

SEMI-DISCRETIZATION AND FULL-DISCRETIZATION WITH IMPROVED ACCURACY FOR CHARGED-PARTICLE DYNAMICS IN A STRONG NONUNIFORM MAGNETIC FIELD

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Abstract. The aim of this paper is to formulate and analyze numerical discretizations of charged-particle dynamics (CPD) in a strong nonuniform magnetic field. A strategy is firstly performed for the two dimensional CPD to construct the semi-discretization and full-discretization which have improved accuracy. This accuracy is improved in the position and in the velocity when the strength of the magnetic field becomes stronger. This is a better feature than the usual so called “uniformly accurate methods”. To obtain this refined accuracy, some reformulations of the problem and two-scale exponential integrators are incorporated, and the improved accuracy is derived from this new procedure. Then based on the strategy given for the two dimensional case, a new class of uniformly accurate methods with simple scheme is formulated for the three dimensional CPD in maximal ordering case. All the theoretical results of the accuracy are numerically illustrated by some numerical tests.

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1. INTRODUCTION

The classical or relativistic description of the natural world is based on describing the interaction of elements of matter *via* force fields. One typical example is the system of plasmas which is composed by charged particles interacting *via* electric and magnetic fields. This system is of paramount importance and applications, comprising in plasma physics, astrophysics and magnetic fusion devices [1, 4]. Motivated by recent interest in numerical methods for the plasmas [2, 12–15, 17–23, 28, 34, 43, 46], this paper is devoted to charged-particle dynamics (CPD) in a strong nonuniform magnetic field. For such system of a large number of charged particles, its behavior can be described by the Vlasov equation [13, 14, 21]:

$$\begin{cases} \partial_t f(t, \mathbf{x}, \mathbf{v}) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{v}) + \left(\mathbf{E}(t, \mathbf{x}) + \mathbf{v} \times \frac{\mathbf{B}(t, \mathbf{x})}{\varepsilon} \right) \cdot \nabla_{\mathbf{v}} f(t, \mathbf{x}, \mathbf{v}) = 0, \\ \nabla_{\mathbf{x}} \cdot \mathbf{E}(t, \mathbf{x}) = \int_{\mathbb{R}^d} f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v} - n_i, \\ f(0, \mathbf{x}, \mathbf{v}) = f_0(\mathbf{x}, \mathbf{v}), \end{cases} \quad \begin{array}{l} 0 < t \leq T, \\ \mathbf{x}, \mathbf{v} \in \mathbb{R}^2 \text{ or } \mathbb{R}^3, \end{array} \quad (1.1)$$

Keywords and phrases. Charged particle dynamics, improved accuracy, strong nonuniform magnetic field, high oscillations, two-scale exponential integrators.

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where $f(t, \mathbf{x}, \mathbf{v})$ depends on the time t , the position $\mathbf{x}$ and the velocity $\mathbf{v}$, and represents the distribution of charged particles under the effects of the strongly external magnetic field $\frac{\mathbf{B}(t, \mathbf{x})}{\varepsilon}$ and the self-consistent electric-field function $\mathbf{E}(t, \mathbf{x})$. Here $0 < \varepsilon \ll 1$ determines the strength of the magnetic field, n_i denotes the ion density of the background, and $f_0(\mathbf{x}, \mathbf{v})$ is a given initial distribution.

For the numerical approximation of the Vlasov model (1.1), consider the Particle-In-Cell (PIC) approach [15, 17–19, 43]:

$$f_p(t, \mathbf{x}, \mathbf{v}) = \sum_{k=1}^{N_p} \omega_k \delta(\mathbf{x} - \mathbf{x}_k(t)) \delta(\mathbf{v} - \mathbf{v}_k(t)), \quad 0 < t \leq T, \quad (1.2)$$

where δ is the Dirac delta function and ω_k is the weight. Plugging (1.2) into (1.1) gives the equation on the characteristics:

$$\begin{cases} \dot{\mathbf{x}}_k(t) = \mathbf{v}_k(t), & \dot{\mathbf{v}}_k(t) = \mathbf{v}_k(t) \times \frac{\mathbf{B}(t, \mathbf{x}_k(t))}{\varepsilon} + \mathbf{E}(t, \mathbf{x}_k(t)), \\ \mathbf{x}_k(0) = \mathbf{x}_{k,0}, & \mathbf{v}_k(0) = \mathbf{v}_{k,0}. \end{cases} \quad 0 < t \leq T, \quad (1.3)$$

In practical computations, the Dirac delta function $\delta(\mathbf{x})$ is usually replaced by the particle shape functions [43] and hence the PIC approximation is accomplished by a particle pusher for (1.3).

For simplicity of notations and without loss of generality, from now on, we are concerned with the numerical solution of the following CPD with the same scheme of (1.3):

$$\dot{x}(t) = v(t), \quad \dot{v}(t) = v(t) \times \frac{B(x(t))}{\varepsilon} + E(x(t)), \quad 0 < t \leq T, \quad x(0) = x_0 \in \mathbb{R}^d, \quad v(0) = v_0 \in \mathbb{R}^d, \quad (1.4)$$

where $x(t) : (0, T] \rightarrow \mathbb{R}^d$ and $v(t) : (0, T] \rightarrow \mathbb{R}^d$ are respectively the unknown position and velocity of a charged particle with the dimension $d = 2$ or 3 , $E(x) \in \mathbb{R}^d$ is a given nonuniform electric-field function, $B(x) \in \mathbb{R}^d$ is a given magnetic field and $0 < \varepsilon \ll 1$ is a dimensionless parameter determining the strength of the magnetic field. For the two dimensional CPD (*i.e.*, $d = 2$), the system (1.4) can be formulated as

$$\dot{x}(t) = v(t), \quad \dot{v}(t) = \frac{b(x(t))}{\varepsilon} J v(t) + E(x(t)), \quad 0 < t \leq T, \quad x(0) = x_0 \in \mathbb{R}^2, \quad v(0) = v_0 \in \mathbb{R}^2, \quad (1.5)$$

with $b(x) : \mathbb{R}^2 \rightarrow \mathbb{R}$ satisfying $|b(x(t))| \geq C > 0$ and $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

For the CPD (1.4) or (1.5), it has a long research history in the physical literature [1, 3, 9, 35, 37]. Meanwhile, the modeling and simulation of CPD is of practical interest in scientific computing. After particle discretization of some kinetic models, the system (1.4) or (1.5) is a core problem which needs to be computed *via* effective numerical algorithms [12–15, 17–23, 34, 43]. Concerning the numerical algorithms for the CPD (1.4) or (1.5), two categories have been in the center of research according to different regimes of magnetic field: *normal magnetic field* $\varepsilon \approx 1$ and *strong magnetic field* $0 < \varepsilon \ll 1$.

Earlier studies are devoted to the normal regime $\varepsilon \approx 1$, comprising the well-known Boris method [5] as well as some further researches on it [24, 28, 40], volume-preserving algorithms [29], symmetric algorithms [25], symplectic algorithms [30, 44, 48, 49], variational integrators [26, 39], splitting integrators [33] and energy-preserving algorithms [7, 8, 36]. However, if those methods are applied to CPD with a strong magnetic field $0 < \varepsilon \ll 1$, this often adds a stringent restriction on the time step used in the numerical algorithms. The error constant of the methods mentioned above is usually proportional to $1/\varepsilon^p$ for some $p > 0$, which is unacceptable for small ε .

In order to handle this restriction, various novel methods with improved accuracy or uniform accuracy have been studied in recent years for CPD under a strong magnetic field with $0 < \varepsilon \ll 1$. An exponential energy-preserving integrator was formulated in [45] for (1.4) in a strong uniform magnetic field and uniform second order accuracy can be derived. In order to improve the asymptotic behaviour of the Boris method as $\varepsilon \rightarrow 0$, two filtered Boris algorithms were developed and analysed in [28] under the maximal ordering scaling [6, 38], *i.e.*, $B = B(\varepsilon x)$. Some splitting methods with uniform error bounds have been proposed and studied in [46].

Combined with the PIC discretization, some effective algorithms have been derived for the CPD (1.4) or (1.5) such as exponential integrators [23], asymptotic preserving schemes [18, 19, 21, 41], uniformly accurate schemes [13–15, 17, 47] and other efficient methods [12, 16, 20, 22].

Among those powerful numerical methods stated above for CPD in a strong magnetic field, the best accuracy is $\mathcal{O}(\varepsilon h^r)$ in the x and $\mathcal{O}(h^r)$ in the v with the time step size h and the order $r = 1, 2$, which is achieved for solving the two dimensional CPD in [13]. The main interest of this paper lies in a novel class of discretizations for solving the two dimensional CPD (1.5), capable of *having improved accuracy which is better than all the existing uniformly accurate algorithms when $0 < \varepsilon < 1$* . More preciously, we prove that *the novel discretizations have the accuracy $\mathcal{O}(\varepsilon^2 h^{2r})$ in the x and $\mathcal{O}(\varepsilon h^{2r})$ in the v , and thus as ε decreases, the method is more accurate in the approximation of both x and v* . This optical accuracy is very competitive in the computation of CPD in a strong nonuniform magnetic field. To get this refined accuracy, some reformulations of the problem and two-scale exponential integrators are incorporated into the formulation of the discretization. Meanwhile, based on the strategy given for the two dimensional case, we obtain a new kind of uniformly accurate algorithms with very simple scheme for the three dimensional CPD (1.4) under the maximal ordering scaling.

The outline of the paper is as follows. In Section 2, we propose the semi-discretization and rigorously prove its improved accuracy for the two dimensional CPD. The full-discretization and its improved accuracy are performed in Section 3. In Section 4, some practical discretizations are constructed and the numerical tests are displayed to support the theoretical results. Section 5 is devoted to the application to the three dimensional CPD in maximal ordering case and a class of uniformly accurate methods is discussed. Some conclusions are drawn in Section 6.

