Classification and Development of Symplectic Algorithms: Postprint

Authors: Sun Lang[1,2], Liu Fuyao[1], Wang Ying[1,2], Sun Wei[1,2,3]

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Abstract

Symplectic algorithms, as the optimal integration tool for studying the long-term qualitative evolution of Hamiltonian systems, have received considerable attention since their inception. Through truncation error analysis of the Hamiltonian function, high-precision symplectic algorithms can be constructed from different perspectives, and automatic adjustment of integration step size and improvement of numerical stability can also be achieved by introducing regularization techniques. Based on their formulation, symplectic algorithms can be divided into explicit and implicit types. When a Hamiltonian system can be decomposed into several integrable parts and the solution of each part can be expressed as explicit functions of time, explicit algorithms can be constructed. Explicit algorithms include four types: non-force-gradient explicit symplectic algorithms, force-gradient symplectic algorithms, symplectic correctors, and high-order-like symplectic algorithms. When the variables of a Hamiltonian system cannot be separated, implicit symplectic algorithms and extended phase-space symmetric algorithms are suitable for solving the problem. The construction methods of these algorithms and their applicable physical models are summarized and compared, the advantages and disadvantages of various symplectic algorithms and their development trends are analyzed, providing a theoretical and numerical computational basis for the efficient and accurate selection of symplectic algorithms to solve practical problems.

Full Text

Classification and Development of Symplectic Algorithms

SUN Lang[1;2], LIU Fu-yao[1], WANG Ying[1;2], SUN Wei[1;2;3]

[1]School of Mathematics, Physics and Statistics, Shanghai University of Engineering Science, Shanghai 201620, China

[2]Center of Application and Research of Computational Physics, Shanghai University of Engineering Science, Shanghai 201620, China
[3]School of Resources and Environment, Anqing Normal University, Anqing 246133, China

Abstract

As the optimal integration tool for studying the long-term qualitative evolution of Hamiltonian systems, symplectic algorithms have attracted considerable attention since their inception. By analyzing the truncation errors of Hamiltonian functions, high-precision symplectic algorithms can be constructed from different perspectives, and regularization techniques can be introduced to achieve automatic step-size adjustment and improved numerical stability. Symplectic algorithms can be classified into explicit and implicit forms based on their representation. When a Hamiltonian system can be decomposed into several integrable parts whose solutions can be expressed as explicit functions of time, explicit algorithms can be constructed. These include non-force-gradient explicit symplectic algorithms, force-gradient symplectic algorithms, symplectic corrections, and pseudo-high-order symplectic algorithms. When the variables of a Hamiltonian system cannot be separated, implicit symplectic algorithms and extended phase space symmetric algorithms are appropriate. This paper systematically compares the construction methods and applicable physical models of these algorithms, analyzes their respective advantages and disadvantages, and provides theoretical and numerical foundations for selecting symplectic algorithms to solve practical problems efficiently and accurately.

Keywords: symplectic algorithm; Hamiltonian system; symplectic correction; force-gradient symplectic algorithm; explicit symplectic-like algorithm in extended phase space

1 Introduction

Hamiltonian systems inherently possess invariant symplectic structure in their physical essence. In the early 1980s, Chinese scholar Feng Kang [1] and Ruth [2] independently proposed numerical integration algorithms that preserve the symplectic structure of Hamiltonian phase flow, addressing the problem that traditional algorithms cannot maintain energy conservation in long-term time integration [4]. The former primarily constructed high-order implicit symplectic algorithms based on the implicit midpoint method for non-separable Hamiltonian systems, while the latter established explicit symplectic algorithms for Hamiltonian systems decomposable into kinetic energy T and potential energy V. The distinction between explicit and implicit symplectic algorithms lies in whether iteration is required during the integration process.

Building upon Ruth's T + V form of explicit symplectic algorithms, research and application of high-order symplectic algorithms developed rapidly [5]. When the Hamiltonian can be decomposed into a dominant unperturbed part H_0 and a minor perturbation part H_1, with both parts being integrable [6], accuracy can be improved by elevating the order of the small parameter in the perturbation term H_1. This approach yields pseudo-high-order symplectic integrators (PSI) [7] and Wisdom-Holman-Touma corrections (WHT) [8].

Force-gradient symplectic algorithms [6] embed force-gradient operators into the Lie operators of the algorithm, effectively avoiding the appearance of negative time coefficients. Ruth [2] and Chin [9, 10] constructed third-order and fourth-order force-gradient symplectic algorithms, respectively. Li Rong and Wu Xin [12–14] combined McLachlan's [11] algorithm optimization ideas to construct optimized third-order and fourth-order force-gradient symplectic algorithms. Chen Yunlong and Wu Xin [15] demonstrated the effectiveness of force-gradient symplectic algorithms for solving the circular restricted three-body problem in rotating coordinate systems.

When Hamiltonian system variables cannot be separated, explicit symplectic algorithms generally cannot be applied directly, and implicit symplectic algorithms become suitable. Commonly used implicit symplectic algorithms include semi-implicit symplectic algorithms [16, 17] and the implicit midpoint method [16–23]. While implicit symplectic algorithms are applicable to arbitrary Hamiltonian systems, their computational efficiency is low, making them unsuitable as the preferred numerical method. To enable the application of explicit symplectic algorithms to non-separable Hamiltonian systems, Pihajoki [24] proposed a phase space extension symmetric algorithm by adding a set of variables identical to the original phase space momentum and coordinates in non-separable Hamiltonian systems, though this approach destroys the system's symplectic structure. Tao [25] improved upon Pihajoki's method by dividing the Hamiltonian system into three parts, where the third part consists of a constraint Hamiltonian formed by the squared differences between the two sets of coordinate-momentum variables, thereby preserving the symplectic structure in the extended phase space. Building on this, Liu and Wu [26, 27] constructed continuous coordinate-momentum permutation phase space extension methods suitable for solving non-separable Hamiltonian problems such as post-Newtonian Hamiltonian problems and rotating Hamiltonian problems, though these methods cannot maintain stable energy in rotating compact binary post-Newtonian Hamiltonian systems. Luo et al. [28, 29] proposed midpoint permutation phase space extension methods, which are superior to both Pihajoki's method and Liu Lei et al.'s method as they impose no requirements on the number of operators and have broader applicability. Wu et al. [30] proposed extended phase space optimized Forest-Ruth algorithms that demonstrated significantly improved accuracy compared to non-optimized algorithms in planar circular restricted three-body problems and compact binary problems, showing that midpoint permutation yields better numerical performance for optimized Forest-Ruth algorithms. Li and Wu [31] combined several permutation methods in extended phase space with Mikkola et al.'s [32, 33] work to propose extended phase space logarithmic Hamiltonian explicit symmetric methods. These methods exhibit high precision and efficiency in models such as the circular restricted three-body problem, third-order post-Newtonian spinning compact binary systems, and Ernst-Schwarzschild black holes. Symplectic algorithms have been widely applied to various astronomical physical models. This paper aims to elaborate on the development, construction, and applicable physical models of the aforementioned symplectic and symplectic-like algorithms.

2 Construction of Symplectic Algorithms

For a T + V decomposition form, assume the Hamiltonian can be expressed as:

$$H(p,q) = T(p) + V(q) = \sum_{i=1}^{n} \frac{p_i^2}{2m_i} + V(q_i),$$

where p and q represent generalized momenta and coordinates, respectively. The corresponding canonical equations of motion are:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad (i = 1, 2, 3, \cdots, n).$$

Alternatively, taking $z = (p, q)$, we have:

$$\dot{z} = J\nabla H(z) = L_H z, \quad (i = 1, 2, 3, \cdots, n),$$

where L_H is the Lie operator, with A and B denoting the Lie derivatives of T and V, respectively:

$$A = \{\cdot, T\} = \sum_{i=1}^{n} \frac{p_i}{m_i} \frac{\partial}{\partial q_i}, \quad B = \{\cdot, V\} = \sum_{i=1}^{n} f_i \frac{\partial}{\partial p_i},$$

where $f_i = -\frac{\partial V}{\partial q_i}$. The symplectic algorithm can then be expressed as a series of compositions of exponentials of Lie operators corresponding to kinetic and potential energies:

$$e^{\tau W} = e^{a_i \tau A} e^{b_i \tau B} + O(\tau^{K+1}) = S_n + O(\tau^{K+1}).$$

Here, a_i and b_i are coefficients determined by specific order conditions, and $O(h^{K+1})$ represents the K-th order truncation error of the Hamiltonian function. When the number of Lie operators equals the number of order conditions, the time coefficients can be easily calculated. Ruth [2] proposed commonly used second-order and third-order symplectic algorithms in the literature. Based on this work, Forest-Ruth fourth-order non-force-gradient symplectic algorithms [3] and Yoshida high-order non-force-gradient symplectic algorithms [5] were subsequently developed.

