang**[1,2]

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Abstract
A new family of high order one-step symplectic integration schemes for separable Hamiltonian systems with Hamiltonians of the form $T(p)+U(q)$ is presented. The new integration methods are defined in terms of an explicitly defined generating function (of the third kind). They are implicit in q (but explicit in p and the internal states), and require the evaluation of the gradients of $T(p)$ and $U(q)$ and the actions of their Hessians on vectors (the later being relatively cheap in the case of many-body problems). A time-symmetric symplectic method is constructed that has order 10 when applied to Hamiltonian systems with quadratic kinetic energy $T(p)$. It is shown by numerical experiments that the new methods have the expected order of convergence.

Keywords High order · Separable Hamiltonian · Quadratic

Mathematics Subject Classification 65L05

✉ Xiongbiao Tu
tuxb@lsec.cc.ac.cn

Ander Murua
Ander.Murua@ehu.es

Yifa Tang
tyf@lsec.cc.ac.cn

1 LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China

2 School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China

3 Konputazio Zientziak eta A. A. Saila, Informatika Fakultatea, UPV/EHU, E-20018 Donostia–San Sebastián, Spain

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1 Introduction

An outstanding property of Hamiltonian systems is the symplecticity and time-symmetry of the flow. The Hamiltonian system in the variables $y = (p, q)$ given in the form

$$\begin{array}{l} \dot{p} = -H_q(p,q) \\ \dot{q} = \quad H_p(p,q) \end{array} \quad \text{or equivalently} \quad \dot{y} = J^{-1}\nabla H(y), \tag{1.1}$$

where $J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$, $p, q \in \mathbb{R}^n$. For the purpose of numerical study, it is natural to look for those discretization systems which preserve as many as possible the characteristic properties and inner symmetries of original continuous systems. Thus, for the Hamiltonian system (1.1), it is natural to search for numerical methods that share symplecticity and time-symmetry.

An important qualitative feature of symplectic integrators is highlighted by the backward error analysis based on modified equations (see [11], Section IX.3 and [18], Section 10.1). If a p order numerical integrator is symplectic when applied to the Hamiltonian system (1.1), then the modified equation is also Hamiltonian [2,22]. The modified Hamiltonian takes the form

$$H_h(y) = H(y) + h^p H_{p+1}(y) + O(h^{p+1}), \tag{1.2}$$

which implies, (under the assumption that the numerical solutions of (1.1) evolve on compact domains), that the symplectic integrator preserves the error of the invariant of Hamiltonian function globally bounded, which convergent to 0 with order p.

Here we focus on symplectic one-step integration schemes that, given a Hamiltonian function $H(y)$, determine a one-parameter family of symplectic maps $\Psi_h : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ such that, for small enough h, $\Psi_h(y(t)) \approx y(t+h)$ for any solution $y(t)$ of the Hamiltonian system (1.1). For linear multi-step methods, the underlying step-transition operator is non-symplectic [23]. Generalizations of the concept of symplecticity for linear multi-step methods are possible [12]. However, the higher dimensionallity of the phase space of the discrete dynamical system typically produce espureus behavior of the numerical solutions.

We are particularly interested in Hamiltonian systems where the kinetic energy is quadratic, that is, with Hamiltonians of the form

$$H(p,q) = \frac{1}{2}p^\top M^{-1} p + U(q), \tag{1.3}$$

where M is an invertible symmetric matrix. Such Hamiltonian systems has a wide range of applications in the fields of celestial mechanics [5,20] and molecular dynamics [3]. Hamiltonians of the form (1.3) fit into the more general format of separable Hamiltonians

$$H(p,q) = T(p) + U(q). \tag{1.4}$$

It is well known [4,9,11,14] that there exist explicit symplectic integrators for Hamiltonian systems with Hamiltonian of the form (1.4). We present a new class of symplectic integration schemes for Hamiltonian systems with Hamiltonian of the form (1.4), and show that it is possible to construct time-symmetric high order symplectic methods for systems with Hamiltonians of the form (1.3) that might outperform existing explicit symplectic methods. While such integrations schemes are not fully explicit, they are defined in terms of an explicitly defined generating function, and can be very efficiently implemented.

A mature theory of generating function has been developed [6,7] (see also [11,18]) that allows one to conveniently construct symplectic integration schemes. Given the matrices $A_\alpha, B_\alpha, C_\alpha, D_\alpha \in \mathbb{R}^{2n\times 2n}$,

$$\alpha = \begin{pmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{pmatrix}, \quad J_{4n} = \begin{pmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{pmatrix}, \quad \tilde{J}_{4n} = \begin{pmatrix} J_{2n} & 0 \\ 0 & -J_{2n} \end{pmatrix}, \tag{1.5}$$

such that $\alpha^\top J_{4n}\alpha = \mu \tilde{J}_{4n}$, $\mu \neq 0$. Consider the formulation

$$A_\alpha \Phi(z) + B_\alpha z = f(C_\alpha \Phi(z) + D_\alpha z), \tag{1.6}$$

where Φ, f are smooth maps from $\mathbb{R}^{2n}$ to $\mathbb{R}^{2n}$, $|C_\alpha \frac{\partial \Phi(z)}{\partial z} + D_\alpha| \neq 0$. Then, Φ is symplectic map if and only if f is gradient map, that is, there exists a function S from $\mathbb{R}^{2n}$ to $\mathbb{R}$ such that $f(w) = \nabla S(w)$. This argument can be immediately derived from the following expression

$$\alpha \begin{pmatrix} \frac{\partial \Phi(z)}{\partial z} \\ I_{2n} \end{pmatrix} = \begin{pmatrix} \frac{\partial f(w)}{\partial w} \\ I_{2n} \end{pmatrix} \frac{\partial w}{\partial z}. \tag{1.7}$$

The t-flow Φ_t of a Hamiltonian system (1.1) is a family of symplectic near-identity maps (for small enough $|t|$), which means Φ_t can be obtained in the formula (1.6) by a generating function $S(w,t)$. Here, $S(w,t)$ is the solution of the Hamilton-Jacobi equation

$$\frac{\partial}{\partial t} S(w,t) = -\mu H(A^\alpha \nabla S(w,t) + B^\alpha w), \tag{1.8}$$

where $(A^\alpha \ B^\alpha)$ is the first row of the blockwise partitioned matrix α^{-1}.

In [16], a family of symplectic integrators for the general Hamiltonian system (1.1) is introduced by considering the generating function (sometimes referred to as Poincare's generating function) corresponding to the choice of $A_\alpha = J_{2n}, B_\alpha = -J_{2n}$, $C_\alpha = D_\alpha = \frac{1}{2} I_{2n}$. one step $y \mapsto \Psi_h(y)$ of the symplectic integrator is defined as

$$\Psi_h(y) = y + J^{-1}\nabla S\left(\frac{1}{2}(y + \Psi_h(y)), h\right), \tag{1.9}$$

with a generating function defined as

$$S(z,h) = h\sum_{i=1}^{s} \alpha_i H(z + h\beta_{i1} J^{-1}\nabla H(z)). \tag{1.10}$$

They determine values of the parameters α_i and β_{i1} that give rise to a fourth order method. In [13], 6th order methods are obtained by generalizing (1.10) as

$$S(z,h) = h\sum_{i=1}^{s} b_i H(Y_i) + \frac{h^2}{2}\sum_{i,j=1}^{s} \beta_{ij}\nabla H(Y_i)^\top J^{-1}\nabla H(Y_j), \tag{1.11}$$

where for $i = 1, ..., s$,

$$Y_i = z + hJ^{-1}\sum_{j=1}^{i-1} \alpha_{ij}\nabla H(Y_j). \tag{1.12}$$

Constructing methods of higher order than 6 was found very difficult due to the lack of appropriate simplifying assumptions for explicitly defined Poincare's generating functions (1.11).

We try to circumvent this problem by considering a different kind of generating function (referred to as generating functions of third kind), corresponding to the choice

$$A_\alpha = -B_\alpha = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}, C_\alpha = \begin{pmatrix} 0 & 0 \\ 0 & I_n \end{pmatrix}, D_\alpha = \begin{pmatrix} I_n & 0 \\ 0 & 0 \end{pmatrix}. \tag{1.13}$$

We thus consider one-step symplectic integrators $(p, q) \mapsto (P, Q) = \Psi_h(p, q)$ defined in terms of a generating function $S(x, y, h)$ as follows

$$\begin{cases} P = p - \frac{\partial S}{\partial Q}(p, Q, h), \\ Q = q + \frac{\partial S}{\partial p}(p, Q, h). \end{cases} \tag{1.14}$$

The actual definition of the generating functions $S(x, y, h)$ of the family of one-step symplectic integrators that we propose for Hamiltonian systems with Hamiltonian of the form (1.4), is given in Sect. 2. Such generating functions are inspired (are a generalization of), the generating functions of third kind corresponding to symplectic partitioned Runge–Kutta methods. Indeed, one step $(p, q) \mapsto (P, Q) = \Psi_h(p, q)$ of a symplectic partitioned Runge–Kutta method for a separable system (1.4) can be expressed [11,18] as (1.14) with $S(x, y, h)$ given by

$$S(x,y,h) = h\sum_{i=1}^{s} \left(b_i U(Q_i) + \hat{b}_i T(P_i)\right) + h^2 \sum_{i,j=1}^{s} \hat{b}_j \alpha_{ji} U_q(Q_i)^\top T_p(P_j), \tag{1.15}$$

where for $i = 1, \ldots, s$,

$$\begin{cases} P_i = x - h \sum_{j=1}^{s} \alpha_{ij} U_q(Q_j), \\ Q_i = y + h \sum_{j=1}^{s} \widehat{\alpha}_{ij} T_p(P_j), \end{cases} \tag{1.16}$$

where the parameters $b_i, \hat{b}_i, \alpha_{ij}$ and $\widehat{\alpha}_{ij}$ are such that $b_i \widehat{\alpha}_{ij} + \hat{b}_j \alpha_{ji} = 0$ for all i, j.