2. SEMI-DISCRETIZATION AND IMPROVED ACCURACY

2.1. Semi-discretization

In this part, we consider the two-scale formulation strategy which has been used in [13, 15]. For the two dimensional CPD (1.5), let us first define some new variables

$$\epsilon = \frac{\varepsilon}{b_0}, \quad q(t) = x(t), \quad p(t) = \epsilon v(t),$$

with $b_0 = b(q(0))$. Then one gets from (1.5) that

$$\dot{q}(t) = \frac{1}{\epsilon} p(t), \quad \dot{p}(t) = \frac{b(q(t))}{\epsilon b_0} J p(t) + \epsilon E(q(t)), \quad q(0) = x_0, \quad p(0) = \epsilon v_0. \quad (2.1)$$

Linearizing this system leads to

$$\dot{q}(t) = \frac{1}{\epsilon} p(t), \quad \dot{p}(t) = \frac{1}{\epsilon} J p(t) + F(q(t), p(t)), \quad q(0) = x_0, \quad p(0) = \epsilon v_0, \quad (2.2)$$

where

$$F(q(t), p(t)) = \frac{b(q(t)) - b_0}{\epsilon b_0} J p(t) + \epsilon E(q(t)).$$

By Lemma 2.4 given in the next subsection, it follows that $p(t) = \epsilon v(t) = \mathcal{O}(\epsilon)$. Then we notice that the function $F(q(t), p(t))$ is bounded.

Then letting

$$u(t) = q(t) - t/\epsilon \varphi_1(-tJ/\epsilon) p(t), \quad w(t) = \varphi_0(-tJ/\epsilon) p(t),$$

with $\varphi_0(z) = e^z$ and $\varphi_1(z) = (e^z - 1)/z$, equation (2.2) can be reformulated as

$$\begin{cases} \dot{u}(t) = -t/\epsilon \varphi_1(-tJ/\epsilon) F(u(t) + t/\epsilon \varphi_1(tJ/\epsilon) w(t), \varphi_0(tJ/\epsilon) w(t)), & u(0) = q(0), \\ \dot{w}(t) = \varphi_0(-tJ/\epsilon) F(u(t) + t/\epsilon \varphi_1(tJ/\epsilon) w(t), \varphi_0(tJ/\epsilon) w(t)), & w(0) = p(0). \end{cases} \quad (2.3)$$

Observing that $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, we deduce that

$$s\varphi_1(sJ) = \begin{pmatrix} \sin(s) & 1 - \cos(s) \\ -1 + \cos(s) & \sin(s) \end{pmatrix} \quad \text{and} \quad \varphi_0(sJ) = \begin{pmatrix} \cos(s) & \sin(s) \\ -\sin(s) & \cos(s) \end{pmatrix}.$$

This shows that $s\varphi_1(sJ)$ and $\varphi_0(sJ)$ are periodic in s on $[0, 2\pi]$. Therefore, the two-scale formulation [10] works for the transformed system (2.3) by considering t/ε as the fast time variable and t as the slow one. With another variable τ to denote the fast time variable t/ε , the two-scale pattern of (2.3) takes the form:

$$\begin{cases} \partial_t X(t, \tau) + \frac{1}{\varepsilon} \partial_\tau X(t, \tau) = -\tau \varphi_1(-\tau J) F(X(t, \tau) + \tau \varphi_1(\tau J) V(t, \tau), \varphi_0(\tau J) V(t, \tau)), \\ \partial_t V(t, \tau) + \frac{1}{\varepsilon} \partial_\tau V(t, \tau) = \varphi_0(-\tau J) F(X(t, \tau) + \tau \varphi_1(\tau J) V(t, \tau), \varphi_0(\tau J) V(t, \tau)), \end{cases} \quad (2.4)$$

where $X(t, \tau)$ and $V(t, \tau)$ are periodic in τ on the torus $\mathbb{T} = [0, 2\pi]$, and they satisfy $X(t, \tau) = u(t)$, $V(t, \tau) = w(t)$ at $\tau = t/\varepsilon$. For this new variable τ , it offers a free degree which can be used in designing initial values. The initial data for (2.4) is derived by using the strategy from [13], which is briefly introduced as follows.

With the notations $U(t, \tau) = [X(t, \tau); V(t, \tau)]$ and

$$f_\tau(U(t, \tau)) = \begin{pmatrix} -\tau \varphi_1(-\tau J) F(X(t, \tau) + \tau \varphi_1(\tau J) V(t, \tau), \varphi_0(\tau J) V(t, \tau)) \\ \varphi_0(-\tau J) F(X(t, \tau) + \tau \varphi_1(\tau J) V(t, \tau), \varphi_0(\tau J) V(t, \tau)) \end{pmatrix}, \quad (2.5)$$

first compute $\underline{U}^{[k]} = \underline{U}^{[0]} - \varepsilon B_0^{[k-1]}(\underline{U}^{[k-1]})$ with $\underline{U}^{[0]} = [x_0; \varepsilon v_0]$. Then the j -th order initial data for (2.4) is defined by

$$[X^0; V^0] := U^{[j]}(\tau) = \underline{U}^{[0]} + \varepsilon B_\tau^{[j]}(\underline{U}^{[j]}) - \varepsilon B_0^{[j]}(\underline{U}^{[j]}), \quad (2.6)$$

where the result of $B_\tau^{[k-1]}$ is derived by the recursion $B_\tau^{[0]} = 0$ and

$$B_\tau^{[k+1]}(U) = L^{-1}(I - \Pi) f_\tau(U + \varepsilon B_\tau^{[k]}(U)) - \frac{L^{-1}}{\varepsilon^{k-1}} \left[B_\tau^{[k]}(U + \varepsilon^k \Pi f_\tau(U + \varepsilon B_\tau^{[k]}(U))) - B_\tau^{[k]}(U) \right].$$

In this paper, I is the identity operator, Π denotes the averaging operator defined by $\Pi \vartheta := \frac{1}{2\pi} \int_0^{2\pi} \vartheta(s) ds$ for some $\vartheta(\cdot)$ on $\mathbb{T}$ and $L := \partial_\tau$ is invertible with inverse defined by $(L^{-1} \vartheta)(\tau) = (I - \Pi) \int_0^\tau \vartheta(s) ds$.

For the two-scale system (2.4), we now discrete t but keep τ , which leads to the following semi-discrete scheme.

Definition 2.1 (Semi-discrete scheme). For solving the CPD system (1.5), the semi-discrete scheme is defined as follows with a time step size h .

Step 1. The initial data of (2.4) is derived from (2.6) with $j = 4^1$ and we denote it as $[X^0; V^0] = U^{[4]}(\tau)$.

Step 2. For solving the two-scale system (2.4), the following s -stage two-scale exponential integrator is considered

$$\begin{aligned} X^{ni} &= \varphi_0(c_i h / \varepsilon \partial_\tau) X^n - h \sum_{j=1}^s \bar{a}_{ij}(h / \varepsilon \partial_\tau) \tau \varphi_1(-\tau J) F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj}), \quad i = 1, 2, \dots, s, \\ V^{ni} &= \varphi_0(c_i h / \varepsilon \partial_\tau) V^n + h \sum_{j=1}^s \bar{a}_{ij}(h / \varepsilon \partial_\tau) \varphi_0(-\tau J) F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj}), \quad i = 1, 2, \dots, s, \\ X^{n+1} &= \varphi_0(h / \varepsilon \partial_\tau) X^n - h \sum_{j=1}^s \bar{b}_j(h / \varepsilon \partial_\tau) \tau \varphi_1(-\tau J) F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj}), \end{aligned}$$

¹We make this choice since exponential integrators up to order four are considered in this paper.

TABLE 1. Stiff order conditions with any bounded operators K and A .

Stiff order conditions	Order
$\psi_1(h/\epsilon\partial_\tau) = 0$	1
$\psi_2(h/\epsilon\partial_\tau) = 0$	2
$\psi_{1,i}(h/\epsilon\partial_\tau) = 0$	2
$\psi_3(h/\epsilon\partial_\tau) = 0$	3
$\sum_{i=1}^s \bar{b}_i(h/\epsilon\partial_\tau) K \psi_{2,i}(h/\epsilon\partial_\tau) = 0$	3
$\psi_4(h/\epsilon\partial_\tau) = 0$	4
$\sum_{i=1}^s \bar{b}_i(h/\epsilon\partial_\tau) K \psi_{3,i}(h/\epsilon\partial_\tau) = 0$	4
$\sum_{i=1}^s \bar{b}_i(h/\epsilon\partial_\tau) K \sum_{j=1}^s \bar{a}_{ij}(h/\epsilon\partial_\tau) A \psi_{2,i}(h/\epsilon\partial_\tau) = 0$	4
$\sum_{i=1}^s \bar{b}_i(h/\epsilon\partial_\tau) c_i K \psi_{2,i}(h/\epsilon\partial_\tau) = 0$	4

$$V^{n+1} = \varphi_0(h/\epsilon\partial_\tau)V^n + h \sum_{j=1}^s \bar{b}_j(h/\epsilon\partial_\tau) \varphi_0(-\tau J) F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj}), \quad (2.7)$$

where $\bar{a}_{ij}(h/\epsilon\partial_\tau)$ and $\bar{b}_j(h/\epsilon\partial_\tau)$ are uniformly bounded functions which will be determined in Section 4.