3.1.1 Unoptimized Non-Force-Gradient Explicit Symplectic Algorithms

Following Ruth's method [2], for integrable and separable Hamiltonian systems, symplectic algorithms are constructed as follows:

(1) First-order explicit symplectic algorithm S_1:

$$e^{\tau A}e^{\tau B}=e^{\tau W}.$$

(2) Second-order explicit symmetric symplectic algorithm: The second-order explicit symmetric symplectic algorithm consists of three single-exponential operators with the form:

$$S_{2X}: e^{\frac{1}{2}\tau A}e^{\tau B}e^{\frac{1}{2}\tau A}=e^{\tau W},$$

$$S_{2Y}: e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B}=e^{\tau W}.$$

(3) Third-order explicit symplectic algorithm: The third-order explicit symplectic algorithm consists of six single-exponential operators with the form S_3:

$$e^{\tau A}e^{-\frac{1}{24}\tau B}e^{-\frac{2}{3}\tau A}e^{\frac{4}{3}\tau B}e^{\frac{3}{4}\tau A}=e^{\tau W}.$$

(4) Fourth-order explicit Forest-Ruth symplectic integrator (FR): The Forest-Ruth algorithm starts from equation (6) and consists of seven single exponentials S_4:

$$e^{A\tau c/2}e^{B\tau c}e^{A(1-c)\tau}e^{B(1-2c)\tau}e^{A(1-c)\tau}e^{B\tau c}e^{A\tau c/2},\quad c=\frac{1}{2-\sqrt[3]{2}}.$$

Another approach for constructing high-order algorithms involves direct multiple compositions of second-order symplectic algorithms. Yoshida [5] symmetrically combined three second-order symplectic algorithms based on Ruth's theory [2] to obtain the fourth-order explicit Yoshida symplectic algorithm S_{YO}:

$$S_{YO}=S_2(c\tau)S_2((1-2c)\tau)S_2(c\tau).$$

In the same year, Forest and Ruth [3] proposed the Forest-Ruth fourth-order symplectic algorithm, which achieves equivalent effectiveness to Yoshida's construction. Following this construction pattern, high-order symplectic algorithms S_{2n+2} can be built [5]:

$$S_{2n+2}=S_{2n}(a\tau)S_{2n}((1-2a)\tau)S_{2n}(a\tau),\quad a=\frac{1}{2-2^{1/(2n+1)}}.$$

3.1.2 Optimized Non-Force-Gradient Explicit Symplectic Algorithms

McLachlan [11] introduced the concept of algorithm optimization in 1992. By minimizing the influence of the main truncation error term, optimized coefficients are obtained to construct optimized second-order and third-order explicit symplectic algorithms. Based on this work, higher-order optimized algorithms such as the fourth-order optimized non-force-gradient algorithm [34] were also developed.

(1) Optimized second-order and third-order explicit symplectic algorithms: The main error function for the second-order explicit symplectic algorithm with unified coefficients is:

$$h_2 = \frac{F'P^2}{24}(1-3a_2) + \frac{F^2P'}{12}\frac{1-4a_2}{8(1-a_2)},$$

where $F = -\frac{\partial V}{\partial q}$, F' and P' represent their derivatives, and a_2 denotes the truncation error term coefficient. McLachlan minimized the sum of squares of the coefficients in h_2, yielding two minima $a_2 = 1 \pm \sqrt{3}/3$, with smaller a_2 values producing smaller errors. Compared with the truncation error constants of unoptimized second-order explicit symplectic algorithms and pseudo-second-order symplectic algorithms, the second-order optimized algorithm improves precision by 0.39, as shown in Table 1 .

McLachlan expressed the main error function for an n-th order symplectic algorithm as:

$$h_n = \left(\sum_{j=1}^{N_f} f_j(a,b) g_i(F,P) \right) \Bigg|_{(q_0;p_0)}.$$

Minimizing the sum of squares of the coefficients yields the third-order optimized symplectic algorithm O_3:

$$e^{a_1\tau A} e^{b_1\tau B} e^{a_2\tau A} e^{b_2\tau B} e^{a_3\tau A} e^{b_3\tau B}.$$

(2) Fourth-order optimized Forest-Ruth algorithm (OFR): Omelyan et al. [34] extended the fourth-order explicit Forest-Ruth algorithm as:

$$S_{OFR} = e^{B\xi h} e^{A(1-2\chi)h/2} e^{B\lambda h} e^{A\chi h} e^{B(1-2(\lambda+\xi))h} e^{A\chi h} e^{B\lambda h} e^{A(1-2\chi)h/2} e^{B\xi h}.$$

Here, ξ, χ, and λ are three step-size coefficients subject to two constraints: the coefficient of operator A, $\alpha(\xi,\chi,\lambda) = 0$, and the coefficient of operator B, $\beta(\xi,\chi,\lambda) = 0$. With one remaining degree of freedom, multiple solutions exist for the step-size coefficients. Following McLachlan's optimization principle, the third-order truncation error of the fourth-order explicit Forest-Ruth algorithm is set to zero while minimizing the sum of squares of the fifth-order truncation error coefficients, yielding the optimal solution:

$$\xi = 0.1720865590295143, \quad \lambda = -0.09156203075515678, \quad \chi = -0.1616217622107222.$$

Under these coefficients, the OFR algorithm's truncation error value is $\gamma_{\min} = 0.00092$, while the fourth-order FR symplectic algorithm's truncation error value is $\gamma_{FR} = 0.039$, representing a significant improvement in precision after optimization.

(3) Optimized fourth-order pseudo-Suzuki integrator (SU): Omelyan et al. [34] constructed the SU algorithm by adding two identical operators at both ends of Yoshida's fourth-order symplectic algorithm, forming a five-operator composition:

$$S_{SU} = S_2(a_1 h) S_2(a_2 h) S_2((1 - 2a_1 - 2a_2)h) S_2(a_2 h) S_2(a_1 h),$$

with $a_1 = 0.3221375960817984$ and $a_2 = 0.5413165481700430$. Considering the order conditions and minimizing the sum of squares of the h^5 truncation error coefficients, the resulting Hamiltonian truncation error value is $\gamma = 0.0011$, which is one order of magnitude less precise than the OFR algorithm.

3.2 H = H_0 + H_1 Decomposition Method

Here, H_0 and H_1 are integrable, with H_0 being the main term and H_1 the perturbation term. The small parameter indicates that H_1 differs from H_0 by order . The detailed decomposition process is described in reference [35].

Defining $A = \{\cdot, H_0\}$ and $B = \{\cdot, H_1\}$, and using the symplectic algorithm construction formula $e^{\tau W} = e^{\tau A} e^{\tau B}$ [2] with repeated application of the Baker-Campbell-Hausdorff (BCH) formula [36, 37], the Hamiltonian error expression becomes:

$$H_{\text{err}} = \varepsilon(a_1 \tau + \cdots) + \varepsilon^2(b_1 \tau^2 + \cdots) + \cdots,$$

where a_1, b_1 are error term coefficients. Three methods for improving symplectic integrator accuracy emerge from this expression: (1) increasing the power of τ to obtain high-order symplectic algorithms; (2) improving the Hamiltonian decomposition and construction methods—smaller yields higher precision, such as Hamiltonian perturbation decomposition [6], time transformation, and extended phase space; (3) increasing the power of to obtain symplectic corrections [8]. If $O(\varepsilon^2 \tau^{n+1})$ terms remain in the error, increasing the power of τ yields pseudo-high-order symplectic methods [7]. These two types of symplectic-like algorithms optimize integration accuracy and efficiency without reducing step size or increasing order.