Compared to symplectic partitioned Runge–Kutta methods, which only require the evaluation of the gradient of the Hamiltonian function, our new methods require in addition the evaluation of the Hessian matrix times a vector. We stress that the later is relatively cheap compared to the evaluation of the gradient in the case of many-body problems.

Also, while there are explicit symplectic partitioned Runge–Kutta methods, our methods are implicit in Q. (The generating function is explicitly defined.) Compared to explicit symplectic methods with a given number s of stages, our methods have far more available parameters that can be used to construct more efficient methods.

Compared to fully implicit Runge–Kutta methods, our methods are only implicit in the approximation Q at the time-grid points (but not in the internal stages), which admits very good starting guesses obtained by interpolating from the data of previous steps.

The plan of the paper is as follows. The definition of the methods is given in Sect. 2.1. An efficient formulation in terms of the gradients and Hessians of $T(p)$ and $U(q)$ is given in Sect. 2.2. In Sect. 2.3, we formulate our integrators for non-necessarily Hamiltonian autonomous ODEs of the form

$$\dot{p} = f(q), \qquad \dot{q} = g(p). \tag{1.17}$$

The order conditions of the proposed integrators for systems of the form (1.17) is characterized in terms of bi-coloured trees in Sect. 2.4. In Sect. 2.5, we characterize the order conditions of time-symmetric methods obtained by composing Ψ_h with its adjoint. In Sect. 3, we focus on the particular case of separable Hamiltonian systems with Hamiltonian of the form (1.3), and present some simplifying assumptions which effectively reduce the number of independent order conditions. We use our simplified order conditions to construct a time-symmetric 10th order symplectic method by utilizing a explicit defined generating function with $s = 5$. In Sect. 4, we show the order of convergence and the numerical behavior of the proposed 10th order method in two particular Hamiltonian problems. Finally, we summarize some concluding remarks in Sect. 5.

2 The new family of symplectic methods

2.1 Definition of the family of symplectic integrators

Given a positive integer s and real numbers $b_i, \hat{b}_i (1 \leq i \leq s)$, $\alpha_{ij}, \widehat{\alpha}_{ij}$ and $\beta_{ij} (1 \leq i, j \leq s)$, one step $(p, q) \mapsto (P, Q) = \Psi_h(p, q)$ of the method is implicitly defined

by (1.14), where the generating function $S(x, y, h)$ is defined as

$$S(x, y, h) = h \sum_{i=1}^{s} \left(b_i U(Q_i) + \hat{b}_i T(P_i) \right) + h^2 \sum_{i,j=1}^{s} \beta_{ij} U_q(Q_i)^\top T_p(P_j), \tag{2.1}$$

where for $i = 1, \ldots, s$,

$$\begin{cases} P_i = x - h \sum\limits_{j=1}^{s} \alpha_{ij} U_q(Q_j), \\ Q_i = y + h \sum\limits_{j=1}^{s} \widehat{\alpha}_{ij} T_p(P_j). \end{cases} \tag{2.2}$$

In practice, we will focus on the case where $S(x, y, h)$ is given as an explicit function of x, y and h. Such case can be achieved when the matrices (α_{ij}), $(\widehat{\alpha}_{ij})$ in (2.2) are, one strictly lower triangular, and the other one lower triangular.

2.2 Efficient formulation in terms of the gradients and Hessians of $T(p)$ and $U(q)$

In order to implement the integration scheme (1.14) with the generating function defined by (2.1) and (2.2), $\frac{\partial S(x,y,h)}{\partial x}$ and $\frac{\partial S(x,y,h)}{\partial y}$ need to be computed. Let us denote, for $i = 1, \ldots, s$,

$$k_i = h U_q(Q_i), \qquad l_i = h T_p(P_i).$$

We thus obtain for the differentials of $P_i, Q_i, k_i, l_i, i = 1, \ldots, s$,

$$\begin{cases} \dfrac{\partial P_i}{\partial x} = I - \sum\limits_{j=1}^{s} \alpha_{ij} \dfrac{\partial k_j}{\partial x}, & \dfrac{\partial k_i}{\partial x} = h \nabla_q^2 U(Q_i) \dfrac{\partial Q_i}{\partial x}, \\ \dfrac{\partial Q_i}{\partial x} = \sum\limits_{j=1}^{s} \widehat{\alpha}_{ij} \dfrac{\partial l_j}{\partial x}, & \dfrac{\partial l_i}{\partial x} = h \nabla_p^2 T(P_i) \dfrac{\partial P_i}{\partial x}. \end{cases} \tag{2.3}$$

$$\begin{cases} \dfrac{\partial P_i}{\partial y} = - \sum\limits_{j=1}^{s} \alpha_{ij} \dfrac{\partial k_j}{\partial y}, & \dfrac{\partial k_i}{\partial y} = h \nabla_q^2 U(Q_i) \dfrac{\partial Q_i}{\partial y}, \\ \dfrac{\partial Q_i}{\partial y} = I + \sum\limits_{j=1}^{s} \widehat{\alpha}_{ij} \dfrac{\partial l_j}{\partial y}, & \dfrac{\partial l_i}{\partial y} = h \nabla_p^2 T(P_i) \dfrac{\partial P_i}{\partial y}. \end{cases} \tag{2.4}$$

Applying the technique of reverse differentiation as in [13], we have that

$$\begin{cases} \dfrac{\partial S(x,\,y,\,h)}{\partial x} = \displaystyle\sum_{i=1}^{s} \big(\hat{b}_i l_i + h\nabla_p^2 T(P_i)u_i\big), \\ \dfrac{\partial S(x,\,y,\,h)}{\partial y} = \displaystyle\sum_{i=1}^{s} \big(b_i k_i + h\nabla_q^2 U(Q_i)v_i\big), \end{cases} \tag{2.5}$$

where, for $i = 1, \ldots, s$,

$$\begin{cases} u_i = \displaystyle\sum_{j=1}^{s} \big((\beta_{ji} + b_j\widehat{\alpha}_{ji})k_j + \widehat{\alpha}_{ji}h\nabla_q^2 U(Q_j)v_j\big), \\ v_i = \displaystyle\sum_{j=1}^{s} \big((\beta_{ij} - \hat{b}_j\alpha_{ji})l_j - \alpha_{ji}h\nabla_p^2 T(P_j)u_j\big). \end{cases} \tag{2.6}$$

2.3 Formulation for autonomous partitioned ODEs

Hamiltonian ODE systems (1.1) with Hamiltonian of the form (1.3) fit into the separable ODE format (1.17) where $f(q) = -U_q(q)$ and $g(p) = T_p(p)$.

We thus have that

$$\begin{cases} -\dfrac{\partial S(p,\,Q,\,h)}{\partial Q} = h\displaystyle\sum_{i=1}^{s} \big(b_i f(Q_i) + f'(Q_i)v_i\big), \\ \dfrac{\partial S(p,\,Q,\,h)}{\partial p} = h\displaystyle\sum_{i=1}^{s} \big(\hat{b}_i g(P_i) + g'(P_i)u_i\big), \end{cases} \tag{2.7}$$

where $f(Q_i) = -U_q(Q_i)$, $g(P_i) = T_p(P_i)$, $f'(Q_i) = -\nabla_q^2 U(Q_i)$, $g'(P_i) = \nabla_p^2 T(P_i)$.

Hence, one step of the method

$$(p, q) \mapsto (P,\, Q) = \Psi_h(p, q) \tag{2.8}$$

can be expressed as

$$\begin{cases} P = p + h\displaystyle\sum_{i=1}^{s} \big(b_i f(Q_i) + f'(Q_i)v_i\big), \\ Q = q + h\displaystyle\sum_{i=1}^{s} \big(\hat{b}_i g(P_i) + g'(P_i)u_i\big), \end{cases} \tag{2.9}$$

where $P_i,\ Q_i,\ u_i,\ v_i\ (i = 1, \ldots, s)$ are defined by

$$\begin{cases} P_i = p + h \sum_{j=1}^{s} \alpha_{ij} f(Q_j), \\ Q_i = Q + h \sum_{j=1}^{s} \widehat{\alpha}_{ij} g(P_j), \end{cases} \tag{2.10}$$

$$\begin{cases} u_i = h \sum_{j=1}^{s} \left(\widehat{\gamma}_{ij} f(Q_j) - \widehat{\alpha}_{ji} f'(Q_j) v_j \right), \\ v_i = h \sum_{j=1}^{s} \left(\gamma_{ij} g(P_j) - \alpha_{ji} g'(P_j) u_j \right), \end{cases} \tag{2.11}$$

and $\gamma_{ij} = \beta_{ij} - \hat{b}_j \alpha_{ji},\ \widehat{\gamma}_{ij} = -\beta_{ji} - b_j \widehat{\alpha}_{ji},\ i, j = 1, 2, \ldots, s$. Observe that P_i, Q_i, u_i, v_i $(i = 1, \ldots, s)$ are explicitly defined when the matrices (α_{ij}), $(\widehat{\alpha}_{ij})$ are lower triangular and one of them strictly triangular.

Actually, (2.9)–(2.11) defines one step $(p, q) \mapsto (P, Q) = \Psi_h(p, q)$ of an integrator for autonomous (non-necessarily Hamiltonian) separable partitioned ODEs of the form (1.17).

It is worth mentioning that in the particular case where

$$b_i \widehat{\alpha}_{ij} + \hat{b}_j \alpha_{ji} = 0, \quad \beta_{ij} = \hat{b}_j \alpha_{ji}, \quad i, j = 1, \ldots, s, \tag{2.12}$$

the scheme (2.8)–(2.11) is just a symplectic partitioned Runge–Kutta scheme. Indeed, (2.12) implies that $\gamma_{ij} = \widehat{\gamma}_{ij} = 0$, for all i, j, hence $u_i = v_i = 0,\ i = 1, \ldots, s$.