Step 3. The numerical solution $x^{n+1} \approx x(t_{n+1})$ and $v^{n+1} \approx v(t_{n+1})$ of (1.5) is defined by

$$x^{n+1} = X^{n+1} + \frac{t_{n+1}}{\epsilon} \varphi_1(t_{n+1}J/\epsilon) V^{n+1}, \quad v^{n+1} = \frac{1}{\epsilon} \varphi_0(t_{n+1}J/\epsilon) V^{n+1},$$

where $t_{n+1} = (n+1)h$.

2.2. Improved accuracy

In this present part, we derive the improved accuracy of the semi-discrete scheme given in Definition 2.1. For simplicity of notations, we shall denote $C > 0$ a generic constant independent of the time step h or ϵ or n . In this section, we use the norm $\|\cdot\|$ of a vector to denote the standard euclidian norm and that of a scalar quantity refers to the absolute value. Meanwhile, let $L_t^\infty := L_t^\infty([0, T])$ and $L_\tau^\infty := L_\tau^\infty([0, 2\pi])$ denote the functional spaces in t and τ variables, respectively. For a smooth periodic function $\vartheta(\tau)$ on $[0, 2\pi]$, define its $W_\tau^{1,\infty}$ -norm as [13] $\|\vartheta\|_{W_\tau^{1,\infty}} := \max\{\|\vartheta\|_{L_\tau^\infty}, \|\partial_\tau \vartheta\|_{L_\tau^\infty}\}$, and for a smooth vector field $\mathcal{V}(\tau) = \begin{pmatrix} \vartheta_1 \\ \vartheta_2 \end{pmatrix}$ on $[0, 2\pi]$, introduce $\|\mathcal{V}\|_{W_\tau^{1,\infty}} := \max\{\|\vartheta_1\|_{W_\tau^{1,\infty}}, \|\vartheta_2\|_{W_\tau^{1,\infty}}\}$. The main result is stated by the following theorem.

Theorem 2.2 (Improved accuracy). *It is assumed that the nonlinear functions $E(x)$ and $b(x)$ are globally Lipschitz functions, i.e.,*

$$\|E(x_1) - E(x_2)\| \leq C\|x_1 - x_2\|, \quad \|b(x_1) - b(x_2)\| \leq C\|x_1 - x_2\|, \quad \text{for all } x_1, x_2 \in \mathbb{R}^2. \quad (2.8)$$

Let $\varphi_k(z) = \int_0^1 \theta^{k-1} e^{(1-\theta)z} / (k-1)! d\theta$ for $k = 2, 3, \dots$ [32] and

$$\psi_j(z) = \varphi_j(z) - \sum_{k=1}^s \bar{b}_k(z) \frac{c_k^{j-1}}{(j-1)!}, \quad \psi_{j,i}(z) = \varphi_j(c_i z) c_i^j - \sum_{k=1}^s \bar{a}_{ik}(z) \frac{c_k^{j-1}}{(j-1)!}, \quad i = 1, 2, \dots, s.$$

Choose $r = 2$ or 4 . Assume that the conditions of order $r - 1$ given in Table 1 are true and for those of order r , the first one has the form $\psi_r(0) = 0$ and the others hold in a weaker form with $\bar{b}_i(0)$ instead of $\bar{b}_i(h/\epsilon\partial_\tau)$ for $1 \leq i \leq s$. Under the conditions stated above, the global error of the semi-discrete scheme given in Definition 2.1 is

$$\|x^n - x(t_n)\| + \|\epsilon v^n - \epsilon v(t_n)\| \leq C\epsilon^2 h^r, \quad 0 \leq n \leq T/h,$$

where C is independent of n, h, ϵ .

Remark 2.3. We note that this improved accuracy is a better feature than the usual so called “uniformly accurate methods” [13–15, 17] when $0 < \varepsilon < 1$. As ε decreases, the accuracy is improved to be $\mathcal{O}(\varepsilon^2 h^r)$ in the x and $\mathcal{O}(\varepsilon h^r)$ in the v , which is very competitive in the scientific computing of CPD with strong nonuniform magnetic field. For the case that $\varepsilon > 1$, normal numerical methods can be considered such as Runge–Kutta methods and they will work well.

To derive this improved accuracy, we first present four lemmas and then give its proof.

Lemma 2.4. Under the assumptions (2.8) and the condition that $\|x_0\| + \|v_0\| \leq C$, the solution of (2.1) satisfies

$$\|q(t)\| + \|p(t)/\epsilon\| \leq C, \quad \text{for all } t \in (0, T]. \quad (2.9)$$

Moreover, we have

$$\|b(q(t)) - b(q(0))\| \leq C\epsilon, \quad \text{for all } t \in (0, T].$$

Proof. This result can be shown in a similar way of [13]. With the new notation $\tilde{p}(t) := e^{-Jt/\epsilon} p(t)$, the system (2.1) reads

$$\dot{q}(t) = \frac{1}{\epsilon} \varphi_0(Jt/\epsilon) \tilde{p}(t), \quad \dot{\tilde{p}}(t) = \varphi_0(-Jt/\epsilon) F(q(t), \varphi_0(Jt/\epsilon) \tilde{p}(t)), \quad q(0) = x_0, \quad \tilde{p}(0) = \epsilon v_0. \quad (2.10)$$

We first take the inner product on both sides of (2.10) with $q(t)$ and $\tilde{p}(t)$ and then use Cauchy–Schwarz inequality to get

$$\frac{d}{dt} \|q(t)\|^2 \leq \frac{2}{\epsilon} \|q(t)\| \|\tilde{p}(t)\|, \quad \frac{d}{dt} \|\tilde{p}(t)\|^2 \leq 2\epsilon \|E(q(t))\| \|\tilde{p}(t)\|.$$

These estimates can be simplified as

$$\frac{d}{dt} \|q(t)\| \leq \frac{2}{\epsilon} \|\tilde{p}(t)\|, \quad \frac{d}{dt} \|\tilde{p}(t)\| \leq 2\epsilon \|E(q(t))\| \leq 2\epsilon \|E(q(0))\| + 2\epsilon C \|q(t)\| + 2\epsilon C \|q(0)\|.$$

The bound (2.9) is deduced from these two inequalities and Gronwall’s inequality.

To prove the second statement, we integrate the first equation in (2.10)

$$q(t) = q(0) + \int_0^t \frac{1}{\epsilon} \varphi_0(J\xi/\epsilon) \tilde{p}(\xi) d\xi = q(0) - J(\varphi_0(Jt/\epsilon) \tilde{p}(t) - \tilde{p}(0)) + J \int_0^t \varphi_0(J\xi/\epsilon) \dot{\tilde{p}}(\xi) d\xi.$$

By inserting the second equation of (2.10), it is obtained that

$$\begin{aligned} q(t) &= q(0) - J(\varphi_0(Jt/\epsilon) \tilde{p}(t) - \tilde{p}(0)) + J \int_0^t \varphi_0(J\xi/\epsilon) \varphi_0(-J\xi/\epsilon) F(q(\xi), \varphi_0(J\xi/\epsilon) \tilde{p}(\xi)) d\xi \\ &= q(0) - J(\varphi_0(Jt/\epsilon) \tilde{p}(t) - \tilde{p}(0)) + J \int_0^t \left(\frac{b(q(\xi)) - b_0}{\epsilon b_0} J \varphi_0(J\xi/\epsilon) \tilde{p}(\xi) + \epsilon E(q(\xi)) \right) d\xi, \end{aligned}$$

so that

$$\|q(t) - q(0)\| \leq \|\varphi_0(Jt/\epsilon) \tilde{p}(t) - \tilde{p}(0)\| + \int_0^t \left\| \frac{b(q(\xi)) - b_0}{\epsilon b_0} J \varphi_0(J\xi/\epsilon) \tilde{p}(\xi) \right\| d\xi + \epsilon T \sup_{0 \leq t \leq T} \|E(q(t))\|$$

$$\leq C\epsilon + C\epsilon \int_0^t \|q(\xi) - q(0)\| d\xi + \epsilon T \sup_{0 \leq t \leq T} \|E(q(t))\|.$$

According to Gronwall's inequality, we obtain the estimate $\|q(t) - q(0)\| \leq C\epsilon$ and this leads to the second result of this lemma. $\square$

Lemma 2.5. *Under the assumptions (2.8), $E(x) \in C^r(\mathbb{R}^2)$ and $b(x) \in C^r(\mathbb{R}^2)$, the solution of (2.4) with the initial value $U^{[r]}(\tau)$ and its derivatives w.r.t. t are bounded by*

$$\begin{aligned} \|X(t, \tau)\|_{L_t^\infty(W_\tau^{1,\infty})} &\leq C, & \|V(t, \tau)\|_{L_t^\infty(W_\tau^{1,\infty})} &\leq C\epsilon, \\ \|\partial_t^k X(t, \tau)\|_{L_t^\infty(W_\tau^{1,\infty})} &\leq C\epsilon, & \|\partial_t^k V(t, \tau)\|_{L_t^\infty(W_\tau^{1,\infty})} &\leq C\epsilon, \end{aligned} \quad (2.11)$$

where $k = 1, 2, \dots, r$ and $0 \leq t \leq t_0$ for some $t_0 > 0$.