Generally, when the Hamiltonian function is decomposed as H = H_0 + H_1, algorithm precision improves significantly compared to T + V decomposition. As shown in Figure 1 [Figure 1: see original paper], using the pure Kepler problem as an example, the numerical precision of algorithms under perturbation decomposition improves by nearly five orders of magnitude compared to T + V decomposition.

3.2.1 Symplectic Correction

Wisdom and Holman [6] established the following second-order symplectic algorithm (second-order Wisdom-Verlet, MV2) in Jacobi coordinates:

$$e^{A+B} = e^{b_N B} \cdots e^{a_1 B} e^{b_1 B} e^{a_0 A} e^{b_0 B}.$$

Here, $N = 1$, $b_0 = b_1 = 1/2$, and $a_0 = 1$. The relationship between the numerical result's Hamiltonian function $\tilde{H}$ and the true Hamiltonian function H is $\tilde{H} = H + H_{\mathrm{err}}$. Wisdom et al. [8] used Lie series operators to construct a generating function W for a canonical transformation, making H_{err} free of first or second-order terms in the perturbation small parameter , thereby constructing symplectic correction formulas. Symplectic correction has the following characteristics: (1) It significantly improves numerical accuracy by eliminating or ^{2} terms from the error without reducing step size or increasing order; (2) It is not strictly symplectic but introduces no dissipative mechanism; (3) It offers high computational efficiency.

The WHT method's process for calculating the generating function W is cumbersome, and the corrector C is only applicable to the aforementioned symplectic algorithm, lacking generality. Mikkola and Palmer [39] derived the generating function W for symplectic correction using the Euler-Maclaurin formula. In the same year, Chambers and Murison [7] established pseudo-high-order symplectic algorithms. Duncan et al. [40, 41] divided the Hamiltonian function in solar system dynamics into three integrable parts using heliocentric coordinates. Malhotra [42] divided the Hamiltonian system into 14 integrable parts when studying tidal evolution of Galilean satellites. Wu et al. [43, 44] generalized the multi-part decomposition of Hamiltonian functions, dividing H_0 into N sub-steps in symplectic algorithms and numerically discussing algorithm accuracy for Hamiltonians with $N + 1$ integrable parts (primarily first and second order).

Wu et al. [44] derived the Hamiltonian error function for symplectic algorithms using Bernoulli polynomials [7]:

$$H_{\mathrm{err}} = \sum_{i=1}^{n} \varepsilon_i B_i + \sum_{i=1}^{n} \sum_{j=1}^{n} \varepsilon_i \varepsilon_j \tau^2 \mathfrak{L}_{B_i} \mathfrak{L}_A B_j - \frac{1}{1440} \varepsilon_i \varepsilon_j \tau^4 \mathfrak{L}_{B_i} \mathfrak{L}_A^3 B_j + \cdots,$$

where $A = L_{H_0}$, $B_i = L_{H_i}$, the commutator $[A, B] = AB - BA$, $[A, B, C] = [A, [B, C]]$, also denoted as $[A, B] = \mathfrak{L}_{AB}$, and $B^{(k)}(x)$ are Bernoulli polynomials satisfying the recurrence relation [8]:

$$B^{(i)}(x) = \sum_{m=0}^{i-1} \frac{B^{(m)}(x)}{m!(i-m+1)!} \quad (B^{(0)}(x) = 1).$$

Equation (20) applies to symplectic algorithms of any order for Hamiltonian systems with n integrable parts. The Hamiltonian truncation error can be directly determined using mathematical software such as MATLAB or Mathematica [44], improving computational efficiency.

(1) First-order symplectic correction in : The first-order correction operator [44] eliminates first-order terms from the truncation error. The first-order corrector expression is:

$$\begin{cases} C_{S1} = \tau \sum_{i=1}^{n} \varepsilon_i \sum_{j=1}^{\infty} \frac{B^{(2j-1)}(1)}{(2j-1)!2^{2j-1}} \mathfrak{L}_{2j-1} AB_i, \\ C_{S2X} = -\sum_{i=1}^{n} \varepsilon_i \sum_{j=1}^{\infty} \frac{B^{(2j)}(0)}{(2j)!2^{2j-1}} \mathfrak{L}_{2j-1} AB_i, \\ C_{S2Y} = -\sum_{i=1}^{n} \varepsilon_i \sum_{j=1}^{\infty} \frac{B^{(2j)}-1}{(2j)!} \mathfrak{L}_{2j-1} AB_i. \end{cases}$$

(2) Second-order symplectic correction in ^{2}: Wu et al. [44] discussed the second-order symplectic correction process for the second-order explicit symplectic algorithm S_{2X}, with derivation applicable to general n-th order symplectic algorithms. The correction formula for S_{2X} regarding ^{2} is:

$$\tilde{S}_{2X} = e^{-C} e^{-C_2} e^{K'} e^{C_2} e^{C},$$

where

$$C_2 \approx \bar{C}_2 = -\sum_{i,j=1}^{n} \varepsilon_i \varepsilon_j \tau^2 \mathfrak{L}_{B_i} \mathfrak{L}_A B_j + c_i \frac{\tau^{n+1}}{n+1} \mathfrak{L}_A^n B_i + c_i \frac{n+2}{5760} \varepsilon_i \varepsilon_j \tau^4 \mathfrak{L}_{B_i} \mathfrak{L}_A^3 B_j + \cdots.$$

In the Sun-Jupiter-Saturn model, numerical comparisons of energy error, computational efficiency, and mean longitude error show that symplectic correction improves computational accuracy by one order of magnitude over explicit symplectic algorithms while providing better numerical stability.

3.2.2 Pseudo-High-Order Symplectic Algorithms

Pseudo-high-order symplectic algorithms form efficient integration methods based on perturbation decomposition. Compared with high-order symplectic algorithms whose sub-steps increase rapidly with time step, pseudo-high-order symplectic algorithms have fewer sub-steps and higher computational efficiency. Chambers and Murison [7] constructed appropriate coefficients from fourth-order and sixth-order symplectic algorithms to eliminate τ^4 or τ^6 terms from the error, yielding:

$$\begin{cases} e^{a_2\tau A} e^{b_1\tau B} e^{a_1\tau A} e^{b_1\tau B} e^{a_2\tau A} = e^{(a_1+2a_2)\tau A + 2b_1\tau B + \varepsilon\tau^3 \frac{b_1}{6}[(a_1+2a_2)^2 - 6a_2(a_1+a_2)]\mathfrak{L}_2 AB} \\ \quad -\varepsilon^2\tau^3 \frac{b_1}{6}(4a_2 - a_1)\mathfrak{L}_2 BA - \varepsilon\tau^5 \frac{b_1}{360}[(a_1+2a_2)^4 - 30a_2^2(a_1+a_2)^2]\mathfrak{L}_2 AB \\ \quad -\varepsilon^2\tau^5 \frac{b_1}{360}(16a_2 - 7a_1)\mathfrak{L}_4 BA + \cdots, \\ a_1 + 2a_2 = 1, \quad 2b_1 = 1, \quad 1 - 6a_2(1-a_2) = 0. \end{cases}$$

When these conditions are satisfied, the τ^3 term can be eliminated. The paper lists pseudo-fourth-order and pseudo-sixth-order symplectic algorithms [7]:

$$\mathrm{PSI}_4 = e^{\frac{1}{2}A(1-\frac{1}{\sqrt{3}})} e^{\tau B} e^{\frac{1}{2}A(1-\frac{2}{\sqrt{3}})} e^{\tau B} e^{\frac{1}{2}A(1-\frac{1}{\sqrt{3}})} = e^{\tau \mathfrak{L}_H} + \varepsilon^2\tau^3 \frac{2-\sqrt{3}}{24} \mathfrak{L}_2 BA - \varepsilon\tau^5 \frac{1}{720} \mathfrak{L}_2 AB + \cdots,$$

$$\mathrm{PSI}_6 = e^{\frac{1}{2}A(1-\frac{\sqrt{3}}{2})}e^{\tau B}e^{\frac{1}{2}A(1-\sqrt{3})}e^{\tau B}e^{\frac{1}{2}A(1-\frac{\sqrt{3}}{2})} = e^{\tau \mathfrak{L}_H + \varepsilon^2\tau^3\frac{13-5\sqrt{3}}{72}\mathfrak{L}_2 BA + O(\varepsilon\tau^7)}.$$