2.4 P-series expansions

In order to obtain order conditions of the method (2.8)–(2.11) applied to the system of autonomous ODEs (1.17), we need to expand $(P, Q) = \Psi_h(p, q)$ as a series in powers of h and compare it with the series in powers of h of the exact h-flow of the system (1.17). This can be achieved by using series indexed by bi-coloured rooted trees as in [11] or in [17]. It is known that, because of the special structure of autonomous ODEs (1.17), the terms in a P-series corresponding to bi-coloured rooted trees having two adjacent vertices of the same colour vanish. Thus, only terms corresponding to the set ST of bi-coloured rooted trees (with, say, black and white vertices) having no edge joining two vertices with the same color need to be considered.

The formulas and statements that follow in the present subsection can be obtained from the results given in [17].

Given a bi-coloured rooted tree $\tau \in ST$, we denote by $|\tau|$ its number of vertices. In what follows, the term bi-coloured rooted tree will refer to elements $\tau \in ST$.

The series expansion in powers of h of the exact h-flow Φ_h and the expansion of one step of the numerical method given by (2.8)–(2.11) are characterized by two

coefficient maps

$$\phi : ST \to \mathbb{R}, \quad \psi : ST \to \mathbb{R}.$$

The numerical method is of order (at least) r if $\psi(\tau) = \phi(\tau)$ for each $\tau \in ST$ with $|\tau| \leq r$.

We denote by $\bullet$ (resp. $\circ$) the bi-coloured rooted tree consisting of a black (resp. white) root, with no additional vertices. Each bi-coloured rooted tree τ with $|\tau| \geq 2$ whose root is black (resp. white) can be represented as $\tau = [\tau_1 \cdots \tau_m]_\bullet$ (resp. $\tau = [\tau_1 \cdots \tau_m]_\circ$) where $\tau_1, \ldots, \tau_m \in ST$ are the bi-coloured rooted trees obtained by removing the root of τ.

The coefficient map $\phi : ST \to \mathbb{R}$ characterizing the h-flow Φ_h is given by $\phi(\tau) = 1/\gamma(\tau)$, where $\gamma : ST \to \mathbb{Z}^+$ is recursively defined by $\gamma(\bullet) = \gamma(\circ) = 1$ and

$$\gamma(\tau) = |\tau|\, \gamma(\tau_1) \cdots \gamma(\tau_m)$$

if $\tau = [\tau_1 \cdots \tau_m]_\bullet$ or $\tau = [\tau_1 \cdots \tau_m]_\circ$.

As for the coefficient map $\psi : ST \to \mathbb{R}$ characterizing one step of the numerical method given by (2.8)–(2.11), it can be obtained, together with the coefficient maps $\eta_i, \boldsymbol{\zeta}_i$ $(i = 1, \ldots, s)$ of (P_i, Q_i) and (u_i, v_i) in (2.9)–(2.11) respectively, as follows:

– For bi-coloured rooted trees with one vertex,

$$\begin{aligned}
&\psi(\bullet) = \sum_{i=1}^{s} b_i, \quad \psi(\circ) = \sum_{i=1}^{s} \hat{b}_i, \\
&\eta_i(\bullet) = \sum_{j=1}^{s} \alpha_{ij}, \quad \eta_i(\circ) = \psi(\circ) + \sum_{j=1}^{s} \widehat{\alpha}_{ij}, \\
&\bar{\zeta}_i(\bullet) = \sum_{j=1}^{s} \widehat{\gamma}_{ij}, \quad \bar{\zeta}_i(\circ) = \sum_{j=1}^{s} \gamma_{ij},
\end{aligned} \tag{2.13}$$

– for each $\tau = [\tau_1 \cdots \tau_m]_\bullet$,

$$\begin{aligned}
\psi(\tau) &= \sum_{i=1}^{s} b_i\, \eta_i(\tau_1) \cdots \eta_i(\tau_m) \\
&\quad + \sum_{i=1}^{s} \sum_{k=1}^{m} \eta_i(\tau_1) \cdots \eta_i(\tau_{k-1}) \bar{\zeta}_i(\tau_k) \eta_i(\tau_{k+1}) \cdots \eta_i(\tau_m), \\
\eta_i(\tau) &= \sum_{j=1}^{s} \alpha_{ij}\, \eta_j(\tau_1) \cdots \eta_j(\tau_m), \\
\bar{\zeta}_i(\tau) &= \sum_{j=1}^{s} \widehat{\gamma}_{ij}\, \eta_j(\tau_1) \cdots \eta_j(\tau_m) \\
&\quad - \sum_{j=1}^{s} \widehat{\alpha}_{ji} \sum_{k=1}^{m} \eta_j(\tau_1) \cdots \eta_j(\tau_{k-1}) \bar{\zeta}_j(\tau_k) \eta_j(\tau_{k+1}) \cdots \eta_j(\tau_m),
\end{aligned} \tag{2.14}$$

Table 1 Bi-coloured rooted trees representing free bi-coloured trees with ≤ 5 vertices

τ	•						
τ	∘						
$\gamma(\tau)$	1	2	3	4	20	10	5

– for each $\tau = [\tau_1 \cdots \tau_m]_\circ$,

$$
\begin{aligned}
\psi(\tau) &= \sum_{i=1}^{s} \hat{b}_i \, \eta_i(\tau_1) \cdots \eta_i(\tau_m) \\
&\quad + \sum_{i=1}^{s} \sum_{k=1}^{m} \eta_i(\tau_1) \cdots \eta_i(\tau_{k-1}) \bar{\zeta}_i(\tau_k) \eta_i(\tau_{k+1}) \cdots \eta_i(\tau_m), \\
\eta_i(\tau) &= \psi(\tau) + \sum_{j=1}^{s} \widehat{\alpha}_{ij} \, \eta_j(\tau_1) \cdots \eta_j(\tau_m), \\
\bar{\zeta}_i(\tau) &= \sum_{j=1}^{s} \gamma_{ij} \, \eta_j(\tau_1) \cdots \eta_j(\tau_m) \\
&\quad - \sum_{j=1}^{s} \alpha_{ji} \sum_{k=1}^{m} \eta_j(\tau_1) \cdots \eta_j(\tau_{k-1}) \bar{\zeta}_j(\tau_k) \eta_j(\tau_{k+1}) \cdots \eta_j(\tau_m).
\end{aligned}
\tag{2.15}
$$

In addition, the symplecticity of numerical methods acts as a simplifying assumption on the order conditions. This is first noticed in [19] for the study of a class of symplectic RK methods. As the class of methods we are considering is by construction symplectic, their corresponding coefficient map $\psi : ST \to \mathbb{R}$ will satisfy the symplecticity conditions [1,11], which induce an equivalence relation $\sim$ in ST.

Two bi-coloured rooted trees are equivalent if they only differ in the location of the root, that is, if they have the same underlying free bi-coloured tree (obtained from the bi-coloured rooted tree by forgetting the location of its root).

We will adopt the definition of canonical representatives of the equivalence classes given in [17]. Let $\widetilde{ST} \subset ST$ be a set of canonical representatives of the equivalence classes of bi-coloured trees. For example, in Table 1, there is only one free bi-coloured tree for two vertices in $\widetilde{ST}$. Hence, the numerical method Ψ_h is of order p if

$$
\psi(\tau) = \frac{1}{\gamma(\tau)} \tag{2.16}
$$

for all $\tau \in \widetilde{ST}$ with $|\tau| \leq p$.

2.5 Order conditions of time-symmetric methods obtained by composing Ψ_h with its adjoint

The methods in such family of integration schemes are not time-symmetric, due to the inherent asymmetry of the definition of one step of the method from its generating functions of third time together with the explicit nature of the proposed generating functions. We thus propose constructing time-symmetric methods by composing a method of the form (2.8)–(2.11) with its adjoint.

For a given integrator Ψ_h, its adjoint [11,18] integrator is defined as $\Psi_h^* = \Psi_{-h}^{-1}$. That is, $(p, q) \mapsto (P, Q) = \Psi_h^*(p, q)$ is such that

$$(p, q) = \Psi_{-h}(P, Q).$$

In the case where $(P, Q) = \Psi_h(p, q)$ is defined as (2.9)–(2.11), $(P^*, Q^*) = \Psi_h^*(p, q)$ is given as

$$\begin{cases} P^* = p + h \sum_{i=1}^{s} \big(b_i f(Q_i) + f'(Q_i)v_i\big), \\ Q^* = q + h \sum_{i=1}^{s} \big(\hat{b}_i g(P_i) + g'(P_i)u_i\big), \end{cases} \tag{2.17}$$

where $P_i,\ Q_i,\ u_i,\ v_i\ (i = 1, 2, \ldots, s)$ are defined by

$$\begin{cases} P_i = P^* - h \sum_{j=1}^{s} \alpha_{ij} f(Q_j), \\ Q_i = q - h \sum_{j=1}^{s} \widehat{\alpha}_{ij} g(P_j), \end{cases} \tag{2.18}$$

$$\begin{cases} u_i = -h \sum_{j=1}^{s} \big(\widehat{\gamma}_{ij} f(Q_j) - \widehat{\alpha}_{ji} f'(Q_j)v_j\big), \\ v_i = -h \sum_{j=1}^{s} \big(\gamma_{ij} g(P_j) - \alpha_{ji} g'(P_j)u_j\big). \end{cases} \tag{2.19}$$

We next give a characterization of the order of the time-symmetric method

$$(p, q) \mapsto (P, Q) = \Psi_{h/2}^* \circ \Psi_{h/2}(p, q), \tag{2.20}$$

together with the order of Ψ_h, in terms of the series expansion in powers of h of $\Psi_h \circ \Phi_{-h}$. Observe that, since in our case both Ψ_h and Φ_h admit a P-series expansion indexed by bi-coloured rooted trees in ST, and the composition of P-series is again a P-series [10], $\Psi_h \circ \Phi_{-h}$ can also be expanded as a P-series.