Proof. According to the Chapman–Enskog expansion, the solution of (2.4) can be partitioned into two parts

$$\begin{aligned} X(t, \tau) &= \underline{X}(t) + \bar{\varphi}(t, \tau) \quad \text{with} \quad \underline{X}(t) = \Pi X(t, \tau), & \Pi \bar{\varphi}(t, \tau) &= 0, \\ V(t, \tau) &= \underline{V}(t) + \bar{\psi}(t, \tau) \quad \text{with} \quad \underline{V}(t) = \Pi V(t, \tau), & \Pi \bar{\psi}(t, \tau) &= 0, \end{aligned}$$

where the averaging operator is defined by $\Pi X(t, \tau) := \frac{1}{2\pi} \int_0^{2\pi} X(t, \tau) d\tau$. These composers satisfy the differential equations

$$\begin{aligned} \dot{\underline{X}}(t) &= \Pi(-\tau\varphi_1(-\tau J)F(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau), \varphi_0(\tau J)V(t, \tau))), \\ \dot{\underline{V}}(t) &= \Pi(\varphi_0(-\tau J)F(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau), \varphi_0(\tau J)V(t, \tau))), \\ \partial_t \bar{\varphi}(t, \tau) + \frac{1}{\epsilon} \partial_\tau \bar{\varphi}(t, \tau) &= (I - \Pi)(-\tau\varphi_1(-\tau J)F(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau), \varphi_0(\tau J)V(t, \tau))), \\ \partial_t \bar{\psi}(t, \tau) + \frac{1}{\epsilon} \partial_\tau \bar{\psi}(t, \tau) &= (I - \Pi)(\varphi_0(-\tau J)F(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau), \varphi_0(\tau J)V(t, \tau))). \end{aligned}$$

For this system, we first derive the bound of its solution, which is accomplished by the initial value (2.6). The first order initial value is

$$\begin{aligned} U^{[1]}(\tau) &= \underline{U}^{[0]} + \epsilon B_\tau^{[1]}(\underline{U}^{[1]}) - \epsilon B_0^{[1]}(\underline{U}^{[1]}) + O(\epsilon^2) \\ &= \underline{U}^{[0]} + \epsilon B_\tau^{[1]}(\underline{U}^{[0]} - \epsilon B_0^{[0]}(\underline{U}^{[0]})) - \epsilon B_0^{[1]}(\underline{U}^{[0]} - \epsilon B_0^{[0]}(\underline{U}^{[0]})) + O(\epsilon^2) \\ &= \underline{U}^{[0]} + \epsilon B_\tau^{[1]}(\underline{U}^{[0]}) - \epsilon B_0^{[1]}(\underline{U}^{[0]}) + O(\epsilon^2) \\ &= \underline{U}^{[0]} + \epsilon L^{-1}(I - \Pi)f_\tau(\underline{U}^{[0]}) - \epsilon L^{-1}(I - \Pi)f_0(\underline{U}^{[0]}) + O(\epsilon^2). \end{aligned}$$

Noticing that Π and $L^{-1}(I - \Pi)$ are bounded operators, one deduces that $U^{[1]}(\tau)$ is uniformly bounded w.r.t. ϵ . This procedure can be continued and the uniform bound (w.r.t. ϵ) can be obtained for $U^{[k]}(\tau)$ with $k = 2, 3, \dots, r$. Using the same strategy as in the proof of Lemma 2.4, we get that for the two-scale problem (2.4), with the initial value $U^{[k]}(\tau)$ for any $k = 0, 1, \dots$, $X(t, \tau) = O(1)$, $V(t, \tau) = O(\epsilon)$ and $X(t, \tau) - X(0, \tau) = O(\epsilon)$. Combining the fact that $b(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau)) - b_0 = O(\epsilon)$ of Lemma 2.4 leads to

$$\begin{aligned} F(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau), \varphi_0(\tau J)V(t, \tau)) &= \frac{b(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau)) - b_0}{\epsilon b_0} J\varphi_0(\tau J)V(t, \tau) \\ &\quad + \epsilon E(X(t, \tau) + \tau\varphi_1(\tau J)V(t, \tau)) = O(\epsilon). \end{aligned} \quad (2.12)$$

Then for the first derivatives $\partial_t X(t, \tau)$ and $\partial_t V(t, \tau)$, they satisfy the equation

$$\begin{aligned}\partial_t(\partial_t X(t, \tau)) + \frac{1}{\epsilon} \partial_\tau(\partial_t X(t, \tau)) &= -\tau \varphi_1(-\tau J)(F_1(\partial_t X(t, \tau) + \tau \varphi_1(\tau J) \partial_t V(t, \tau)) + F_2 \varphi_0(\tau J) \partial_t V(t, \tau)), \\ \partial_t(\partial_t V(t, \tau)) + \frac{1}{\epsilon} \partial_\tau(\partial_t V(t, \tau)) &= \varphi_0(-\tau J)(F_1(\partial_t X(t, \tau) + \tau \varphi_1(\tau J) \partial_t V(t, \tau)) + F_2 \varphi_0(\tau J) \partial_t V(t, \tau)),\end{aligned}\quad (2.13)$$

where $F_j = \partial_{U_j} F(U_1, U_2) |_{U_1=X(t,\tau)+\tau\varphi_1(\tau J)V(t,\tau), U_2=\varphi_0(\tau J)V(t,\tau)}$ for $j = 1, 2$. The initial value of (2.13) is given by

$$\begin{aligned}[\partial_t X(t, \tau)|_{t=0}; \partial_t V(t, \tau)|_{t=0}] &= -\frac{1}{\epsilon} \partial_\tau [X^0; V^0] + \begin{pmatrix} -\tau \varphi_1(-\tau J) F(X^0 + \tau \varphi_1(\tau J) V^0, \varphi_0(\tau J) V^0) \\ \varphi_0(-\tau J) F(X^0 + \tau \varphi_1(\tau J) V^0, \varphi_0(\tau J) V^0) \end{pmatrix} \\ &= -\frac{1}{\epsilon} \partial_\tau \left(\epsilon L^{-1} (I - \Pi) f_\tau(\underline{U}^{[0]}) - \epsilon L^{-1} (I - \Pi) f_0(\underline{U}^{[0]}) \right) + O(\epsilon) \\ &= (I - \Pi) \left(f_0(\underline{U}^{[0]}) - f_\tau(\underline{U}^{[0]}) \right) + O(\epsilon) = O(\epsilon).\end{aligned}$$

This initial value and the fact that $F_1 = O(\epsilon), F_2 = O(\epsilon)$ yield

$$\|\partial_t X(t, \tau)\|_{L^\infty_\tau(L^\infty)} \leq C\epsilon, \quad \|\partial_t V(t, \tau)\|_{L^\infty_\tau(L^\infty)} \leq C\epsilon.$$

In an analogous way, we can derive the bounds of the j th derivatives $\partial_t^j X(t, \tau)$ and $\partial_t^j V(t, \tau)$ with $j = 2, 3, \dots, r$.

By differentiating the above system with respect to τ and in a similar way, we obtain the bounds with $W_\tau^{1,\infty}$ estimates. The proof of this lemma is complete. $\square$

Lemma 2.6 (Boundedness of the schemes). *If (x_0, v_0) is uniformly bounded, there exists a sufficiently small $0 < h_0 \leq 1$ such that when $h \leq h_0$, we have the following bounds for the integrator (2.7) with $i = 1, 2, \dots, s$*

$$\|X^{ni}\|_{L^\infty_\tau} \leq C, \quad \|V^{ni}/\epsilon\|_{L^\infty_\tau} \leq C, \quad \|X^{n+1}\|_{L^\infty_\tau} \leq C, \quad \|V^{n+1}/\epsilon\|_{L^\infty_\tau} \leq C, \quad 0 \leq n < T/h.$$

Proof. For all ϵ and h , it is true that $\|\varphi_0(h/\epsilon \partial_\tau)\|_{L^\infty_\tau} = 1$, and $\|\varphi_j(h/\epsilon \partial_\tau)\|_{L^\infty_\tau}$ for $j = 1, 2, \dots$, are uniformly bounded. According to the fact that the coefficients of exponential integrators are composed of φ -functions, we have $\|\bar{a}_{ij}(h/\epsilon \partial_\tau)\|_{L^\infty_\tau} \leq C$ and $\|\bar{b}_j(h/\epsilon \partial_\tau)\|_{L^\infty_\tau} \leq C$ for $i, j = 1, 2, \dots, s$, where the constant C is independent of h, ϵ .

We first prove the boundedness for a single time step of explicit methods. Assume that the numerical solution satisfies $\|X^n\|_{L^\infty_\tau} \leq C$ and $\|V^n/\epsilon\|_{L^\infty_\tau} \leq C$, then we have the estimates for $n+1$:

$$\begin{aligned}\|X^{ni}\|_{L^\infty_\tau} &\leq \|X^n\|_{L^\infty_\tau} + hC \sum_{j=1}^{i-1} \|F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj})\|_{L^\infty_\tau}, \quad i = 1, 2, \dots, s, \\ \|V^{ni}\|_{L^\infty_\tau} &\leq \|V^n\|_{L^\infty_\tau} + hC \sum_{j=1}^{i-1} \|F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj})\|_{L^\infty_\tau}, \quad i = 1, 2, \dots, s, \\ \|X^{n+1}\|_{L^\infty_\tau} &\leq \|X^n\|_{L^\infty_\tau} + hC \sum_{j=1}^s \|F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj})\|_{L^\infty_\tau}, \\ \|V^{n+1}\|_{L^\infty_\tau} &\leq \|V^n\|_{L^\infty_\tau} + hC \sum_{j=1}^s \|F(X^{nj} + \tau \varphi_1(\tau J) V^{nj}, \varphi_0(\tau J) V^{nj})\|_{L^\infty_\tau}.\end{aligned}$$

Based on the bounds of F and $X^n, V^n/\epsilon$, the boundedness of $X^{n+1}, V^{n+1}/\epsilon$ is immediately obtained.