Higher-order algorithms such as eighth-order and tenth-order can also be constructed. Pseudo-high-order symplectic algorithms maintain stable system energy [45, 46] and demonstrate significantly better computational efficiency than conventional symplectic algorithms of the same order [11, 39]. From the perspective of truncation error terms, they can be viewed as partial corrections to second-order symplectic algorithms. Beyond a certain order, the precision of pseudo-high-order symplectic algorithms no longer improves with increasing order. Laskar and Robutel [47] noted that pseudo-sixth-order or eighth-order algorithms yield the best numerical results. Wu et al. [44] conducted numerical simulations of the pseudo-fourth-order symplectic algorithm PSI_4, its corrected version, and the conventional fourth-order symplectic algorithm S_4 in the Sun-Jupiter-Saturn three-body model, showing that all three exhibit energy error precision of the same order of magnitude.

4 Force-Gradient Symplectic Algorithms

Conventional symplectic algorithms inevitably produce negative integration step sizes during integration, but irreversible mechanical problems require all positive step sizes. Ruth [2] introduced the force-gradient operator $[\hat{V}, \hat{T}, \hat{V}]$ into the operator composition of third-order symplectic algorithms, ensuring all integration sub-step coefficients are positive. Chin et al. [9, 10, 48–50] extended force-gradient symplectic algorithms to fourth order, achieving 10–80 times higher precision than conventional symplectic algorithms of the same order [9], with successful applications in circular restricted three-body problems, time-dependent gravitational field problems [10], and quantum mechanical problems [48]. Sun et al. [51] constructed two types of fourth-order force-gradient symplectic algorithms containing third-derivative terms based on Chin's fourth-order force-gradient symplectic algorithm, demonstrating improved precision and computational efficiency in numerical simulations of the Hénon-Heiles system, quadrupole core-shell model, and oblateness-affected restricted three-body problem. Xu and Wu [52, 53] applied this force-gradient symplectic algorithm to solve perturbed two-body problems and perturbed N-body problems in Jacobi coordinates. Omelyan et al. [54, 55] introduced optimization ideas into force-gradient symplectic algorithms, constructing third-order and fourth-order optimized force-gradient symplectic algorithms in symmetric composition form and applying them to celestial mechanics, molecular dynamics, and quantum mechanics, showing significant numerical precision improvements over conventional symplectic algorithms, though negative step-size coefficients remained unavoidable.

Li Rong et al. [12–14, 56, 57] constructed asymmetric third-order and fourth-order optimized force-gradient symplectic algorithms with all-positive step-size coefficients, demonstrating clear precision advantages in solving perturbed Kepler chaotic problems [57] and stationary Schrödinger equation energy eigenvalue problems [12–14, 56]. Chen Yunlong and Wu Xin [15] rigorously demonstrated that force-gradient symplectic algorithms remain suitable for solving problems where kinetic energy T in the rotating coordinate system's center-of-mass frame is not a strict quadratic function of momentum P.

The force-gradient operator is defined as:

$$[C] = [B, A, B] = \{\cdot, \{\{V, T\}, V\}\} = 2 \sum_{i,j=1}^{n} V_i V_{ij} T_{jk} \frac{\partial}{\partial p_k},$$

where A and B are as defined in equation (4), $V_k = \frac{\partial V}{\partial q_k}$, $V_{ij} = \frac{\partial^2 V}{\partial q_i \partial q_j}$, and $T_{jk} = \frac{\partial^2 T}{\partial p_j \partial p_k}$. Force-gradient symplectic algorithms can be constructed by combining operators C with A and B:

$$e^{\tau W} = e^{\tau(A+B)} = e^{a_i \tau A} e^{b_i \tau B + c_i \tau^3 C}.$$

4.1 Non-Optimized Force-Gradient Symplectic Algorithms

(1) Third-order force-gradient symplectic algorithm F_3:

$$e^{\frac{2}{3}\tau A} e^{\frac{3}{4}\tau B} e^{\frac{2}{3}\tau A} e^{\frac{3}{4}\tau B + \frac{1}{48}\tau^3 C} = e^{\tau W}.$$

This algorithm has all positive integration step sizes, but the complex computation of the force-gradient operator C limited its early adoption.

(2) Fourth-order force-gradient symplectic algorithm F_4: Chin and collaborators developed the force-gradient symplectic algorithm to fourth order [9, 10, 48–50]:

Algorithm A:

$$e^{\frac{1}{6}\tau B} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{4}\tau B + \frac{1}{72}\tau^3 C} e^{\frac{1}{2}(2-\sqrt{3})\tau A} e^{\frac{3}{4}\tau B + \frac{1}{48}(2-\sqrt{3})\tau^3 C} e^{\frac{1}{6}\tau B} = e^{\tau W}.$$

Algorithm B:

$$e^{\frac{1}{8}\tau B} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{8}\tau B + \frac{1}{384}\tau^3 C} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{8}\tau B + \frac{1}{192}\tau^3 C} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{8}\tau B + \frac{1}{384}\tau^3 C} e^{\frac{1}{8}\tau B} = e^{\tau W}.$$

Algorithm C:

$$e^{\frac{1}{6}\tau B} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{4}\tau B + \frac{1}{72}\tau^3 C} e^{\frac{1}{2}(2-\sqrt{3})\tau A} e^{\frac{3}{4}\tau B + \frac{1}{48}(2-\sqrt{3})\tau^3 C} e^{\frac{1}{6}\tau B} = e^{\tau W}.$$

Algorithm D:

$$e^{\frac{1}{8}\tau B} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{8}\tau B + \frac{1}{384}\tau^3 C} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{8}\tau B + \frac{1}{192}\tau^3 C} e^{\frac{1}{2}(1-\frac{1}{\sqrt{3}})\tau A} e^{\frac{3}{8}\tau B + \frac{1}{384}\tau^3 C} e^{\frac{1}{8}\tau B} = e^{\tau W}.$$

Compared with conventional fourth-order symplectic algorithms, precision improves by 10–80 times. Xu and Wu [52] followed Yoshida's approach for constructing standard high-order symplectic algorithms, symmetrically combining operator C with A and B in two different ways to obtain two new classes of fourth-order force-gradient symplectic algorithms.

(a) When the force-gradient operator is nested in the center:

$$e^{a_1\tau A}e^{b_1\tau B}e^{a_2\tau A}e^{b_2\tau B+b_3\tau^3 C}e^{a_2\tau A}e^{b_1\tau B}e^{a_1\tau A}=e^W.$$

(b) When the force-gradient operator is nested at both ends:

$$e^{b_1\tau B+b_2\tau^3 C}e^{a_1\tau A}e^{b_3\tau B}e^{a_2\tau A}e^{b_3\tau B}e^{a_1\tau A}e^{b_1\tau B+b_2\tau^3 C}=e^W.$$

Using the BCH formula, cyclic derivation starting from the middle of the combined operators yields the specific expression for W. Applying optimization principles produces a series of new positive integration coefficients, as shown in Table 2 and Table 3 . Algorithms A1 and B1 correspond to Chin's fourth-order algorithms C and D. Xu and Wu [52] applied these two new fourth-order force-gradient symplectic algorithms to solve perturbed Kepler problems and N-body problems in Jacobi coordinates, and deeply studied chaotic motion of charged particles in planetary magnetospheres. As shown in Figure 2 [Figure 2: see original paper], the numerical performance of force-gradient symplectic algorithms shows no significant difference between the two decomposition forms, while perturbation decomposition significantly improves algorithm precision. In perturbation decomposition, computing the force-gradient operator $[H_0]$ is simpler than computing H_0 and does not add substantial computational cost compared to H_1, making it highly recommended for studying N-body Hamiltonian problems in Jacobi coordinates [15, 53].