Theorem 2.1 *Let $\bar{\psi} : ST \to \mathbb{R}$ be the coefficient map corresponding to the P-series expansion of $\Psi_h \circ \Phi_{-h}$, and let r be an even number and $r' \leq r$. The symplectic integrator Ψ_h is order at least r' if*

$$\bar{\psi}(\tau) = 0 \tag{2.21}$$

for all $\tau \in \widetilde{ST}$ with $|\tau| \leq r'$. If in addition (2.21) holds for all $\tau \in \widetilde{ST}$ with odd $|\tau| < r$, then the time-symmetric symplectic method (2.20) is of order at least r.

Proof The integrator Ψ_h is of order r' if $\Psi_h = \Phi_h + \mathcal{O}(h^{r'+1})$ which is equivalent to $\Psi_h \circ \Phi_{-h} = I_{id} + \mathcal{O}(h^{r'+1})$, where I_{id} is identity map. Hence, Ψ_h is of order r' if (2.21) holds for all $\tau \in ST$ with $|\tau| \leq r'$. Since $\Psi_h \circ \Phi_{-h}$ is symplectic, then it is enough to restrict to bi-coloured rooted trees in the set $\widetilde{ST}$ of canonical representatives.

The method (2.20) is of order r if $\Psi_h^* \circ \Psi_h = \Phi_{2h} + \mathcal{O}(h^{r+1})$ which is equivalent (since $\Phi_{2h} = \Phi_h \circ \Phi_h$ and $\Phi_h^{-1} = \Phi_{-h}$) to

$$\Psi_h \circ \Phi_{-h} - \Psi_{-h} \circ \Phi_h = \mathcal{O}(h^{r+1}). \tag{2.22}$$

The terms in the left-hand side of (2.22) corresponding to even powers of h identically vanish. Similarly, the terms corresponding to odd powers of h in the series expansions of $\Psi_h \circ \Phi_{-h}$ and $-\Psi_{-h} \circ \Phi_h$ coincide. Since $\bar{\psi} : ST \to \mathbb{R}$ are the coefficient map corresponding to the P-series expansion of $\Psi_h \circ \Phi_{-h}$, the time-symmetric method (2.20) is of order at least r if $\bar{\psi}(\tau) = 0$ for all $\tau \in ST$ with odd $|\tau| < r$. Again, it is enough to consider only bi-coloured rooted trees in the set $\widetilde{ST}$ of canonical representatives. Indeed, by symplecticity of $\Psi_h \circ \Phi_{-h}$, if $\tau, \tau' \in ST$ are two equivalent bi-coloured rooted trees with their roots located in adjacent vertices of their corresponding free bi-coloured tree, then $\bar{\psi}(\tau) + \bar{\psi}(\tau') = \bar{\psi}(\tau_1)\bar{\psi}(\tau_2)$ where τ_1 and τ_2 are the bi-coloured rooted trees obtained from that free bi-coloured tree by removing the edge connecting the vertices where the roots of τ and τ' are located respectively. If $|\tau| = |\tau'|$ is odd, then either $|\tau_1|$ or $|\tau_2|$ is odd as well. This allows us to prove by induction on r that, if (2.21) holds for all $\tau \in \widetilde{ST}$ with odd $|\tau| < r$, then (2.21) holds for all $\tau \in ST$ with odd $|\tau| < r$. □

The required P-series coefficients $\bar{\psi}(\tau)$ of $\Psi_h \circ \Phi_{-h}$ can be obtained from the P-series coefficient maps $\psi, \phi : ST \to \mathbb{R}$ by using the known formulas for the composition of P-series [10,17]. Alternatively, they can be obtained similarly to the coefficients $\psi(\tau)$ in previous subsection as follows:

– For bi-coloured rooted trees with one vertex,

$$\begin{aligned}
\bar{\psi}(\bullet) &= -1 + \sum_{i=1}^{s} b_i, \quad \bar{\psi}(\circ) = -1 + \sum_{i=1}^{s} \hat{b}_i, \\
\bar{\eta}_i(\bullet) &= -1 + \sum_{j=1}^{s} \alpha_{ij}, \quad \bar{\eta}_i(\circ) = \bar{\psi}(\circ) + \sum_{j=1}^{s} \widehat{\alpha}_{ij}, \\
\bar{\bar{\zeta}}_i(\bullet) &= \sum_{j=1}^{s} \widehat{\gamma}_{ij}, \quad \bar{\bar{\zeta}}_i(\circ) = \sum_{j=1}^{s} \gamma_{ij},
\end{aligned} \tag{2.23}$$

– for each $\tau = [\tau_1 \cdots \tau_m]_\bullet$,

$$\begin{aligned}
\bar{\psi}(\tau) &= \frac{(-1)^{|\tau|}}{\gamma(\tau)} + \sum_{i=1}^{s} b_i\, \bar{\eta}_i(\tau_1)\cdots\bar{\eta}_i(\tau_m) \\
&\quad + \sum_{i=1}^{s}\sum_{k=1}^{m} \bar{\eta}_i(\tau_1)\cdots\bar{\eta}_i(\tau_{k-1})\bar{\bar{\xi}}_i(\tau_k)\bar{\eta}_i(\tau_{k+1})\cdots\bar{\eta}_i(\tau_m), \\
\bar{\eta}_i(\tau) &= \frac{(-1)^{|\tau|}}{\gamma(\tau)} + \sum_{j=1}^{s} \alpha_{ij}\, \bar{\eta}_j(\tau_1)\cdots\bar{\eta}_j(\tau_m), \\
\bar{\bar{\xi}}_i(\tau) &= \sum_{j=1}^{s} \widehat{\gamma}_{ij}\, \bar{\eta}_j(\tau_1)\cdots\bar{\eta}_j(\tau_m) \\
&\quad - \sum_{j=1}^{s} \widehat{\alpha}_{ji} \sum_{k=1}^{m} \bar{\eta}_j(\tau_1)\cdots\bar{\eta}_j(\tau_{k-1})\bar{\bar{\xi}}_j(\tau_k)\bar{\eta}_j(\tau_{k+1})\cdots\bar{\eta}_j(\tau_m),
\end{aligned} \tag{2.24}$$

– for each $\tau = [\tau_1 \cdots \tau_m]_\circ$,

$$\begin{aligned}
\bar{\psi}(\tau) &= \frac{(-1)^{|\tau|}}{\gamma(\tau)} + \sum_{i=1}^{s} \hat{b}_i\, \bar{\eta}_i(\tau_1)\cdots\bar{\eta}_i(\tau_m) \\
&\quad + \sum_{i=1}^{s}\sum_{k=1}^{m} \bar{\eta}_i(\tau_1)\cdots\bar{\eta}_i(\tau_{k-1})\bar{\bar{\xi}}_i(\tau_k)\bar{\eta}_i(\tau_{k+1})\cdots\bar{\eta}_i(\tau_m), \\
\bar{\eta}_i(\tau) &= \bar{\psi}(\tau) + \sum_{j=1}^{s} \widehat{\alpha}_{ij}\, \bar{\eta}_j(\tau_1)\cdots\bar{\eta}_j(\tau_m), \\
\bar{\bar{\xi}}_i(\tau) &= \sum_{j=1}^{s} \gamma_{ij}\, \bar{\eta}_j(\tau_1)\cdots\bar{\eta}_j(\tau_m) \\
&\quad - \sum_{j=1}^{s} \alpha_{ji} \sum_{k=1}^{m} \bar{\eta}_j(\tau_1)\cdots\bar{\eta}_j(\tau_{k-1})\bar{\bar{\xi}}_j(\tau_k)\bar{\eta}_j(\tau_{k+1})\cdots\bar{\eta}_j(\tau_m).
\end{aligned} \tag{2.25}$$

Bi-coloured rooted trees $\tau \in \widetilde{ST}$ with odd $|\tau| \le 5$ are displayed in Table 1. In Tables 2 and 3, bi-coloured rooted trees $\tau \in \widetilde{ST}$ with $|\tau| = 7$ are displayed.

Table 2 Bi-coloured rooted trees representing free bi-coloured trees with 7 vertices

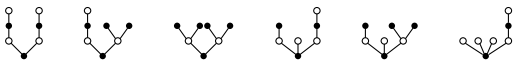
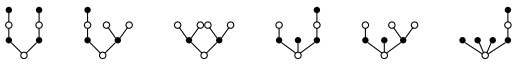
τ	
τ	
$\gamma(\tau)$	252	126	63	84	42	42

Table 3 Bi-coloured rooted trees representing free bi-coloured trees with 7 vertices

τ	
τ	
$\gamma(\tau)$	21 56 28 14 7

3 Methods for Hamiltonians with quadratic kinetic energy

We now consider the particular Hamiltonian systems where the kinetic energy is quadratic, that is, with Hamiltonians of the form

$$H(p,q) = \frac{1}{2}\, p^{\top} M^{-1} p + U(q), \tag{3.1}$$

where M is a invertible symmetric matrix.

In that case, the terms in the P-series expansion of Ψ_h, Φ_h, and $\Psi_h \circ \Phi_{-h}$ corresponding to the bi-coloured rooted trees having a white vertex with more than two edges vanish. So the order conditions corresponding to such trees need not be considered. Our goal is to construct a time-symmetric method that is of order 10 for systems with Hamiltonians of the form (3.1). We next consider some simplifying assumptions with the aim of further reducing the number of independent order conditions required to attain order 10.