Then for a single time step of implicit methods, iterative solutions are needed. In this paper we consider the fixed point iterative pattern:

$$\begin{aligned}
 (X^{ni})^{[0]} &= \varphi_0(c_i h / \epsilon \partial_\tau) X^n - h \sum_{j=1}^s \bar{a}_{ij}(h / \epsilon \partial_\tau) \tau \varphi_1(-\tau J) F(X^n + \tau \varphi_1(\tau J) V^n, \varphi_0(\tau J) V^n), \\
 (V^{ni})^{[0]} &= \varphi_0(c_i h / \epsilon \partial_\tau) V^n + h \sum_{j=1}^s \bar{a}_{ij}(h / \epsilon \partial_\tau) \varphi_0(-\tau J) F(X^n + \tau \varphi_1(\tau J) V^n, \varphi_0(\tau J) V^n), \\
 (X^{ni})^{[m+1]} &= \varphi_0(h / \epsilon \partial_\tau) X^n - h \sum_{j=1}^s \bar{b}_j(h / \epsilon \partial_\tau) \tau \varphi_1(-\tau J) F\left((X^{nj})^{[m]} + \tau \varphi_1(\tau J)(V^{nj})^{[m]}, \varphi_0(\tau J)(V^{nj})^{[m]}\right), \\
 (V^{ni})^{[m+1]} &= \varphi_0(h / \epsilon \partial_\tau) V^n + h \sum_{j=1}^s \bar{b}_j(h / \epsilon \partial_\tau) \varphi_0(-\tau J) F\left((X^{nj})^{[m]} + \tau \varphi_1(\tau J)(V^{nj})^{[m]}, \varphi_0(\tau J)(V^{nj})^{[m]}\right), \\
 & \qquad \qquad \qquad m = 0, 1, \dots \quad (2.14)
 \end{aligned}$$

With the boundedness of $X^n, V^n / \epsilon$, the coefficients and the nonlinear function F , it is easy to derive the boundedness of $(X^{ni})^{[m+1]}, (V^{ni})^{[m+1]} / \epsilon$ and then of $X^{n+1}, V^{n+1} / \epsilon$.

Finally, considering the above results and using the mathematical induction, the boundedness of explicit or implicit numerical solutions (2.7) as shown in this lemma over a long time interval is arrived. $\square$

Lemma 2.7 (Remainders). *Inserting the exact solution of (2.4) into the numerical approximation (2.7), we get*

$$\begin{aligned}
 X(t_n + c_i h, \tau) &= \varphi_0(c_i h / \epsilon \partial_\tau) X(t_n, \tau) - h \sum_{j=1}^s \bar{a}_{ij}(h / \epsilon \partial_\tau) \tau \varphi_1(-\tau J) G(X(t_n + c_j h, \tau), V(t_n + c_j h, \tau)) + \Delta_X^{ni}, \\
 V(t_n + c_i h, \tau) &= \varphi_0(c_i h / \epsilon \partial_\tau) V(t_n, \tau) + h \sum_{j=1}^s \bar{a}_{ij}(h / \epsilon \partial_\tau) \varphi_0(-\tau J) G(X(t_n + c_j h, \tau), V(t_n + c_j h, \tau)) + \Delta_V^{ni}, \\
 X(t_n + h, \tau) &= \varphi_0(h / \epsilon \partial_\tau) X(t_n, \tau) - h \sum_{j=1}^s \bar{b}_j(h / \epsilon \partial_\tau) \tau \varphi_1(-\tau J) G(X(t_n + c_j h, \tau), V(t_n + c_j h, \tau)) + \delta_X^{n+1}, \\
 V(t_n + h, \tau) &= \varphi_0(h / \epsilon \partial_\tau) V(t_n, \tau) + h \sum_{j=1}^s \bar{b}_j(h / \epsilon \partial_\tau) \varphi_0(-\tau J) G(X(t_n + c_j h, \tau), V(t_n + c_j h, \tau)) + \delta_V^{n+1}, \quad (2.15)
 \end{aligned}$$

where $\Delta_X^{ni}, \Delta_V^{ni}, \delta_X^{n+1}, \delta_V^{n+1}$ are the remainders and $G(X, V) := F(X + \tau \varphi_1(\tau J) V, \varphi_0(\tau J) V)$. Under the conditions of Theorem 2.2 and the local assumptions of $X^n = X(t_n, \tau), V^n = V(t_n, \tau)$, the remainders are bounded for $i = 1, 2, \dots, s$ and $0 \leq n < T/h$

$$\|\Delta_X^{ni}\|_{W_\tau^{1,\infty}} \leq C\epsilon^2 h^r, \quad \|\Delta_V^{ni}\|_{W_\tau^{1,\infty}} \leq C\epsilon^2 h^r, \quad \|\delta_X^{n+1}\|_{W_\tau^{1,\infty}} \leq C\epsilon^2 h^{r+1}, \quad \|\delta_V^{n+1}\|_{W_\tau^{1,\infty}} \leq C\epsilon^2 h^{r+1}.$$

Proof. Since the variable τ plays essentially no role in subsequent computations of the proof, we shall omit it for brevity. From the Duhamel principle, it is clear that

$$\begin{aligned}
 X(t_n + c_i h) &= \varphi_0(c_i h / \epsilon \partial_\tau) X(t_n) - \int_0^{c_i h} e^{(\theta - c_i h) \frac{\partial_\tau}{\epsilon}} \tau \varphi_1(-\tau J) G(X(t_n + \theta), V(t_n + \theta)) d\theta, \\
 V(t_n + c_i h) &= \varphi_0(c_i h / \epsilon \partial_\tau) V(t_n) + \int_0^{c_i h} e^{(\theta - c_i h) \frac{\partial_\tau}{\epsilon}} \varphi_0(-\tau J) G(X(t_n + \theta), V(t_n + \theta)) d\theta, \\
 X(t_n + h) &= \varphi_0(h / \epsilon \partial_\tau) X(t_n) - \int_0^h e^{(\theta - h) \frac{\partial_\tau}{\epsilon}} \tau \varphi_1(-\tau J) G(X(t_n + \theta), V(t_n + \theta)) d\theta,
 \end{aligned}$$

$$V(t_n + h) = \varphi_0(h/\epsilon\partial_\tau)V(t_n) + \int_0^h e^{(\theta-h)\frac{\partial_\tau}{\epsilon}} \varphi_0(-\tau J)G(X(t_n + \theta), V(t_n + \theta)) d\theta.$$

Subtracting this expression from (2.15) gives the equations of remainders

$$\begin{aligned} [\Delta_X^{ni}; \Delta_V^{ni}] &= [X(t_n + c_i h); V(t_n + c_i h)] - (\varphi_0(c_i h/\epsilon\partial_\tau) \otimes \text{diag}(1, 1))[X(t_n); V(t_n)] \\ &\quad + h \sum_{j=1}^s (\bar{a}_{ij}(h/\epsilon\partial_\tau) \otimes \text{diag}(1, 1))G(t_n + c_j h), \\ [\delta_X^{n+1}; \delta_V^{n+1}] &= [X(t_n + h); V(t_n + h)] - (\varphi_0(h/\epsilon\partial_\tau) \otimes \text{diag}(1, 1))[X(t_n); V(t_n)] \\ &\quad + h \sum_{j=1}^s (\bar{b}_j(h/\epsilon\partial_\tau) \otimes \text{diag}(1, 1))G(t_n + c_j h), \end{aligned}$$

where we use the notation $G(t) := [-\tau\varphi_1(-\tau J)G(X(t), V(t)); \varphi_0(-\tau J)G(X(t), V(t))]$ and the Kronecker product $\otimes$. Applying Taylor expansions, one gets

$$\begin{aligned} [\delta_X^{n+1}; \delta_V^{n+1}] &= h\epsilon \int_0^1 (\varphi_0((1-\xi)c_i h/\epsilon\partial_\tau) \otimes \text{diag}(1, 1)) \sum_{j=0}^{\infty} \frac{(\xi c_i h)^j}{j!} \frac{d^j}{dt^j} G(t_n) d\xi \\ &\quad - h\epsilon \sum_{k=1}^s (\bar{b}_k(h/\epsilon\partial_\tau) \otimes \text{diag}(1, 1)) \sum_{j=0}^{\infty} \frac{c_k^j h^j}{j!} \frac{d^j}{dt^j} G(t_n) \\ &= h\epsilon \sum_{j=0}^{\infty} h^j (\psi_j(h/\epsilon\partial_\tau) \otimes \text{diag}(1, 1)) \frac{d^j}{dt^j} G(t_n). \end{aligned}$$

Following the analysis of [31], the bounds of δ_X^{n+1} and δ_V^{n+1} given in this lemma are deduced from the stiff order conditions presented in Theorem 2.2 and the bound (2.11). In an analogous way, we proceed for the bound of Δ_X^{ni} and Δ_V^{ni} , and the proof of Lemma 2.7 is complete. $\square$

Proof of Theorem 2.2. Based on the above preparations, we are ready to derive the error bounds of Theorem 2.2. Before presenting the proof, we note here that how the previous lemmas (Lems. 2.4–2.7) fit together to get the improved accuracy.

- To derive the global errors given in Theorem 2.2, the boundedness and local errors of numerical solutions are needed which are estimated by Lemmas 2.6 and 2.7, respectively.
- In the study of local errors, we consider the Taylor series of nonlinearity which includes the solution of (2.4) and its derivatives w.r.t. t . Thus the local errors depend on the bounds of the solution of (2.4) and its derivatives which are derived by Lemma 2.5.
- To get the estimates proposed in Lemma 2.5, we use the result of Lemma 2.4 and the improved bounds on $\partial_t^k V(t, \tau)$, $\partial_t^k V(t, \tau)$ with $k = 1, 2, \dots, r$ lead to improved bounds of local errors given in Lemma 2.7, which finally result in the improved accuracy of Theorem 2.2.