4.2 Optimized Force-Gradient Symplectic Algorithms

(1) Third-order optimized force-gradient symplectic algorithm: Solving for Lie operator coefficients only applies to symmetric symplectic algorithms, complicating the construction of asymmetric force-gradient symplectic algorithms. Li Rong et al. constructed asymmetric third-order and fourth-order optimized force-gradient symplectic algorithms [12–14, 52]. Following Chin's approach, the following asymmetric operator combination was constructed:

$$e^{b_1\tau B+k\tau^3 C}e^{a_1\tau A}e^{b_1\tau B}e^{a_2\tau A}e^{b_2\tau B}=e^{\tau W}.$$

Using the BCH formula to obtain order condition relationships and applying optimization principles (i.e., adding additional constraints [13] to minimize the sum of squares of fourth-order truncation error coefficients), new third-order optimized force-gradient symplectic algorithms were obtained:

Algorithm SOF3X:

$$\begin{cases} e^{b_1\tau B+k\tau^3 C}e^{a_1\tau A}e^{b_2\tau B}e^{a_2\tau A}e^{b_3\tau B}=e^{\tau W}, \\ a_1=0.60482187531038, \quad a_2=0.39517812468962, \\ k=0.01644283046910, \quad b_1=0.22443677474275, \\ b_2=0.69731396562925, \quad b_3=0.07824925962800. \end{cases}$$

Algorithm SOF3Y:

$$\begin{cases} e^{a_1\tau A}e^{b_1\tau B+k\tau^3 C}e^{a_2\tau A}e^{b_2\tau B}e^{a_3\tau A}=e^{\tau W}, \\ a_1=0.17270717029761, \quad a_2=0.58190681989921, \\ a_3=0.24538600980318, \quad b_1=0.43755113617833, \\ b_2=0.56244886382167, \quad k=0.011172965730361. \end{cases}$$

Li Rong [12] conducted numerical comparisons of the newly constructed third-order optimized force-gradient symplectic algorithm with other symplectic algorithms in harmonic oscillator, pendulum, Kepler two-body, Hénon-Heiles systems, and quantum mechanical models. In classical mechanical models, this algorithm demonstrates absolute precision advantages in energy error calculations and can accurately identify chaotic orbits in the Hénon-Heiles system, effectively avoiding false chaotic phenomena caused by numerical errors. In stationary Schrödinger equation energy eigenvalue problems, the algorithm also shows clear precision advantages, even achieving higher precision than fourth-order standard symplectic algorithms.

(2) Fourth-order optimized force-gradient symplectic algorithm: Omelyan et al. [54, 55] constructed symmetric fourth-order optimized force-gradient symplectic algorithms as follows:

$$\text{OF4}: e^{\frac{1}{6}\tau B-\frac{17}{18000}\tau^3 C}e^{\frac{1}{2}\tau A}e^{\frac{3}{4}\tau B+\frac{71}{4500}\tau^3 C}e^{\frac{1}{2}\tau A}e^{\frac{1}{6}\tau B-\frac{17}{18000}\tau^3 C}=e^{\tau W}.$$

Li Rong [12] obtained two fourth-order symplectic algorithms by symmetrically combining the third-order optimized force-gradient symplectic algorithm:

Algorithm OF4X:

$$e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B+k\tau^3 C}e^{a_3\tau A}e^{\frac{1}{2}\tau B+k\tau^3 C}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}=e^{\tau W}.$$

Algorithm OF4Y:

$$e^{\frac{\tilde{b}_1}{2}\tau B}e^{\frac{\tilde{a}_2}{2}\tau A}e^{\frac{\tilde{b}_2}{2}\tau B}e^{\frac{\tilde{a}_3}{2}\tau A}e^{\bar{b}_3\tau B+l\tau^3 C}e^{\frac{\tilde{a}_3}{2}\tau A}e^{\frac{\tilde{b}_2}{2}\tau B}e^{\frac{\tilde{a}_2}{2}\tau A}e^{\frac{\tilde{b}_1}{2}\tau B}=e^{\tau W}.$$

Numerical analysis and comparison in classical mechanical models such as Kepler two-body and perturbed two-body problems, as well as quantum mechanical Morse potential models, show that the new fourth-order force-gradient algorithms exhibit excellent numerical precision, even significantly superior to existing fourth-order optimized force-gradient symplectic algorithm OF4 [55].

In the planar circular restricted three-body problem in rotating coordinates, kinetic energy T is not a strict quadratic form of momentum P due to cross terms between momentum and coordinates from the rotating frame, complicating the incorporation of force-gradient operators. Chen Yunlong and Wu Xin [15] rigorously demonstrated that the force-gradient operator in rotating coordinates maintains the same form as in the center-of-mass frame—it represents the gradient of gravitational force rather than the gradient of the combined gravitational and inertial forces. Only operator A changes to:

$$-T_{q_i} = (p_x + y)\frac{\partial}{\partial p_x} + (p_y - x)\frac{\partial}{\partial p_y},$$

while operator C in equation (26) remains applicable. Numerical results from applying fourth-order force-gradient symplectic algorithms, optimized fourth-order force-gradient symplectic algorithms, and Forest-Ruth symplectic algorithms to this problem show that the optimized fourth-order force-gradient symplectic algorithm achieves the best precision.

5.1 Construction of Implicit Symplectic Algorithms

When a system's Hamiltonian variables cannot be separated, explicit algorithms generally cannot be applied directly. Consider a non-separable Hamiltonian:

$$H(p,q) = H_0(p,q) + H_1(p,q),$$

with canonical equations:

$$\dot{p} = -\frac{\partial H(p,q)}{\partial q} = f(p,q), \quad \dot{q} = \frac{\partial H(p,q)}{\partial p} = g(p,q).$$

Using time step τ and first-order Euler forward difference formulas for the entire Hamiltonian system yields first-order implicit symplectic algorithms M_1 and M_1^*, and second-order implicit midpoint method M_2 [2]:

(1) First-order position implicit Euler method:

$$q_{n+1} = q_n + \tau f(p_n, q_{n+1}), \quad p_{n+1} = p_n + \tau g(p_n, q_{n+1}).$$

(2) First-order momentum implicit Euler method:

$$M_1^* : q_{n+1} = q_n + \tau f(q_n, p_{n+1}), \quad p_{n+1} = p_n + \tau g(q_n, p_{n+1}).$$

(3) Second-order implicit midpoint method:

$$q_{n+1} = q_n + \tau f\left(\frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2}\right),$$
$$p_{n+1} = p_n + \tau g\left(\frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2}\right).$$

(4) Second-order explicit-implicit mixed symplectic algorithm: Operator A has an analytical solution, while B is solved iteratively using the implicit midpoint method, combining to form:

$$\text{MSI1} : \tilde{S}_2 = \exp\left(\frac{\tau}{2}B\right)\exp(\tau A)\exp\left(\frac{\tau}{2}B\right),$$
$$\text{MSI2} : \tilde{S}_2^* = \exp\left(\frac{\tau}{2}A\right)\exp(\tau B)\exp\left(\frac{\tau}{2}A\right).$$

(5) High-order implicit symplectic algorithms: Following Yoshida's [5] and Ruth's [2] approach for constructing high-order explicit symplectic algorithms, high-order implicit symplectic algorithms can be constructed for the global Hamiltonian function:

$$S_4(YO) = \tilde{S}_2(c\tau)\tilde{S}_2((1-2c)\tau)\tilde{S}_2(c\tau),$$

$$S_4^*(YO) = \tilde{S}_2^*(c\tau)\tilde{S}_2^*((1-2c)\tau)\tilde{S}_2^*(c\tau),$$

$$S_4(FR) = A\left(\frac{c}{2}\tau\right)B(c\tau)A\left(\frac{1-c}{2}\tau\right)A(c\tau)B\left(\frac{1-c}{2}\tau\right)B(1-2c\tau)A\left(\frac{1-c}{2}\tau\right)A(1-2c\tau)B\left(\frac{1-c}{2}\tau\right)B(c\tau$$

$$S_4^*(FR) = B\left(\frac{c}{2}\tau\right)A(c\tau)B\left(\frac{1-c}{2}\tau\right)B(c\tau)A\left(\frac{1-c}{2}\tau\right)A(1-2c\tau)B\left(\frac{1-c}{2}\tau\right)B(1-2c\tau)A\left(\frac{1-c}{2}\tau\right)A(c\tau$$

where $c = \frac{1}{2} - \frac{2^{1/3}}{2}$.