3.1 Simplifying assumptions

We will consider schemes (2.8)–(2.11) such that their corresponding P-series coefficient maps η_i, $\bar{\zeta}_i$ $(i = 1, \ldots, s)$ satisfy the following

$$\eta_i(\,\overset{\bullet}{\circ}\,) = \frac{1}{2}\eta_i(\circ)^2 \quad \text{and} \quad \bar{\zeta}_i(\,\overset{\bullet}{\circ}\,) = \eta_i(\circ)\bar{\zeta}_i(\circ). \tag{3.2}$$

By assuming that the integrator (2.8)–(2.11) is at least of second order, so that $\psi(\circ) = 1$ and $\psi(\,\overset{\bullet}{\circ}\,) = \frac{1}{2}$, such simplifying assumptions read

$$\frac{1}{2} + \sum_{j=1}^{s} \widehat{\alpha}_{ij}\, c_j = \frac{\hat{c}_i^2}{2}, \quad \sum_{j=1}^{s} (\gamma_{ij}\, c_j - \alpha_{ji}\, d_j) = \hat{c}_i\, \hat{d}_i, \tag{3.3}$$

for $i = 1, \ldots, s$, where

$$c_i = \sum_{j=1}^{s} \alpha_{ij}, \quad \hat{c}_i = 1 + \sum_{j=1}^{s} \widehat{\alpha}_{ij}, \quad d_i = \sum_{j=1}^{s} \widehat{\gamma}_{ij}, \quad \hat{d}_i = \sum_{j=1}^{s} \gamma_{ij}. \tag{3.4}$$

Next proposition shows the effect of the simplifying assumptions (3.2) on the coefficient maps $\psi, \eta_i, \bar{\zeta}_i$ (resp. $\bar{\psi}, \bar{\eta}_i, \bar{\bar{\zeta}}_i$) of the scheme given in (2.13)–(2.15) [resp. (2.23)–(2.25)].

Proposition 3.1 *If $\tau, \tau' \in ST$ are such that τ' can be obtained from τ by replacing a subtree* $\curlywedge$ *whose root is joined (by and edge of τ) to a given vertex of τ, by two white vertices joined to the same vertex, then $\phi(\tau') = 2\phi(\tau)$. If (3.2) holds, then $\psi(\tau') = 2\psi(\tau)$ and $\bar{\psi}(\tau') = 2\bar{\psi}(\tau)$ for $i = 1, \ldots, s$, $\eta_i(\tau') = 2\eta_i(\tau)$, $\bar{\zeta}_i(\tau') = 2\bar{\zeta}_i(\tau)$, $\bar{\eta}_i(\tau') = 2\bar{\eta}_i(\tau)$, $\bar{\bar{\zeta}}_i(\tau') = 2\bar{\bar{\zeta}}_i(\tau)$.*

Proof The result for the P-series coefficients $\phi(\tau) = 1/\gamma(\tau)$ of the h-flow is standard. The result for $\psi, \eta_i, \bar{\zeta}_i$ (resp. $\bar{\psi}, \bar{\eta}_i, \bar{\bar{\zeta}}_i$) follows trivially from (2.13)–(2.15) [resp. (2.23)–(2.25)] in the case where the subtree $\curlywedge$ that is transformed in two white vertices is joined to the root of τ. The cases where that subtree is joined to a vertex that is from a topological distance of k vertices from the root are proven by induction on k. □

Proposition 3.1 clearly implies that, under the assumption that (3.2) holds, then the order condition of any bi-coloured rooted tree that is equivalent (in the sense of having the same underlying free bi-coloured rooted tree) to a bi-coloured rooted tree having one or more subtrees of the form $\curlywedge$ need not be considered.

3.2 Order conditions for a time-symmetric method of order 10

Our goal is to construct a time-symmetric symplectic scheme

$$(p, q) \mapsto (P, Q) = \Psi^*_{h/2} \circ \Psi_{h/2}(p, q), \tag{3.5}$$

(with Ψ_h determined by (2.8)–(2.11)), that is of order 10 when applied to Hamiltonian systems with Hamiltonian of the form (3.1). Recall that time-symmetry (in addition to being a property of the flow of the system that is convenient to preserve by the numerical integrator) helps to reduce the number of independent order conditions that are required to attain a given order. In addition, we will require that Ψ_h itself is of order 5.

The characterization of the order conditions given in Theorem 2.1 in terms of the coefficients $\bar{\psi}(\tau)$ (and the auxiliary ones $\bar{\eta}_i$ and $\bar{\bar{\zeta}}_i$, $i = 1, \ldots, s$) determined by (2.23)–(2.25) is still valid, but now fewer bi-coloured rooted trees (of odd number of vertices) need to be considered:

- Since we aim at applying our integrators to Hamiltonian systems with Hamiltonian of the form (3.1), the order conditions corresponding to bi-coloured rooted trees having a white vertex with more than two edges need not be considered. For example, in Table 1, the fourth tree in the second row is missing.
- In addition, the map $(P, Q) = \Psi_h(p, q)$ given by (2.9)–(2.11) will be chosen so that the simplifying assumptions (3.3)–(3.4) hold true, and thus Proposition 3.1 can be applied. This implies that the order conditions of bi-coloured rooted trees

Table 4 Relevant bi-coloured rooted trees with 9 vertices

k	1	2	3	4	5
$\tau_{9,k}$					
$\gamma(\tau_{9,k})$	1296	5184	864	144	648
k	6	7	8	9	
$\tau_{9,k}$					
$\gamma(\tau_{9,k})$	108	324	54	9	

(that are equivalent to some bi-coloured rooted trees) having one or more subtrees of the form need not be considered.

For instance, an arbitrary time-symmetric method (3.5), with Ψ_h determined by (2.8)–(2.11) not necessarily satisfying our simplifying assumptions (3.2), will be of order 8 for arbitrary Hamiltonian systems with separable Hamiltonian, if (2.21) holds for the 32 bi-coloured rooted trees $\tau \in \widetilde{ST}$ with odd $|\tau| \leq 7$ (Tables 1, 2, 3). Under the assumptions (3.2), only 11 trees need to be considered for systems with Hamiltonians of the form (3.1). As for order 10, there are 94 bi-coloured free trees with 9 vertices, but only 9 of them are additionally required for Hamiltonians of the form (3.1), provided that the simplifying assumptions hold. Their canonical representatives are displayed in Table 4.

Summing up, given a symplectic method (2.8)–(2.11) satisfying the simplifying assumptions (3.2), our time-symmetric method (3.5) will be of order 10 while Ψ_h being of order 5 if

$$\bar{\psi}(\tau) = 0 \tag{3.6}$$

holds for the 20 surviving bi-coloured rooted trees τ with 1, 2, 3, 4, 5, 7, and 9 vertices. More precisely,

$$\bar{\psi}(\bullet) = -1 + \sum_{i=1}^{s} b_i,$$

$$\bar{\psi}(\circ) = -1 + \sum_{i=1}^{s} \hat{b}_i,$$

$$\bar{\psi}(\,\overset{\circ}{\bullet}\,) = \frac{1}{2} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\circ) + \bar{\zeta}_i(\circ)\big),$$

$$\bar{\psi}(\,\overset{\circ}{\bullet}\!\!\overset{\circ}{\diagdown}) = -\frac{1}{3} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\circ)^2 + 2\bar{\eta}_i(\circ)\bar{\zeta}_i(\circ)\big),$$

$$\bar{\psi}(\,\overset{\circ}{\bullet}\!\!\overset{\circ}{\diagdown}\!\!\overset{\circ}{\diagdown}) = \frac{1}{4} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\circ)^3 + 3\bar{\eta}_i(\circ)^2\bar{\zeta}_i(\circ)\big),$$

$$\bar{\psi}(\tau_{4,1}) = -\frac{1}{20} + \sum_{i=1}^{s} \big(\hat{b}_i \bar{\eta}_i(\tau_{3,1})^2 + 2\bar{\eta}_i(\tau_{3,1})\bar{\zeta}_i(\tau_{3,1})\big),$$

$$\bar{\psi}(\tau_{5,1}) = -\frac{1}{5} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\circ)^4 + 4\bar{\eta}_i(\circ)^3 \bar{\zeta}_i(\circ)\big),$$

$$\bar{\psi}(\tau_{5,2}) = -\frac{1}{252} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\tau_{4,2})^2 + 2\bar{\eta}_i(\tau_{4,2})\bar{\zeta}_i(\tau_{4,2})\big),$$

$$\bar{\psi}(\tau_{5,3}) = -\frac{1}{63} + \sum_{i=1}^{s} \big(\hat{b}_i \bar{\eta}_i(\tau_{4,3})^2 + 2\bar{\eta}_i(\tau_{4,3})\bar{\zeta}_i(\tau_{4,3})\big),$$

$$\begin{aligned}\bar{\psi}(\tau_{5,4}) = -\frac{1}{42} + \sum_{i=1}^{s} \big(&b_i \bar{\eta}_i(\circ)^3 \bar{\eta}_i(\tau_{4,2}) + \bar{\eta}_i(\circ)^3 \bar{\zeta}_i(\tau_{4,2}) \\ &+3\bar{\eta}_i(\circ)^2 \bar{\eta}_i(\tau_{4,2})\bar{\zeta}_i(\circ)\big),\end{aligned}$$

$$\bar{\psi}(\tau_{6,1}) = -\frac{1}{7} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\circ)^6 + 6\bar{\eta}_i(\circ)^5 \bar{\zeta}_i(\circ)\big),$$

$$\bar{\psi}(\tau_{9,1}) = -\frac{1}{1296} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\tau_{5,1})^2 + 2\bar{\eta}_i(\tau_{5,1})\bar{\zeta}_i(\tau_{5,1})\big),$$

$$\bar{\psi}(\tau_{9,2}) = -\frac{1}{5184} + \sum_{i=1}^{s} \big(\hat{b}_i \bar{\eta}_i(\tau_{5,2})^2 + 2\bar{\eta}_i(\tau_{5,2})\bar{\zeta}_i(\tau_{5,2})\big),$$