Define the error functions by

$$e_X^n := X(t_n, \tau) - X^n, \quad e_V^n := V(t_n, \tau) - V^n, \quad E_X^{ni} := X(t_n + c_i h, \tau) - X^{ni}, \quad E_V^{ni} := V(t_n + c_i h, \tau) - V^{ni}.$$

Subtracting the scheme of the method (2.7) from (2.15) gives the error recursions

$$E_X^{ni} = \varphi_0(c_i h/\epsilon\partial_\tau)e_X^n + h \sum_{j=1}^s \bar{a}_{ij}(h/\epsilon\partial_\tau)\delta G^{nj} + \Delta_X^{ni},$$

$$\begin{aligned}
E_V^{ni} &= \varphi_0(c_i h / \epsilon \partial_\tau) e_V^n + h \sum_{j=1}^s \bar{a}_{ij}(h / \epsilon \partial_\tau) \delta G^{nj} + \Delta_V^{ni}, \\
e_X^{n+1} &= \varphi_0(h / \epsilon \partial_\tau) e_X^n + h \sum_{j=1}^s \bar{b}_j(h / \epsilon \partial_\tau) \delta G^{nj} + \delta_X^{n+1}, \\
e_V^{n+1} &= \varphi_0(h / \epsilon \partial_\tau) e_V^n + h \sum_{j=1}^s \bar{b}_j(h / \epsilon \partial_\tau) \delta G^{nj} + \delta_V^{n+1},
\end{aligned}$$

where $\delta G^{nj} = G(X(t_n + c_j h, \tau), V(t_n + c_j h, \tau)) - G(X^{nj}, V^{nj})$. This and the results given in Lemma 2.7 contribute with

$$\begin{aligned}
\|e_X^{n+1}\|_{L_\tau^\infty} &\leq \|e_X^n\|_{L_\tau^\infty} + hC \sum_{j=1}^s \|\delta G^{nj}\|_{L_\tau^\infty} + C\epsilon^2 h^{r+1}, \\
\|e_V^{n+1}\|_{L_\tau^\infty} &\leq \|e_V^n\|_{L_\tau^\infty} + hC \sum_{j=1}^s \|\delta G^{nj}\|_{L_\tau^\infty} + C\epsilon^2 h^{r+1}.
\end{aligned}$$

It stems from F that $\|\delta G^{nj}\|_{L_\tau^\infty} \leq C(\epsilon \|E_X^{nj}\|_{L_\tau^\infty} + \|E_V^{nj}\|_{L_\tau^\infty})$, and based on which, it is further arrived

$$\begin{aligned}
\|e_X^{n+1}\|_{L_\tau^\infty} &\leq \|e_X^n\|_{L_\tau^\infty} + hC \sum_{j=1}^s \left(\epsilon \|E_X^{nj}\|_{L_\tau^\infty} + \|E_V^{nj}\|_{L_\tau^\infty} \right) + C\epsilon^2 h^{r+1}, \\
\|e_V^{n+1}\|_{L_\tau^\infty} &\leq \|e_V^n\|_{L_\tau^\infty} + hC \sum_{j=1}^s \left(\epsilon \|E_X^{nj}\|_{L_\tau^\infty} + \|E_V^{nj}\|_{L_\tau^\infty} \right) + C\epsilon^2 h^{r+1}.
\end{aligned} \tag{2.16}$$

Similar result can be obtained for E_X^{ni} and E_V^{ni} in an analogous way as follows:

$$\begin{aligned}
\|E_X^{ni}\|_{L_\tau^\infty} &\leq \|e_X^n\|_{L_\tau^\infty} + hC \sum_{j=1}^s \left(\epsilon \|E_X^{nj}\|_{L_\tau^\infty} + \|E_V^{nj}\|_{L_\tau^\infty} \right) + C\epsilon^2 h^r, \\
\|E_V^{ni}\|_{L_\tau^\infty} &\leq \|e_V^n\|_{L_\tau^\infty} + hC \sum_{j=1}^s \left(\epsilon \|E_X^{nj}\|_{L_\tau^\infty} + \|E_V^{nj}\|_{L_\tau^\infty} \right) + C\epsilon^2 h^r.
\end{aligned}$$

Based on the above results, one gets

$$\sum_{i=1}^s \left(\|E_X^{ni}\|_{L_\tau^\infty} + \|E_V^{ni}\|_{L_\tau^\infty} \right) \leq s\|e_X^n\|_{L_\tau^\infty} + s\|e_V^n\|_{L_\tau^\infty} + 2shC \sum_{j=1}^s \left(\epsilon \|E_X^{nj}\|_{L_\tau^\infty} + \|E_V^{nj}\|_{L_\tau^\infty} \right) + C\epsilon^2 h^r.$$

If the stepsize h satisfies $h\epsilon \leq \frac{1}{4sC}$, it is straightforward to show that

$$\sum_{j=1}^s \left(\|E_X^{nj}\|_{L_\tau^\infty} + \|E_V^{nj}\|_{L_\tau^\infty} \right) \leq 2s\|e_X^n\|_{L_\tau^\infty} + 2s\|e_V^n\|_{L_\tau^\infty} + C\epsilon^2 h^r.$$

Inserting this into (2.16) and using Gronwall inequality eventually leads to

$$\|e_X^{n+1}\|_{L_\tau^\infty} \leq C\epsilon^2 h^r, \quad \|e_V^{n+1}\|_{L_\tau^\infty} \leq C\epsilon^2 h^r.$$

This bound, Lemma 2.6 and the transformations of Section 2.1 immediately complete the proof of Theorem 2.2. $\square$

3. FULL-DISCRETIZATION AND ITS ACCURACY

In the present section, by using the Fourier pseudospectral method in τ , we first present the full-discretization for solving the CPD (1.5) and then derive its accuracy.

3.1. Full-discretization

To use the Fourier method in the variable τ , we introduce $\tau_l = \frac{2\pi}{N_\tau}l$ with an even positive integer N_τ and $l \in \mathcal{M} := \{-N_\tau/2, -N_\tau/2 + 1, \dots, N_\tau/2\}$. Then the Fourier spectral method is proposed by considering the trigonometric polynomials

$$X^\mathcal{T}(t, \tau) = (X_j^\mathcal{T}(t, \tau))_{j=1,2}, \quad V^\mathcal{T}(t, \tau) = (V_j^\mathcal{T}(t, \tau))_{j=1,2},$$

with

$$X_j^\mathcal{T}(t, \tau) = \sum_{k \in \mathcal{T}} \widehat{X}_{k,j}(t) e^{ik\tau}, \quad V_j^\mathcal{T}(t, \tau) = \sum_{k \in \mathcal{T}} \widehat{V}_{k,j}(t) e^{ik\tau}, \quad (t, \tau) \in [0, T] \times [-\pi, \pi],$$

such that

$$\begin{cases} \partial_t X^\mathcal{T}(t, \tau) + \frac{1}{\varepsilon} \partial_\tau X^\mathcal{T}(t, \tau) = -\tau \varphi_1(-\tau J) F(X^\mathcal{T}(t, \tau) + \tau \varphi_1(\tau J) V^\mathcal{T}(t, \tau), \varphi_0(\tau J) V^\mathcal{T}(t, \tau)), \\ \partial_t V^\mathcal{T}(t, \tau) + \frac{1}{\varepsilon} \partial_\tau V^\mathcal{T}(t, \tau) = \varphi_0(-\tau J) F(X^\mathcal{T}(t, \tau) + \tau \varphi_1(\tau J) V^\mathcal{T}(t, \tau), \varphi_0(\tau J) V^\mathcal{T}(t, \tau)), \end{cases}$$

where $\widehat{X}_{k,j}(t)$ and $\widehat{V}_{k,j}(t)$ are referred to the discrete Fourier coefficients of $X_j^\mathcal{M}$ and $V_j^\mathcal{M}$, respectively. Collecting all the coefficients in $D := 2(N_\tau + 1)$ dimensional coefficient vectors $\widehat{\mathbf{X}}(t) = (\widehat{X}_{k,j}(t))$, $\widehat{\mathbf{V}}(t) = (\widehat{V}_{k,j}(t))$ implies a system of ordinary differential equations (ODEs)

$$\begin{cases} \frac{d}{dt} \widehat{\mathbf{X}}(t) = i\Omega \widehat{\mathbf{X}}(t) + \mathcal{F} \left(\mathbf{S}^- F \left(\mathcal{F}^{-1} \widehat{\mathbf{X}}(t) + \mathbf{S}^+ \mathcal{F}^{-1} \widehat{\mathbf{V}}(t), \mathbf{C}^+ \mathcal{F}^{-1} \widehat{\mathbf{V}}(t) \right) \right), \\ \frac{d}{dt} \widehat{\mathbf{V}}(t) = i\Omega \widehat{\mathbf{V}}(t) + \mathcal{F} \left(\mathbf{C}^- F \left(\mathcal{F}^{-1} \widehat{\mathbf{X}}(t) + \mathbf{S}^+ \mathcal{F}^{-1} \widehat{\mathbf{V}}(t), \mathbf{C}^+ \mathcal{F}^{-1} \widehat{\mathbf{V}}(t) \right) \right), \end{cases} \quad (3.1)$$

where $\mathcal{F}$ is the discrete Fast Fourier Transform (FFT), $\mathbf{S}^\pm = \text{diag}(\pm \tau_l \varphi_1(\pm \tau_l J))_{l=0,1,\dots,N_\tau}$, $\mathbf{C}^\pm = \text{diag}(\varphi_0(\pm \tau_l J))_{l=0,1,\dots,N_\tau}$, and $\Omega = \text{diag}(\Omega_1, \Omega_2)$ with $\Omega_1 = \Omega_2 := \frac{1}{\varepsilon} \text{diag}(\frac{N_\tau}{2}, \frac{N_\tau}{2} - 1, \dots, -\frac{N_\tau}{2})$.

The full-discretization of (1.5) is stated as follows.