Global implicit symplectic algorithms suffer from unsatisfactory computational efficiency. If variable separation makes H_0 integrable while H_1 remains non-integrable, explicit-implicit mixed symplectic algorithms constructed according to equations (44)–(46) clearly outperform fully implicit symplectic algorithms in efficiency.

Zhong et al. [18–21] applied second-order implicit midpoint methods and their symmetric combinations to solve entire post-Newtonian Hamiltonian systems, with numerical experiments showing that explicit-implicit mixed midpoint embedding methods consistently outperform fully implicit midpoint methods in energy precision while offering better computational efficiency. Zhong and Wu [19] further optimized the midpoint embedding method to improve computational precision. For spinning post-Newtonian Hamiltonian systems:

$$H(r, p, S_1, S_2) = H_{\text{Kep}} + H_{\text{PN}},$$

where the Keplerian and post-Newtonian parts are:

$$H_{\text{Kep}} = \frac{p^2}{2} - \frac{1}{r}, \quad H_{\text{PN}} = H_{1\text{PN}} + H_{2\text{PN}} + H_{\text{SO}} + H_{\text{SS}}.$$

Introducing Wu and Xie's [18] canonical rotational coordinates for rotational scalars yields a new canonical Hamiltonian function $\Gamma(r, \theta, p, \xi)$. The implicit midpoint method is applied directly to solve for variables $\Gamma(r, \theta, p, \xi)$, denoted as S_{2A}. Additionally, Zhong and Wu [19] obtained analytical solutions for the Keplerian part and numerical solutions for the post-Newtonian part, applying the implicit midpoint method to the numerical portion and constructing fourth-order canonical explicit-implicit mixed symplectic algorithms following Yoshida's approach:

$$\begin{cases} S_{2B} = \phi_{\tau/2} \circ \phi_{\tau} \circ \phi_{\tau/2}, \\ S_{4B} = \phi_{c\tau/2} \circ \phi_{(1-2c)\tau/2} \circ \phi_{c\tau}, \\ \tilde{S}_{4B} = \phi_{\xi\tau} \circ \phi_{\chi\tau} \circ \phi_{\lambda\tau} \circ \phi_{(1-2\chi)\tau/2} \circ \phi_{(1-2(\lambda+\xi))\tau} \circ \phi_{(1-2\chi)\tau/2} \circ \phi_{\lambda\tau} \circ \phi_{\chi\tau} \circ \phi_{\xi\tau}, \end{cases}$$

where $c = \frac{1}{2} - 2^{1/3}$, $\xi = 0.1720865590295143$, $\chi = -0.09156203075515678$, and $\lambda = -0.1616217622107222$.

Mei et al. [22, 23] conducted theoretical analysis of fourth-order Forest-Ruth type explicit-implicit mixed symplectic algorithms and fourth-order Yoshida explicit-implicit mixed symplectic algorithms, proving that the former achieves only second-order accuracy in most cases, while the latter can reach fourth-order accuracy. The same conclusion was reached in one-dimensional non-separable systems $H = (p^2 + q^2) + \cos p \sin q$ and compact binary post-Newtonian Hamiltonian systems. They noted that in practical computations, when part of the Hamiltonian is integrable with easily obtainable analytical solutions, the $S_4(FR)$ algorithm or Yoshida's algorithm $S_4(YO)$ combining analytical and implicit numerical solutions should be used to achieve high precision and efficiency. When separable Hamiltonian variables are partially integrable but analytical solutions are difficult to obtain, or when Hamiltonian variables are partially non-integrable, Yoshida's algorithm $S_4(YO)$ combining analytical and implicit numerical solutions should be employed.

Lubich et al. [58] proposed fourth-order non-canonical explicit-implicit mixed symplectic algorithms primarily applied to spinning compact binary post-Newtonian Hamiltonian systems, dividing the Hamiltonian into three main components: orbital H_{Orb}, spin-orbit H_{SO}, and spin-spin H_{SS}:

$$H = H_{\text{Orb}} + H_{\text{SO}} + H_{\text{SS}}.$$

Following Suzuki's [17] approach of using five compositions of second-order integrators to construct fourth-order algorithms:

$$h = \phi^*_{H_{\text{SS}}} \circ \phi^*_{H_{\text{SO}}} \circ \phi_{H_{\text{Orb}}} \circ \phi_{H_{\text{SO}}} \circ \phi_{H_{\text{SS}}}.$$

Each component is then further decomposed into 2, 3, or 4 parts and solved using explicit-implicit mixed symplectic algorithms. Extending equation (54) to fourth order:

$$\phi_H^{4\text{th}} = \phi_H^{\gamma_0 h} \circ \phi_H^{\gamma_1 h} \circ \phi_H^{\gamma_1 h} \circ \phi_H^{\gamma_0 h},$$

where $\gamma_0 = \frac{1}{4-4^{1/3}}$ and $\gamma_1 = -\frac{4^{1/3}}{4-4^{1/3}}$.

5.2 Comparison of Numerical Stability of Several Implicit Symplectic Algorithms

When both parts of the Hamiltonian are integrable, Liu Fu-yao et al. [59] analyzed and compared the numerical stability of first-order implicit symplectic algorithm M_1^*, implicit midpoint method M_2, first-order explicit algorithm, and second-order explicit algorithm by applying them to linear Hamiltonian systems:

$$H = \frac{p^2}{2} + \frac{q^2}{2} + \frac{(y^2 - x^2)}{2}.$$

Compared with T + V decomposition, the stable regions of each algorithm expand under $H_0 + H_1$ decomposition. In 2009, Liu Fu-yao and Qian Xiao-ming [60] compared the numerical stability of two explicit-implicit mixed symplectic algorithms proposed by Liao [16], which embed first-order implicit symplectic algorithm M_1^* and implicit midpoint method M_2 into first-order and second-order explicit symplectic algorithms, respectively. The former demonstrates superior numerical stability.

Zhong Shuang-ying [61] compared the numerical performance of explicit-implicit mixed symplectic algorithms MSI1 and MSI2 using one-dimensional coupled oscillators, classical circular restricted three-body problems, and post-Newtonian approximated compact binary systems as numerical test cases. In both the one-dimensional coupled oscillator model and the circular restricted three-body problem, MSI2 demonstrates significantly better stability than MSI1. The two algorithms perform very differently under different Hamiltonian decompositions: under T + V decomposition, both embedding methods maintain numerical stability; under $H_0 + H_1$ decomposition, MSI1 fails to maintain numerical stability in both regular and chaotic orbits. In spinning compact binary post-Newtonian Hamiltonian systems, MSI1 has slightly higher computational efficiency than MSI2 but inferior stability. Considering all factors, midpoint embedding methods are more suitable for solving various relativistic post-Newtonian dynamics problems.

Implicit symplectic algorithms are applicable to any Hamiltonian system and are ideal choices when classical algorithms exhibit poor stability. However, due to iterative solving processes, computational efficiency is greatly reduced, so they should not be the first-choice numerical method.