$$\begin{aligned}\bar{\psi}(\tau_{9,3}) = -\frac{1}{864} + \sum_{i=1}^{s} \big(&\hat{b}_i \bar{\eta}_i(\tau_{5,2})\bar{\eta}_i(\tau_{4,3}) + \bar{\eta}_i(\tau_{5,2})\bar{\zeta}_i(\tau_{4,3}) \\ &+\bar{\eta}_i(\tau_{4,3})\bar{\zeta}_i(\tau_{5,2})\big),\end{aligned}$$

$$\bar{\psi}(\tau_{9,4}) = -\frac{1}{144} + \sum_{i=1}^{s} \big(\hat{b}_i \bar{\eta}_i(\tau_{4,3})^2 + 2\bar{\eta}_i(\tau_{4,3})\bar{\zeta}_i(\tau_{4,3})\big),$$

$$\begin{aligned}\bar{\psi}(\tau_{9,5}) = -\frac{1}{648} + \sum_{i=1}^{s} \big(&b_i \bar{\eta}_i(\circ)\bar{\eta}_i(\tau_{4,2})\bar{\eta}_i(\tau_{3,1}) + \bar{\eta}_i(\circ)\bar{\eta}_i(\tau_{4,2})\bar{\zeta}_i(\tau_{3,1}) \\ &+\bar{\eta}_i(\circ)\bar{\eta}_i(\tau_{3,1})\bar{\zeta}_i(\tau_{4,2}) + \bar{\eta}_i(\tau_{4,2})\bar{\eta}_i(\tau_{3,1})\bar{\zeta}_i(\circ)\big),\end{aligned}$$

$$\begin{aligned}\bar{\psi}(\tau_{9,6}) = -\frac{1}{108} + \sum_{i=1}^{s} \big(&b_i \bar{\eta}_i(\circ)^4 \bar{\eta}_i(\tau_{3,1}) + \bar{\eta}_i(\circ)^4 \bar{\zeta}_i(\tau_{3,1}) \\ &+4\bar{\eta}_i(\circ)^3 \bar{\eta}_i(\tau_{3,1})\bar{\zeta}_i(\circ)\big),\end{aligned}$$

$$\begin{aligned}\bar{\psi}(\tau_{9,7}) = -\frac{1}{324} + \sum_{i=1}^{s} \big(&b_i \bar{\eta}_i(\circ)^2 \bar{\eta}_i(\tau_{4,2})^2 + 2\bar{\eta}_i(\circ)^2 \bar{\eta}_i(\tau_{4,2})\bar{\zeta}_i(\tau_{4,2}) \\ &+2\bar{\eta}_i(\circ)\bar{\eta}_i(\tau_{4,2})^2 \bar{\zeta}_i(\circ)\big),\end{aligned}$$

$$\bar{\psi}(\tau_{9,8}) = -\frac{1}{54} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\circ)^5 \bar{\eta}_i(\overset{\circ}{\circ}\!\!\bullet) + \bar{\eta}_i(\circ)^5 \bar{\zeta}_i(\overset{\circ}{\circ}\!\!\bullet) + 5\bar{\eta}_i(\circ)^4 \bar{\eta}_i(\overset{\circ}{\circ}\!\!\bullet) \bar{\zeta}_i(\circ) \big),$$

$$\bar{\psi}(\tau_{9,9}) = -\frac{1}{9} + \sum_{i=1}^{s} \big(b_i \bar{\eta}_i(\circ)^8 + 8\bar{\eta}_i(\circ)^7 \bar{\zeta}_i(\circ) \big),$$

where $\tau_{9,k}$ are displayed in Table 4, and for each $i = 1, \ldots, s$,

$$\bar{\eta}_i(\bullet) = -1 + \sum_{j=1}^{s} \alpha_{ij},$$

$$\bar{\eta}_i(\circ) = \bar{\psi}(\circ) + \sum_{j=1}^{s} \widehat{\alpha}_{ij},$$

$$\bar{\eta}_i(\overset{\circ}{\bullet}\!\!\diagup) = \frac{1}{2} + \sum_{j=1}^{s} \alpha_{ij} \bar{\eta}_j(\circ),$$

$$\bar{\eta}_i(\overset{\circ}{\circ}\!\!\bullet) = \bar{\psi}(\overset{\circ}{\circ}\!\!\bullet) + \sum_{j=1}^{s} \widehat{\alpha}_{ij} \bar{\eta}_j(\overset{\circ}{\bullet}\!\!\diagup),$$

$$\bar{\eta}_i(\overset{\circ}{\diagdown}\!\!\overset{\circ}{\diagup}) = -\frac{1}{3} + \sum_{j=1}^{s} \alpha_{ij} \bar{\eta}_j(\circ)^2,$$

$$\bar{\eta}_i(\overset{\circ}{\bullet}\!\!\overset{\circ}{\circ}) = \bar{\psi}(\overset{\circ}{\bullet}\!\!\overset{\circ}{\circ}) + \sum_{j=1}^{s} \widehat{\alpha}_{ij} \bar{\eta}_j(\overset{\circ}{\diagdown}\!\!\overset{\circ}{\diagup}),$$

$$\bar{\eta}_i(\overset{\circ}{\bullet}\!\!\overset{\circ}{\circ}\!\!\diagup) = \frac{1}{24} + \sum_{j=1}^{s} \alpha_{ij} \bar{\eta}_j(\overset{\circ}{\circ}\!\!\bullet),$$

$$\bar{\eta}_i(\overset{\circ}{\diagdown}\!\!\overset{\circ}{\diagup}\!\!\overset{\circ}{\diagup}) = \frac{1}{4} + \sum_{j=1}^{s} \alpha_{ij} \bar{\eta}_j(\circ)^3,$$

$$\bar{\zeta}_i(\bullet) = \sum_{j=1}^{s} \widehat{\gamma}_{ij},$$

$$\bar{\zeta}_i(\circ) = \sum_{j=1}^{s} \gamma_{ij},$$

$$\bar{\zeta}_i(\overset{\circ}{\bullet}\!\!\diagup) = \sum_{j=1}^{s} \big(\widehat{\gamma}_{ij} \bar{\eta}_j(\circ) - \widehat{\alpha}_{ji} \bar{\zeta}_j(\circ) \big),$$

$$\bar{\zeta}_i(\overset{\circ}{\circ}\!\!\bullet) = \sum_{j=1}^{s} \big(\gamma_{ij} \bar{\eta}_j(\overset{\circ}{\bullet}\!\!\diagup) - \alpha_{ji} \bar{\zeta}_j(\overset{\circ}{\bullet}\!\!\diagup) \big),$$

$$\bar{\zeta}_i(\circ\!\!\curlyvee\!\!\circ) = \sum_{j=1}^{s} \big(\widehat{\gamma}_{ij}\bar{\eta}_j(\circ)^2 - 2\widehat{\alpha}_{ji}\bar{\eta}_j(\circ)\bar{\zeta}_j(\circ)\big),$$

$$\bar{\zeta}_i(\curlyvee) = \sum_{j=1}^{s} \big(\gamma_{ij}\bar{\eta}_j(\circ\!\!\curlyvee\!\!\circ) - \alpha_{ji}\bar{\zeta}_j(\circ\!\!\curlyvee\!\!\circ)\big),$$

$$\bar{\zeta}_i(\circ\!\!\curlyvee\!\!\circ) = \sum_{j=1}^{s} \big(\widehat{\gamma}_{ij}\bar{\eta}_j(\circ\!\!\curlyvee) - \widehat{\alpha}_{ji}\bar{\zeta}_j(\circ\!\!\curlyvee)\big),$$

$$\bar{\zeta}_i(\circ\!\!\curlyvee\!\!\curlyvee\!\!\circ) = \sum_{j=1}^{s} \big(\widehat{\gamma}_{ij}\bar{\eta}_j(\circ)^3 - 3\widehat{\alpha}_{ji}\bar{\eta}_j(\circ)^2\bar{\zeta}_j(\circ)\big).$$

3.3 Construction of a time-symmetric 10th order method with underlying 5th order method

With the aim to show that 10th order methods exist, we fix $s = 5$, choose two vectors $(c_1, \ldots, c_s)$ and $(\hat{c}_1, \ldots, \hat{c}_s)$,

Since we want the underlying scheme (2.8)–(2.11) to be implicit only on Q, we require $(\widehat{\alpha}_{ij})$ to be a strictly lower triangular matrix, and (α_{ij}) lower triangular. We thus have $2(s^2 + s)$ parameters $((b_i), (\widehat{b}_i), (\alpha_{ij}), (\widehat{\alpha}_{ij}), (\beta_{ij}))$ to be determined for a method with s stages. As we aim at determining an underlying method (2.8)–(2.11) satisfying the simplifying assumptions (3.3)–(3.4), which is of order 5, and such that the time-symmetric composition (3.5) is of order 10. We thus have $20+2s$ constraints.