Definition 3.1 (Fully discrete scheme). The initial data of (2.4) is derived from (2.6) with $j = 4$ and we denote it as $[X^0; V^0] = U^{[4]}(\tau)$. Choose a time step size h and a positive even number N_τ . The full-discretization of (1.5) is defined as follows.

- The first step is to compute the initial value of (3.1) by $[\widehat{X}^0; \widehat{V}^0] = [\mathcal{F}(X^0); \mathcal{F}(V^0)]$.
- For solving the ODEs (3.1) with the initial value $[\widehat{X}^0; \widehat{V}^0]$, we consider the same s -stage two-scale exponential integrator as semi-discretization, that is for $M = i\Omega$

$$\begin{aligned} \widehat{X}^{ni} &= \varphi_0(c_i h M) \widehat{X}^n + h \sum_{j=1}^s \bar{a}_{ij}(h M) \mathcal{F} \left(\mathbf{S}^- F \left(\mathcal{F}^{-1} \widehat{X}^{nj} + \mathbf{S}^+ \mathcal{F}^{-1} \widehat{V}^{nj}, \mathbf{C}^+ \mathcal{F}^{-1} \widehat{V}^{nj} \right) \right), \quad i = 1, 2, \dots, s, \\ \widehat{V}^{ni} &= \varphi_0(c_i h M) \widehat{V}^n + h \sum_{j=1}^s \bar{a}_{ij}(h M) \mathcal{F} \left(\mathbf{C}^- F \left(\mathcal{F}^{-1} \widehat{X}^{nj} + \mathbf{S}^+ \mathcal{F}^{-1} \widehat{V}^{nj}, \mathbf{C}^+ \mathcal{F}^{-1} \widehat{V}^{nj} \right) \right), \quad i = 1, 2, \dots, s, \\ \widehat{X}^{n+1} &= \varphi_0(h M) \widehat{X}^n + h \sum_{j=1}^s \bar{b}_j(h M) \mathcal{F} \left(\mathbf{S}^- F \left(\mathcal{F}^{-1} \widehat{X}^{nj} + \mathbf{S}^+ \mathcal{F}^{-1} \widehat{V}^{nj}, \mathbf{C}^+ \mathcal{F}^{-1} \widehat{V}^{nj} \right) \right), \\ \widehat{V}^{n+1} &= \varphi_0(h M) \widehat{V}^n + h \sum_{j=1}^s \bar{b}_j(h M) \mathcal{F} \left(\mathbf{C}^- F \left(\mathcal{F}^{-1} \widehat{X}^{nj} + \mathbf{S}^+ \mathcal{F}^{-1} \widehat{V}^{nj}, \mathbf{C}^+ \mathcal{F}^{-1} \widehat{V}^{nj} \right) \right). \end{aligned}$$

– The full-discretization $x^{n+1} \approx x(t_{n+1})$ and $v^{n+1} \approx v(t_{n+1})$ of (1.5) is formulated as

$$x^{n+1} = \mathbf{X}^{n+1} + \frac{t_{n+1}}{\epsilon} \varphi_1(t_{n+1}J/\epsilon) \mathbf{V}^{n+1}, \quad v^{n+1} = \frac{1}{\epsilon} \varphi_0(t_{n+1}J/\epsilon) \mathbf{V}^{n+1},$$

where $\mathbf{X}^{n+1}$ and $\mathbf{V}^{n+1}$ are obtained by the Fourier pseudospectral method

$$\mathbf{X}^{n+1} = \sum_{\ell \in \mathcal{M}} \left(\widehat{X^{n+1}} \right)_{\ell} e^{i\ell t_{n+1}/\epsilon}, \quad \mathbf{V}^{n+1} = \sum_{\ell \in \mathcal{M}} \left(\widehat{V^{n+1}} \right)_{\ell} e^{i\ell t_{n+1}/\epsilon}.$$

3.2. Improved accuracy

Theorem 3.2 (Improved accuracy). *For a smooth periodic function $\vartheta(\tau)$ on $\mathbb{T}$, denote the Soblev space $\mathcal{H}^m(\mathbb{T}) = \{\vartheta(\tau) \in \mathcal{H}^m : \partial_{\tau}^l \vartheta(0) = \partial_{\tau}^l \vartheta(2\pi), l = 0, 1, \dots, m\}$. Assume that the exact solution $X(t, \tau)$ and $V(t, \tau)$ of the system (2.4) satisfy that $X(t, \tau), V(t, \tau) \in \mathbb{C}^r([0, T], \mathcal{H}^{m_0}(\mathbb{T}))$ with $m_0 \geq 0$. Under the conditions of Theorem 2.2, the global error of the fully discrete scheme is bounded as*

$$\|X(t_n, \tau) - \mathbf{X}^n\|_{L_{\tau}^{\infty}} + \|\varepsilon V(t_n, \tau) - \varepsilon \mathbf{V}^n\|_{L_{\tau}^{\infty}} \leq C(\varepsilon^2 h^r + (2\pi/N_{\tau})^{m_0}), \quad 0 \leq n \leq T/h,$$

where C is a generic constant independent of n, h, N_{τ}, ϵ .

Proof. To prove this result, we introduce an intermediate algorithm (IA) and by which, the conclusions of this theorem are converted to the estimations for IA. To this end, consider the following trigonometric polynomials

$$X^{\mathcal{M}}(t, \tau) = (X_j^{\mathcal{M}}(t, \tau))_{j=1,2}, \quad V^{\mathcal{M}}(t, \tau) = (V_j^{\mathcal{M}}(t, \tau))_{j=1,2},$$

with

$$X_j^{\mathcal{M}}(t, \tau) = \sum_{k \in \mathcal{M}} \widetilde{X_{k,j}}(t) e^{ik\tau}, \quad V_j^{\mathcal{M}}(t, \tau) = \sum_{k \in \mathcal{M}} \widetilde{V_{k,j}}(t) e^{ik\tau}, \quad (t, \tau) \in [0, T] \times [0, 2\pi],$$

such that

$$\begin{aligned} \partial_t X^{\mathcal{M}}(t, \tau) + \frac{1}{\epsilon} \partial_{\tau} X^{\mathcal{M}}(t, \tau) &= -\tau \varphi_1(-\tau J) F(X^{\mathcal{M}}(t, \tau) + \tau \varphi_1(\tau J) V^{\mathcal{M}}(t, \tau), \varphi_0(\tau J) V^{\mathcal{M}}(t, \tau)), \\ \partial_t V^{\mathcal{M}}(t, \tau) + \frac{1}{\epsilon} \partial_{\tau} V^{\mathcal{M}}(t, \tau) &= \varphi_0(-\tau J) F(X^{\mathcal{M}}(t, \tau) + \tau \varphi_1(\tau J) V^{\mathcal{M}}(t, \tau), \varphi_0(\tau J) V^{\mathcal{M}}(t, \tau)). \end{aligned}$$

Here $\widetilde{X_{k,j}}$ and $\widetilde{V_{k,j}}$ are the Fourier transform coefficients of the periodic functions $X_j^{\mathcal{M}}$ and $V_j^{\mathcal{M}}$, respectively. According to the Fourier functions' orthogonality and collecting all the $\widetilde{X_{k,j}}, \widetilde{V_{k,j}}$ in $(N_{\tau} + 1)$ -periodic coefficient vectors $\widetilde{\mathbf{X}}(t) = (\widetilde{X_{k,j}}(t))$, $\widetilde{\mathbf{V}}(t) = (\widetilde{V_{k,j}}(t))$, one gets

$$\begin{aligned} \frac{d}{dt} \widetilde{\mathbf{X}}(t) &= i\Omega \widetilde{\mathbf{X}}(t) + \mathcal{F} \left(\mathbf{S}^{-} F \left(\mathcal{F}^{-1} \widetilde{\mathbf{X}}(t) + \mathbf{S}^{+} \mathcal{F}^{-1} \widetilde{\mathbf{V}}(t), \mathbf{C}^{+} \mathcal{F}^{-1} \widetilde{\mathbf{V}}(t) \right) \right), \\ \frac{d}{dt} \widetilde{\mathbf{V}}(t) &= i\Omega \widetilde{\mathbf{V}}(t) + \mathcal{F} \left(\mathbf{C}^{-} F \left(\mathcal{F}^{-1} \widetilde{\mathbf{X}}(t) + \mathbf{S}^{+} \mathcal{F}^{-1} \widetilde{\mathbf{V}}(t), \mathbf{C}^{+} \mathcal{F}^{-1} \widetilde{\mathbf{V}}(t) \right) \right). \end{aligned} \quad (3.2)$$