6 Extended Phase Space Explicit Symplectic Algorithms

Pihajoki [24] proposed a phase space extension method. In non-separable Hamiltonian systems, a set of momentum and coordinates $(\tilde{p}, \tilde{q})$ identical to the original space is added to obtain a new separable Hamiltonian:

$$\Gamma(p, \tilde{p}, q, \tilde{q}) = H_1(\tilde{p}, q) + H_2(p, \tilde{q}).$$

The two parts on the right side are independent and integrable, allowing analytical solutions. From canonical equations:

$$\dot{\tilde{q}} = \{\tilde{p}, H_1\}, \quad \dot{q} = \{p, H_1\}, \quad \dot{p} = -\frac{\partial H_1}{\partial q} = \{q, H_1\}, \quad \dot{\tilde{p}} = -\frac{\partial H_2}{\partial \tilde{q}} = \{\tilde{q}, H_2\}.$$

Explicit symplectic algorithms can be applied. At the initial moment, (p, q) and $(\tilde{p}, \tilde{q})$ are equal, but they diverge during integration. Pihajoki modified the second-order explicit symplectic algorithm (equation 8) as:

$$\Phi_2(h) = M_2 e^{hH_1/2} e^{hH_2/2} M_1 e^{hH_2/2} e^{hH_1/2} = \tilde{Q}(h/2) P(h/2) Q(h/2) \tilde{P}(h/2) M_1 \tilde{P}(h/2) Q(h/2) P(h/2) \tilde{Q}(h/2),$$

$$\Phi_2^*(h) = M_2 e^{hH_2/2} e^{hH_1/2} M_1 e^{hH_1/2} e^{hH_2/2} = M_2 Q(h/2)\tilde{P}(h/2)\tilde{Q}(h/2)P(h/2)M_1 P(h/2)\tilde{Q}(h/2)\tilde{P}(h/2)Q(h/2).$$

Here, M_1 and M_2 represent permutation mappings between the two sets of variables:

$$\tilde{\alpha}_{M_i} = \alpha_{M_i}, \quad \tilde{\beta}_{M_i} = \beta_{M_i}, \quad i = 1, 2.$$

Additionally, projection operator W is needed to return the extended phase space solution to the original phase space:

$$\alpha_W = \tilde{\alpha}_W = \beta_W = \tilde{\beta}_W = \mathbf{I}_n,$$

where $\mathbf{I}_n$ are $n \times n$ diagonal matrices. The method is originally symplectic-symmetric, but the symplectic structure is no longer preserved after projection onto the original phase space.

6.1 High-Order Continuous Coordinate-Momentum Permutation Phase Space Extension Explicit Symplectic-Like Algorithms

Liu and Wu [26] constructed explicit high-order symplectic-like algorithms using even multiple compositions, differing from Yoshida's approach for constructing high-order symplectic algorithms. Six even low-order algorithms were used to construct high-order algorithm S_{4A}:

$$\begin{cases} S_4 = \bar{S}_2(\lambda_1 h)\bar{S}_2(\lambda_2 h)\bar{S}_2(\lambda_3 h)M_1 \times \bar{S}_2(\lambda_3 h)\bar{S}_2(\lambda_2 h)\bar{S}_2(\lambda_1 h)M_2, \\ S_6 = \bar{S}_4(\lambda_1 h)\bar{S}_4(\lambda_2 h)\bar{S}_4(\lambda_3 h)M_1 \times \bar{S}_4(\lambda_3 h)\bar{S}_4(\lambda_2 h)\bar{S}_4(\lambda_1 h)M_2, \\ S_{2j+2} = \bar{S}_{2j}(\lambda_1 h)\bar{S}_{2j}(\lambda_2 h)\bar{S}_{2j}(\lambda_3 h)M_1 \times \bar{S}_{2j}(\lambda_3 h)\bar{S}_{2j}(\lambda_2 h)\bar{S}_{2j}(\lambda_1 h)M_2, \\ \lambda_1 = \lambda_2 = \lambda = \frac{1}{2(2-2^{1/(2j+1)})}, \quad \lambda_3 = \frac{1}{2} - 2\lambda. \end{cases}$$

This construction pattern consists of four parts: coordinate permutation, integration of three even low-order leapfrog formats without permutation, momentum permutation, and integration of three even low-order leapfrog formats without permutation [26].

In planar circular restricted three-body problems, Chin's [9] simple model, and non-rotating compact binary post-Newtonian Hamiltonian systems, high-order continuous coordinate-momentum permutation phase space extension explicit symplectic-like algorithms demonstrate superior numerical precision over Yoshida's fourth-order explicit symplectic algorithm, Chin's [9] explicit symplectic algorithm, and explicit-implicit mixed symplectic algorithms, with computational efficiency far exceeding that of explicit-implicit mixed symplectic algorithms. These explicit symplectic-like algorithms are also suitable for solving non-separable Hamiltonian systems such as post-Newtonian Hamiltonian problems and rotating Hamiltonian problems.

6.2 Midpoint Permutation Phase Space Extension Explicit Symplectic-Like Algorithms

The high-order symplectic-like algorithms proposed by Liu and Wu [26] require two triple compositions to achieve high precision and can fail in certain orbit integrations of rotating compact binary post-Newtonian Hamiltonian systems [52]. Luo et al. [28, 29] replaced continuous coordinate-momentum permutation with a single midpoint permutation (the midpoint between original variables and their corresponding extended variables), adjusting the values of original variables and their extended counterparts to their midpoint at each integration step:

$$p \leftarrow \frac{p+\tilde{p}}{2}, \quad \tilde{p} \leftarrow \frac{p+\tilde{p}}{2}, \quad q \leftarrow \frac{q+\tilde{q}}{2}, \quad \tilde{q} \leftarrow \frac{q+\tilde{q}}{2}.$$

Combined with Yoshida's triple composition, high-order symplectic-like algorithms S_{4B} are constructed:

$$S_4 = M_{1/2} \otimes \bar{S}_2(\lambda_3 h)\bar{S}_2(\lambda_2 h)\bar{S}_2(\lambda_1 h),$$

$$S_{2j+2} = M_{1/2} \otimes \bar{S}_{2j}(\lambda_3 h)\bar{S}_{2j}(\lambda_2 h)\bar{S}_{2j}(\lambda_1 h),$$

where $\lambda_1 = \lambda_2 = \lambda = \frac{1}{2-2^{1/(2j+1)}}$ and $\lambda_3 = \frac{1}{2} - 2\lambda$.

Using non-spinning second-order post-Newtonian approximated compact binaries without gravitational dissipation as a model, the newly constructed midpoint permutation phase space extension method S_{4B} demonstrates the highest numerical precision among periodic and chaotic orbits compared with implicit midpoint method IM4 and continuous coordinate-momentum permutation phase space extension method S_{4A}. In chaotic orbits, S_{4A} exhibits dramatic error divergence at half the integration time. Due to differences between H_1 and H_2, errors in both Hamiltonian components accumulate continuously during permutation processes in chaotic orbits, causing S_{4A} to fail.

Midpoint permutation methods can be extended to non-conservative gravitational dissipative Hamiltonian systems. Using spinning compact binaries with 2.5PN post-Newtonian approximation including gravitational dissipation, damped harmonic oscillators, and dust particles subject to Poynting-Robertson drag as models, midpoint permutation methods maintain optimal superiority, with computational precision, efficiency, and universality superior to other algorithms, warranting widespread adoption.

6.3 Extended Phase Space Optimized Forest-Ruth Algorithms

Wu Ya-lin et al. combined optimization ideas with phase space extension concepts to construct several optimized phase space extension symplectic-like algorithms, conducting numerical comparisons with other symplectic algorithms in one-dimensional non-separable integrable systems, planar circular restricted three-body problems, and third-order post-Newtonian non-spinning compact binary systems [30, 62].