Hence, for $s = 4$, we have 4 more parameters than equations. However we have not been able to find any solution of that system of polynomial equations. We thus fix $s = 5$, and proceed as follows. We choose at random an strictly lower triangular matrix $(\widehat{\alpha}_{ij})$ and a lower triangular matrix (α_{ij}) such that the first equality in (3.3) (with c_i and $\hat{c}_i$ given in (3.4)) holds. Then, the 20 order conditions and the s simplifying assumptions in the right-hand equality in (3.3) are linear in the parameters of the method that are not determined so far, that is, the entries of the $s \times s$ matrix (β_{ij}) and the two vectors $(b_1, \ldots, b_s)$ and $(\hat{b}_1, \ldots, \hat{b}_s)$. Actually, we have an underdetermined system of 25 linear equations with $s^2 + 2s$ unknowns. We compute (by means of Penrose's pseudo-inverse) the solution that minimizes the entries of (b_i), $(\widehat{b}_i)$, (β_{ij}) in the least squares sense. We repeatedly apply that process until a solution with reasonably small values of the parameters is obtained. We finally use that solution as a starting guess of a local minimization algorithm to minimize in the least squares sense the entries of (b_i), $(\widehat{b}_i)$, (α_{ij}), $(\widehat{\alpha}_{ij})$, (β_{ij}) subject to our $20 + 2s$ constraints. A solution obtained this way is shown next. (The entries of (b_i), $(\widehat{b}_i)$, (β_{ij}) are given as rational approximations that are accurate to 30 decimal digits.)

$$b = \left(\tfrac{79528452594427}{386833405960979}, \tfrac{179619393320206}{717409375724581}, \tfrac{309681925308569}{1457507220827293}, \tfrac{184104799644601}{1265839638241819}, \tfrac{243774183543697}{1309734794251835}\right),$$

$$\hat{b} = \left(\tfrac{134982025613281}{856310414670211}, \tfrac{109103259075824}{465584013540749}, \tfrac{98570501656192}{544519467509031}, \tfrac{233403115094213}{946365272264325}, \tfrac{203587841462900}{1128676441563873}\right),$$

$$\alpha = \begin{bmatrix} \frac{789}{1114} & 0 & 0 & 0 & 0 \\ -\frac{88}{729} & \frac{157343}{198288} & 0 & 0 & 0 \\ \frac{4}{241} & \frac{9}{148} & -\frac{126827}{918451} & 0 & 0 \\ \frac{11}{252} & -\frac{35}{271} & \frac{142}{353} & -\frac{569861659}{5375877948} & 0 \\ -\frac{2}{317} & \frac{4}{295} & -\frac{9}{257} & \frac{101}{837} & \frac{1075768155334}{13538012904855} \end{bmatrix},$$

$$\widehat{\alpha} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ -\frac{325}{557} & 0 & 0 & 0 & 0 \\ -\frac{115901117}{129086325} & \frac{46777472}{129086325} & 0 & 0 & 0 \\ -\frac{105}{404} & -\frac{90472501705}{195368240717} & -\frac{96250749591}{781472962868} & 0 & 0 \\ -\frac{65}{1083} & -\frac{17}{368} & -\frac{1142528784789967}{12733222902177600} & \frac{2052082132758907}{12733222902177600} & 0 \end{bmatrix},$$

$$\beta = \begin{bmatrix} \frac{10846865048720}{154621659615453} & \frac{200092830817094}{1041215810642403} & -\frac{9075135198727}{955800339152999} & -\frac{112731853571272}{1711667121556705} & -\frac{22282103883473}{875662058306578} \\ \frac{497761452818450}{2124356303065639} & -\frac{547570929196952}{3565057102686285} & -\frac{10824793235937}{1712088519188863} & \frac{110265031898277}{868975611673961} & -\frac{4329638758393}{463468420400887} \\ \frac{19753390670156}{1045118056635089} & \frac{91519141738531}{646606242893693} & \frac{238213366737873}{2045376887929309} & -\frac{208672069835317}{711918285271484} & \frac{22318397231703}{726005457849671} \\ \frac{39146818853558}{993278772571567} & -\frac{32117007460523}{681170618194107} & -\frac{19248244465552}{639378376498825} & \frac{159678125697655}{1207908196468101} & -\frac{76915371229387}{611530411975323} \\ -\frac{8060156497242}{445547130616549} & -\frac{396145793969596}{3774913235893365} & \frac{72235313246467}{898704158675425} & -\frac{54898005606614}{2162876624381563} & -\frac{18534289090223}{491074839296518} \end{bmatrix}.$$

4 The numerical experiments

In this section, we check (for a two-body problem, and for an 9-body problem representing to the solar system) that the time-symmetric symplectic method presented in Sect. 3.3 actually exhibits over 10th order behaviour.

In the case of Hamiltonians of the form $H(p,q) = \frac{1}{2}p^\top p + U(q)$, we obtain the following simple form of symplectic integrator $(p,q) \mapsto (P,Q) = \Psi_h(p,q)$

$$\begin{cases} P = p + h\sum_{i=1}^{s}\big(b_i f(Q_i) + v_i\big), \\ Q = q + hp + h^2\sum_{i=1}^{s}\big(\hat{d}_i f(Q_i) - \hat{c}_i v_i\big), \\ Q_i = Q + h\hat{c}_i p + h^2\sum_{j=1}^{s} a_{ij} f(Q_j), \\ v_i = f'(Q_i)\big[h\, cr_i\ p + h^2\sum_{j=1}^{s}\big(\eta_{ij} f(Q_j) + a_{ji} v_j\big)\big], \end{cases}$$

where $\hat{d}_i = \sum_{j=1}^{s}(\widehat{\gamma}_{ji} + \hat{b}_j\alpha_{ji})$, $\hat{c}_i = \sum_{j=1}^{s}\widehat{\alpha}_{ij}$, $cr_i = \sum_{j=1}^{s}\gamma_{ij}$, $\eta_{ij} = \sum_{k=1}^{s}(\gamma_{ik}\alpha_{kj} - \alpha_{ki}\widehat{\gamma}_{kj})$, $a_{ij} = \sum_{k=1}^{s}\widehat{\alpha}_{ik}\alpha_{kj}$, and (a_{ij}) is a strictly lower triangular matrix.

Observe that Q_i, v_i $(i = 1, \ldots, s)$ and P are explicitly defined as functions of h, p, q, and Q, so that Q is implicitly defined with an equation of the form

$$Q = q + hp + h^2 G(p, q, Q, h). \tag{4.1}$$

Equation (4.1) can be solved for small enough step-sizes h by simple fixed-point iteration. Similarly, the adjoint Ψ_h^* of Ψ_h is implicit only on P, which can be computed by fixed point iteration for small enough step-sizes h.

We compare our method (that we denote as Ψ^{10}) with the 10th order Gauss–Runge–Kutta method Ψ^{grk} (the 5-stage implicit Runge–Kutta with Gauss-Legendre collocation nodes) and a 10th order explicit symplectic integrator Ψ^{ss} (obtained from Stormer–Verlet as basic integrator by applying the very efficient composition scheme of 35 stages constructed by Sofroniou and Spaletta [21]).

In our current implementation of the 10th order integrator $\Psi_h^{10} = \Psi_{h/2}^* \circ \Psi_{h/2}$, in the computation of $\Psi_{h/2}$ (resp. $\Psi_{h/2}^*$), we apply fixed point iteration for Q (resp. for P) with starting value obtained as the truncated Taylor expansion of degree 6 for the exact solution. As for the implicit Runge–Kutta method Ψ^{grk}, we apply fixed point iteration adapted for separable problems with starting values computed by extrapolation from the previous step (see [11]).

4.1 The two-body problem

The gravitational two-body problem, can be recast, after eliminating the center of masses and the linear momentum, as a Hamiltonian system with Hamiltonian function

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^1 + q_2^2}}, \tag{4.2}$$

i.e.

$$\begin{cases} \dot{p}_i = -\dfrac{q_i}{(q_1^2 + q_2^2)^{3/2}}, \\ \dot{q}_i = p_i, \end{cases} \qquad i = 1, 2. \tag{4.3}$$

The exact solution of the Kepler problem (4.3) with initial conditions

$$q_1(0) = r_0, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = v_0 \tag{4.4}$$

describes an elliptic orbit with semi-major axis $a = 1/(2/r_0 - v_0^2)$, and eccentricity $e = 1 - r_0/a$ provided that $a > 0$. The exact solution is

$$q_1(t) = \frac{cos(E(t)) - e}{1 - e}\, r_0, \quad q_2(t) = \frac{1 - e}{\omega}\, sin(E(t))\, v_0$$

(with $p_1(t) = q_1'(t)$ and $p_2(t) = q_2'(t)$) where $E(t)$ is the solution of the Kepler equation

$$E(t) - e\, sin(E(t)) = a^{-3/2}\, t. \tag{4.5}$$

Clearly, it is a periodic solution with period $T = 2\pi\, a^{3/2}$.

We have integrated the considered initial value problem (4.3)–(4.4) with $r_0 = 4$ and $v_0 = \sqrt{13/40}$ (in which case one has $a = 40/7$, $e = 3/10$) over a time interval

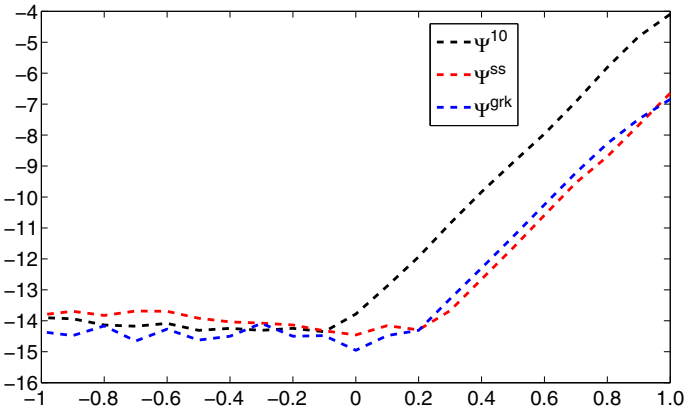


Fig. 1 Maximum energy variation $\mathrm{err}_H(h)$ versus step-size $h = T/n$ in double logarithmic scale

$t \in [0, T]$, with $T = 2\pi\, a^{3/2}$ (i.e., over one period) by applying Ψ^{10}, Ψ^{ss} and Ψ^{grk} with different step-sizes $h = T/n$. We denote the maximum energy variation

$$\mathrm{err}_H(T/n) = \max_{k=1,\ldots,n} \left| \frac{H(p^k, q^k) - H(p^0, q^0)}{H(p^0, q^0)} \right|. \tag{4.6}$$

The maximum variation in energy along the trajectory versus the step-size in double logarithmic scale is displayed in Fig. 1. We also consider the maximum global error in positions (position error, for short)

$$\mathrm{err}_q(T/n) = \max_{k=1,\ldots,n} ||q^n - q(T)||_2. \tag{4.7}$$

The position error versus the step size $h = T/n$ in double logarithmic scale is displayed in Fig. 2. A 10th order behavior can be observed (both in Figs. 1 and 2) for the three integrators.

4.2 The numerical experiment 2

We now consider a simple point mass model of the Solar System: a main massive body (the Sun) and the eight planets orbiting the Sun following almost Keplerian trajectories, which is a Hamiltonian system with Hamiltonian

$$H(p, q) = \frac{1}{2} \sum_{i=0}^{8} \frac{1}{m_i} p_i^\top p_i - G \sum_{i=1}^{8} \sum_{j=0}^{i-1} \frac{m_i m_j}{||q_i - q_j||}, \tag{4.8}$$

where p and q are the supervectors composed by the vectors $p_i, q_i \in \mathbb{R}^3$, $i = 0, 1, \ldots, 8$.

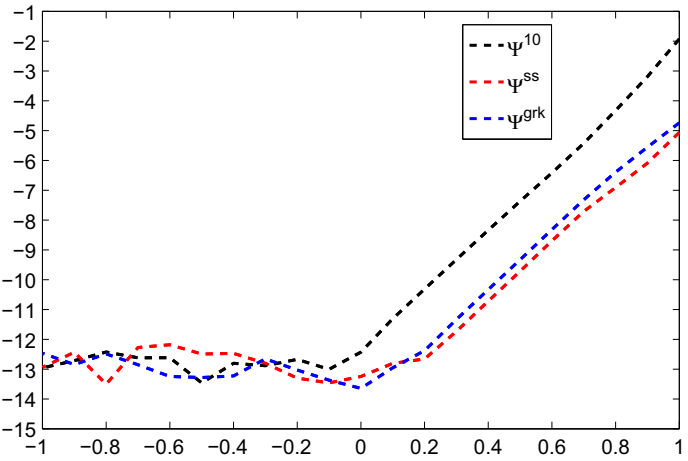


Fig. 2 Position errors $\mathrm{err}_q(h)$ versus step-size $h = T/n$ in double logarithmic scale

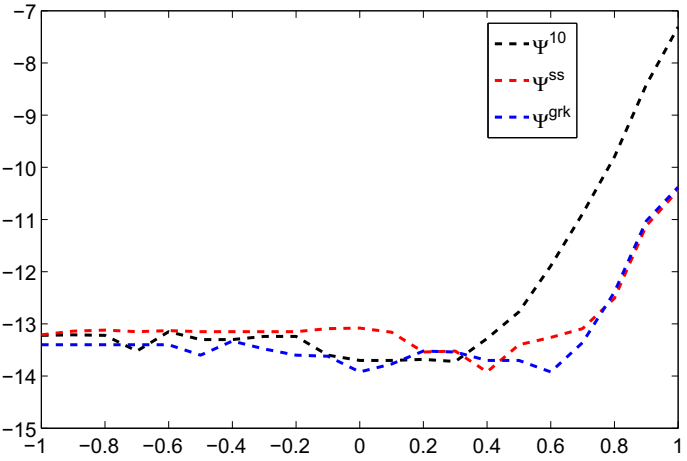


Fig. 3 Maximum energy variation $\mathrm{err}_H(h)$ versus the step-size $h = T/n$ in double logarithmic scale

The distances are in astronomical units (1[A.U.]=149 597870[km]), times in earth days. The initial conditions and mass parameters (see "Appendix A" Table 5) have been taken from INPOP10 [8] (http://www.imcce.fr/inpop/).

We have integrated the initial value problem over a time interval $[0, T]$ with $T = 10^4$ with different step-sizes $h = T/n$. We denote the maximum energy variation by

$$\mathrm{err}_H(T/n) = \max_{k=1,\ldots,n} \left| \frac{H(p^k, q^k) - H(p^0, q^0)}{H(p^0, q^0)} \right|. \tag{4.9}$$

Maximum variation in energy along the trajectory versus the step-size in double logarithmic scale is displayed in Fig. 3. The efficiency diagram of maximum variation in energy along the trajectory versus CPU time is displayed in Fig. 4, the maximum

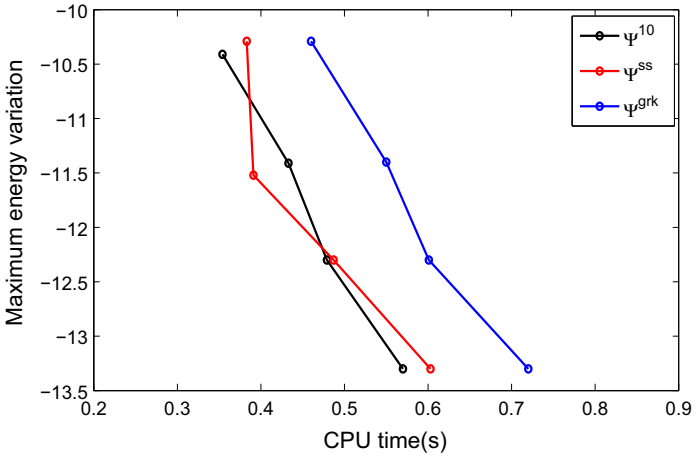


Fig. 4 Maximum energy variation $\mathrm{err}_H(h)$ versus cpu time, the maximum energy variation in logarithmic scale

energy variation in logarithmic scale. We observe in Fig. 4 that our integrator Ψ^{10} is clearly more efficient than Ψ^{grk}. On the other hand, the efficiency of our current implementation of Ψ^{10} is similar to that of the integrator Ψ^{ss} (slightly better for high precision). However, the implementation of the explicit integrator Ψ^{ss} essentially cannot be improved, while there is still room for improvement in the implementation of Ψ^{10}. Actually, we believe that the current implementation of our implicit integrator can be considerably improved, by computing cheap good initial guesses based on the results of the previous step (as it is already done in our implementation of Ψ^{grk}), and by solving the implicit equations required at each step by a Newton-like iteration (instead of by fixed point iteration) that uses some good (and relatively cheap) approximation of the inverse of the required Jacobian matrix in terms of Hessian matrix (by using similar techniques to those proposed in [15], adapted to the mono-implicit structure of our integrators).

5 Concluding remarks

We have presented a new class of one-step symplectic integration schemes for Hamiltonian systems with Hamiltonians of the form $H(p,q) = T(p) + U(q)$. Our new integration methods are constructed in terms of an explicitly defined generating function (of the third kind), which automatically determines a symplectic map. Such family of methods are closely related to the methods introduced in [13,16]. The order conditions of such methods are studied in terms of bi-coloured trees, and some simplifying assumptions are proposed that reduces the number of independent conditions.

In particular, a family of time-symmetric 10th order symplectic integration methods is constructed for the special separable Hamiltonian systems with Hamiltonians of the form $H(p,q) = \frac{1}{2}p^\top M^{-1}p + U(q)$.

Compared to explicit symplectic partitioned Runge–Kutta methods, which only require the evaluation of the gradient of the Hamiltonian function, our new methods require in addition the evaluation of the Hessian matrix times a vector. For many-body problems, one evaluation of the gradient of the potential together with the action of its Hessian on vectors is typically cheaper than two evaluations of the gradient [15].

It must be stressed that, while we have obtained a 10th order method with $s = 5$ stages that locally minimize the size of the method parameters in the least squares sense, a more extensive exploration of the space of parameters should be made, optimizing the methods in a multi-objective sense (taking into account, in addition to the size of the coefficients, for instance, the size of the residuals of the leading local error coefficients). We plan to do this n the near future, together with an optimized careful implementation (along the lines mentioned at the end of previous section) of the application of our integrators to many-body problems.

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Appendix A

Table 5 The initial values of the sun and the eight planets in the Solar System in the rectangular coordinates (x, y, x)

Celestial body	G*mass	Initial position	Initial velocity
Sun	0.2959122083684144D-03	− 0.7136455863204587D-02	0.5378460509916422D-05
		− 0.2647034369379783D-02	− 0.6758188010324566D-05
		− 0.9229892505496660D-03	− 0.3032853127487478D-05
Mercury	0.4912547451450812D-10	− 0.1372300604044608D+00	0.2137177410373583D-01
		− 0.4032407549582179D+00	− 0.4933057845768988D-02
		− 0.2014122961813283D+00	− 0.4850465824782499D-02
Venus	0.7243452486162703D-09	− 0.7254387523043796D+00	0.8034959695360596D-03
		− 0.4892128064383859D-01	− 0.1849859566689047D-01
		0.2371764876743381D-01	− 0.8372768202283038D-02
Earth	0.8997011603631609D-09	− 0.1842952397799571D+00	− 0.1719773059711599D-01
		0.8847598247153874D+00	− 0.2909600200841075D-02
		0.3838137291658033D+00	− 0.1261542481279748D-02
Mars	0.9549535105779258D-10	0.1383579466034955D+01	0.6768779851778725D-03
		− 0.1245817406488680D-02	0.1380727932292873D-01
		− 0.3788315570928926D-01	0.6314867592550115D-02

Table 5 continued

Celestial body	G*mass	Initial position	Initial velocity
Jupiter	0.2825345842083778D-06	0.3994040727569959D+01	−0.4562935030967951D-02
		0.2733931551497335D+01	0.5874704016500655D-02
		0.1074589534370346D+01	0.2629270097583528D-02
Saturn	0.8459715185680659D-07	0.6399272407330191D+01	−0.4286973415229299D-02
		0.6172010777712233D+01	0.3521586379637339D-02
		0.2273847748703642D+01	0.1638898666195764D-02
Uranus	0.1292024916781969D-07	0.1442472013917530D+02	0.2683482937370634D-02
		−0.1250891021661682D+02	0.2455247222284456D-02
		−0.5682605953506514D+01	0.1037377699162441D-02
Neptune	0.1524358900784276D-07	0.1680491152960319D+02	0.2584652661920899D-02
		−0.2298275092881995D+02	0.1661666325918560D-02
		−0.9825343431971598D+01	0.6157837652766749D-03

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