6.3.1 Several Extended Phase Space Symplectic-Like Algorithms

(1) Continuous coordinate-momentum permutation extended phase space optimized algorithm: The middle operators of FR algorithm and its optimized version OFR were split following Liu and Wu's [26] high-order symplectic-like algorithm construction, modifying equations (10) and (16) to:

$$\text{EFR} = M_2 e^{Ach/2} e^{Bch} e^{A(1-c)h/2} e^{B(1-2c)h/2} M_1 e^{B(1-2c)h/2} e^{A(1-c)h/2} e^{Bch} e^{Ach/2},$$

$$\text{EOFR} = M_2 e^{B\xi h} e^{A(1-2\chi)h/2} e^{B\lambda h} e^{A\chi h} e^{B(1-2(\lambda+\xi))h/2} M_1 e^{B(1-2(\lambda+\xi))h/2} e^{A\chi h} e^{B\lambda h} e^{A(1-2\chi)h/2} e^{B\xi h}.$$

(2) Midpoint permutation extended phase space optimized algorithm: Following Luo et al.'s [29] midpoint permutation method, equations (10), (11), (16), and (17) are modified to:

$$\text{MFR} = M \otimes \text{FR}, \quad \text{MOFR} = M \otimes \text{OFR},$$

$$\text{MSU} = M \otimes \text{SU}.$$

(3) Tao's symplectic explicit algorithm: Tao [25] modified Pihajoki's method by reformulating the non-separable Hamiltonian system as:

$$\Gamma(p, \tilde{p}, q, \tilde{q}) = H_1(\tilde{p}, q) + H_2(p, \tilde{q}) + \omega H_3(p, \tilde{p}, q, \tilde{q}).$$

Here, the ωH_3 term is an artificially added constraint Hamiltonian function, where ω is a parameter controlling the separation between old and new phase space variables. H_1 and H_2 have analytical solutions, and operators A and B from Section 2 remain applicable, with H_3 being integrable. Operator $\bar{B}$ is defined as:

$$e^{h\bar{B}} = e^{\frac{h}{2}B} e^{hD} e^{\frac{h}{2}B},$$

where D is the operator for the H_3 component. This yields a new second-order explicit symplectic algorithm:

$$\bar{S}_2(h) = e^{\frac{h}{2}A} e^{h\bar{B}} e^{\frac{h}{2}A}.$$

Wu Ya-lin et al. applied Tao's method to modify FR and Suzuki algorithms:

$$\text{TYO} = \bar{S}_2(ah)\bar{S}_2((1-a)h)\bar{S}_2(ah),$$

$$\text{TSU} = \bar{S}_2(a_1 h)\bar{S}_2(a_2 h)\bar{S}_2((1-2a_1-2a_2)h)\bar{S}_2(a_2 h)\bar{S}_2(a_1 h).$$

Since no permutation factor is included, the algorithm's symplectic structure remains intact, with ωH_3 serving to constrain and regulate old and new space variables. The choice of ω significantly impacts precision.

6.3.2 Numerical Tests of Algorithms Numerical comparisons of the above algorithms in one-dimensional non-separable Hamiltonian systems, planar circular restricted three-body problems, and third-order post-Newtonian non-spinning compact binary systems show precision ranking from high to low as: M OFR MSU > MFR MYO > IM4 > EOFR TSU > EFR TYO. Overall, optimized algorithms achieve higher precision than unoptimized versions. All algorithms combined with midpoint permutation outperform those combined with Tao's method, reaching the precision of optimized fourth-order conventional explicit symplectic algorithms, while fourth-order implicit symplectic algorithms have the lowest computational efficiency. The TSU algorithm's precision depends on coefficient ω, achieving fourth-order precision when $\omega = 100$.

6.4 Extended Phase Space Logarithmic Hamiltonian Explicit Symmetric Method

Logarithmic Hamiltonian symplectic algorithms can adjust step sizes to avoid numerical distortion in high-eccentricity orbit problems, with simpler construction than general time-transformed symplectic algorithms. Extended phase space enables explicit symplectic algorithms to be applied to non-separable Hamiltonian systems with ideal precision. Li and Wu [31, 63] combined these ideas with Mikkola et al.'s [32, 64, 65] logarithmic Hamiltonian method by adding a constant or function, then incorporating Pihajoki's phase space extension concept to construct extended phase space logarithmic Hamiltonian symplectic-like algorithms with broader applicability. The basic Hamiltonian form is:

$$\Gamma(p, \tilde{p}, q, \tilde{q}, p_0, q_0) = \ln(T + p_0 + C) - \ln(U + C),$$

where $p_0 = -H$, $q_0 = t$, C is an integration constant with $C > 0$. When $C = 0$, this reduces to the logarithmic Hamiltonian method constructed and used by Mikkola and Su Xiang-ning [66]. Time transformation functions are $g = T + p_0 + C$ and $g = U + C$. When kinetic and potential parts of the Hamiltonian are separable, conventional explicit symplectic algorithms can be used; when inseparable, extended phase space concepts can be considered.

6.4.1 Extended Phase Space Logarithmic Hamiltonian Symplectic Algorithms Based on whether the system explicitly contains time t, Hamiltonian functions can be extended as:

(1) Time-independent:

$$\psi(p_0, p, \tilde{p}, q, \tilde{q}) = \Lambda_1(p_0, p, \tilde{q}) + \Lambda_2(p_0, \tilde{p}, q).$$

(2) Time-dependent:

$$\psi^*(p_0, p, \tilde{p}, \tilde{p}_0, q, \tilde{q}, q_0, \tilde{q}_0) = \Lambda_1(p_0, \tilde{q}_0, p, \tilde{q}) + \Lambda_2(\tilde{p}_0, q_0, \tilde{p}, q),$$

where $\tilde{p}_0, \tilde{q}_0$ are physical quantities in the extended phase space corresponding to p_0, q_0.

6.4.2 Numerical Tests Fourth-order explicit symplectic algorithm FR, fourth-order implicit midpoint method IS4 (identical to IM4 in Section 6.3.2), and three extended phase space algorithms S_{4A}, S_{4B}, and S_{4C} were applied to perturbed Kepler two-body problems, circular restricted three-body problems, and non-spinning third-order post-Newtonian compact binary systems. In all three models, algorithm S_{4C} consistently performs best. While implicit midpoint method IS4 also demonstrates excellent computational precision, it has the highest computational cost. Algorithm S_{4B} achieves precision comparable to IS4 with the lowest computational cost. Extended phase space logarithmic Hamiltonian explicit symplectic-like algorithms offer significant advantages in numerical stability, precision, and computational efficiency, and are applicable to high-eccentricity orbits.

This paper primarily compares the above algorithms in circular restricted three-body problems: fourth-order explicit symplectic algorithm FR, fourth-order implicit midpoint method IS4, continuous coordinate-momentum permutation phase space extension explicit algorithm EFR and its optimized version EOFR, midpoint permutation phase space extension explicit algorithm MFR and its optimized version MOFR. As shown in Figure 3 [Figure 3: see original paper], for low-eccentricity orbits, fourth-order explicit symplectic algorithm FR maintains stable energy error with high precision during long-term integration, but for high-eccentricity orbits, energy error begins to grow after long integration. When $c = 0$, continuous coordinate-momentum permutation EFR fourth-order algorithm and its optimized version EOFR are unsuitable for high-eccentricity orbits, with errors growing in short time. When $c = 1.7$, the precision of all phase space extension methods improves, and EFR and EOFR algorithms prevent linear energy error growth in high-eccentricity orbits, indicating that coefficient c selection is crucial. Additionally, midpoint permutation phase space extension methods MFR and MOFR achieve the highest computational efficiency, while fourth-order implicit algorithm IS4 has the lowest efficiency.

7 Summary and Outlook

Since their inception, symplectic algorithms—particularly explicit symplectic algorithms for separable Hamiltonian systems—have been widely applied in dynamical astronomy, demonstrating unparalleled advantages over traditional algorithms. In quantitative astronomical computations, symplectic algorithms can effectively control the continuous rapid growth of along-track orbit errors. However, for algorithms of the same order, symplectic algorithms have larger truncation errors than traditional methods such as Runge-Kutta, making their advantages less prominent in short-term integrations. Symplectic correction and pseudo-high-order symplectic algorithms improve algorithm precision without reducing integration step size through error correction, while time-transformed symplectic algorithms use variable step sizes to resolve numerical distortion issues in close encounters and high-eccentricity orbits. For non-separable Hamiltonian systems, implicit symplectic algorithms are highly suitable. Compared with traditional algorithms, they also guarantee system symplectic structure and energy error stability, but their computational efficiency is significantly reduced due to multiple iterations during integration. Extended phase space symplectic-like algorithms have developed rapidly in recent years, with Luo et al.'s [28, 29] midpoint permutation extended phase space method currently being the most ideal, offering high precision, efficiency, and broad applicability. Subsequently proposed extended phase space optimized FR algorithms [30, 62] and extended phase space logarithmic Hamiltonian explicit symplectic-like algorithms [31, 63] have confirmed this. Force-gradient symplectic algorithms, as a unique class of symplectic algorithms, offer great advantages in solving time-reversible Hamiltonian systems but face difficulties when Hamiltonian variables are non-separable.

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Note: Figure translations are in progress. See original paper for figures.