Then the IA is defined by

$$\begin{aligned} X_{\mathcal{M},j}^{ni}(\tau) &= \sum_{k \in \mathcal{M}} \widetilde{X_{k,j}^{ni}} e^{ik\tau}, & V_{\mathcal{M},j}^{ni}(\tau) &= \sum_{k \in \mathcal{M}} \widetilde{V_{k,j}^{ni}} e^{ik\tau}, & i &= 1, 2, \dots, s, \\ X_{\mathcal{M},j}^{n+1}(\tau) &= \sum_{k \in \mathcal{M}} \widetilde{X_{k,j}^{n+1}} e^{ik\tau}, & V_{\mathcal{M},j}^{n+1}(\tau) &= \sum_{k \in \mathcal{M}} \widetilde{V_{k,j}^{n+1}} e^{ik\tau}, & n &= 0, 1, \dots, T/h - 1, \end{aligned}$$

where the following s -stage exponential integrator is applied to solving (3.2):

$$\begin{aligned}\widetilde{X^{ni}} &= \varphi_0(c_i h M) \widetilde{X^n} + h \sum_{j=1}^s \bar{a}_{ij}(hM) \mathcal{F}\left(\mathbf{S}^- F\left(\mathcal{F}^{-1} \widetilde{X^{nj}} + \mathbf{S}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}, \mathbf{C}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}\right)\right), \quad i = 1, 2, \dots, s, \\ \widetilde{V^{ni}} &= \varphi_0(c_i h M) \widetilde{V^n} + h \sum_{j=1}^s \bar{a}_{ij}(hM) \mathcal{F}\left(\mathbf{C}^- F\left(\mathcal{F}^{-1} \widetilde{X^{nj}} + \mathbf{S}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}, \mathbf{C}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}\right)\right), \quad i = 1, 2, \dots, s, \\ \widetilde{X^{n+1}} &= \varphi_0(hM) \widetilde{X^n} + h \sum_{j=1}^s \bar{b}_j(hM) \mathcal{F}\left(\mathbf{S}^- F\left(\mathcal{F}^{-1} \widetilde{X^{nj}} + \mathbf{S}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}, \mathbf{C}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}\right)\right), \\ \widetilde{V^{n+1}} &= \varphi_0(hM) \widetilde{V^n} + h \sum_{j=1}^s \bar{b}_j(hM) \mathcal{F}\left(\mathbf{C}^- F\left(\mathcal{F}^{-1} \widetilde{X^{nj}} + \mathbf{S}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}, \mathbf{C}^+ \mathcal{F}^{-1} \widetilde{V^{nj}}\right)\right).\end{aligned}\quad (3.3)$$

To study the accuracy of the fully discrete scheme, consider the standard projection operator $P_{\mathcal{M}} : L^2([-\pi, \pi]) \rightarrow Y_{\mathcal{M}} := \text{span}\{e^{ik\tau}, k \in \mathcal{M}, \tau \in [-\pi, \pi]\}$ as $(P_{\mathcal{M}}v)(\tau) = \sum_{k \in \mathcal{M}} \tilde{v}_k e^{ik\tau}$. With the notations $\mathbf{X}^{ni} = \sum_{\ell \in \mathcal{M}} (\widetilde{X^{ni}})_{\ell} e^{i\ell(t_n + c_i h)/\varepsilon}$ and $\mathbf{V}^{ni} = \sum_{\ell \in \mathcal{M}} (\widetilde{V^{ni}})_{\ell} e^{i\ell(t_n + c_i h)/\varepsilon}$, define the error functions of our fully discrete scheme by

$$\begin{aligned}e_X^n(\tau) &:= X(t_n, \tau) - \mathbf{X}^n, & E_X^{ni}(\tau) &:= X(t_n + c_i h, \tau) - \mathbf{X}^{ni}, \\ e_V^n(\tau) &:= V(t_n, \tau) - \mathbf{V}^n, & E_V^{ni}(\tau) &:= V(t_n + c_i h, \tau) - \mathbf{V}^{ni},\end{aligned}$$

and the projected errors of the intermediate algorithm as

$$\begin{aligned}e_{\mathcal{M},X}^n(\tau) &:= P_{\mathcal{M}}X(t_n, \tau) - X_{\mathcal{M}}^n, & E_{\mathcal{M},X}^{ni}(\tau) &:= P_{\mathcal{M}}X(t_n + c_i h, \tau) - X_{\mathcal{M}}^{ni}, \\ e_{\mathcal{M},V}^n(\tau) &:= P_{\mathcal{M}}V(t_n, \tau) - V_{\mathcal{M}}^n, & E_{\mathcal{M},V}^{ni}(\tau) &:= P_{\mathcal{M}}V(t_n + c_i h, \tau) - V_{\mathcal{M}}^{ni}.\end{aligned}$$

Based on the estimates on projection error [42] and the triangle inequality, it follows that

$$\begin{aligned}\|e_X^n\|_{L_{\tau}^{\infty}} &\leq \|e_{\mathcal{M},X}^n\|_{L_{\tau}^{\infty}} + \|X_{\mathcal{M}}^n - \mathbf{X}^n\|_{L_{\tau}^{\infty}} + \|X(t_n, \tau) - P_{\mathcal{M}}X(t_n, \tau)\|_{L_{\tau}^{\infty}} \leq \|e_{\mathcal{M},X}^n\|_{L_{\tau}^{\infty}} + C(2\pi/N_{\tau})^{m_0}, \\ \|E_X^{ni}\|_{L_{\tau}^{\infty}} &\leq \|E_{\mathcal{M},X}^{ni}\|_{L_{\tau}^{\infty}} + \|X_{\mathcal{M}}^{ni} - \mathbf{X}^{ni}\|_{L_{\tau}^{\infty}} + \|X(t_n + c_i h, \tau) - P_{\mathcal{M}}X(t_n + c_i h, \tau)\|_{L_{\tau}^{\infty}} \\ &\leq \|E_{\mathcal{M},X}^{ni}\|_{L_{\tau}^{\infty}} + C(2\pi/N_{\tau})^{m_0}.\end{aligned}$$

Similar results can be derived for e_V^n , E_V^{ni} . Therefore, the estimations for e_X^n , e_V^n and E_X^{ni} , E_V^{ni} can be turned to estimate the estimations for $e_{\mathcal{M},X}^n$, $e_{\mathcal{M},V}^n$ and $E_{\mathcal{M},X}^{ni}$, $E_{\mathcal{M},V}^{ni}$.

The error system of the intermediate algorithm is given by

$$\begin{aligned}e_{\mathcal{M},X}^{n+1}(\tau) &= \sum_{k \in \mathcal{M}} \left(\widetilde{e_{\mathcal{M},X}^{n+1}} \right)_k e^{ik\tau}, & E_{\mathcal{M},X}^{ni}(\tau) &= \sum_{k \in \mathcal{M}} \left(\widetilde{E_{\mathcal{M},X}^{ni}} \right)_k e^{ik\tau}, \\ e_{\mathcal{M},V}^{n+1}(\tau) &= \sum_{k \in \mathcal{M}} \left(\widetilde{e_{\mathcal{M},V}^{n+1}} \right)_k e^{ik\tau}, & E_{\mathcal{M},V}^{ni}(\tau) &= \sum_{k \in \mathcal{M}} \left(\widetilde{E_{\mathcal{M},V}^{ni}} \right)_k e^{ik\tau},\end{aligned}$$

where

$$\begin{aligned}\widetilde{e_{\mathcal{M},X}^{n+1}} &= \varphi_0(hM) \widetilde{e_{\mathcal{M},X}^n} + h \sum_{j=1}^s \bar{b}_j(hM) \Delta \widetilde{f_X^{nj}} + \widetilde{\delta_X^{n+1}}, & \widetilde{E_{\mathcal{M},X}^{ni}} &= \varphi_0(c_i h M) \widetilde{e_{\mathcal{M},X}^n} + h \sum_{j=1}^s \bar{a}_{ij}(hM) \Delta \widetilde{f_X^{nj}} + \widetilde{\Delta_X^{ni}}, \\ \widetilde{e_{\mathcal{M},V}^{n+1}} &= \varphi_0(hM) \widetilde{e_{\mathcal{M},V}^n} + h \sum_{j=1}^s \bar{b}_j(hM) \Delta \widetilde{f_V^{nj}} + \widetilde{\delta_V^{n+1}}, & \widetilde{E_{\mathcal{M},V}^{ni}} &= \varphi_0(c_i h M) \widetilde{e_{\mathcal{M},V}^n} + h \sum_{j=1}^s \bar{a}_{ij}(hM) \Delta \widetilde{f_V^{nj}} + \widetilde{\Delta_V^{ni}},\end{aligned}$$

and

$$\begin{aligned}\widetilde{G}(X, V) &= F(\mathcal{F}^{-1}X + \mathbf{S}^+ \mathcal{F}^{-1}V, \mathbf{C}^+ \mathcal{F}^{-1}V), \\ \widetilde{\Delta f_X^{nj}} &= \mathcal{F} \mathbf{S}^- \left(\widetilde{G}(P_{\mathcal{M}}X(t_n + c_j h, \tau), P_{\mathcal{M}}V(t_n + c_j h, \tau)) - \widetilde{G}(X_{\mathcal{M}}^{nj}, V_{\mathcal{M}}^{nj}) \right), \\ \widetilde{\Delta f_V^{nj}} &= \mathcal{F} \mathbf{C}^- \left(\widetilde{G}(P_{\mathcal{M}}X(t_n + c_j h, \tau), P_{\mathcal{M}}V(t_n + c_j h, \tau)) - \widetilde{G}(X_{\mathcal{M}}^{nj}, V_{\mathcal{M}}^{nj}) \right).\end{aligned}$$

Here the remainders $\widetilde{\delta_X^{n+1}}$, $\widetilde{\Delta_X^{ni}}$ and $\widetilde{\delta_V^{n+1}}$, $\widetilde{\Delta_V^{ni}}$ are determined by inserting the exact solution of (3.2) into the numerical approximation (3.3), *i.e.*,

$$\begin{aligned}\widetilde{\mathbf{X}(t_n + c_i h)} &= \varphi_0(c_i h M) \widetilde{\mathbf{X}(t_n)} + h \sum_{j=1}^s \bar{a}_{ij}(h M) \mathcal{F} \mathbf{S}^- \widetilde{G}(\widetilde{\mathbf{X}(t_n + c_j h)}, \widetilde{\mathbf{V}(t_n + c_j h)}) + \widetilde{\Delta_X^{ni}}, \\ \widetilde{\mathbf{V}(t_n + c_i h)} &= \varphi_0(c_i h M) \widetilde{\mathbf{V}(t_n)} + h \sum_{j=1}^s \bar{a}_{ij}(h M) \mathcal{F} \mathbf{C}^- \widetilde{G}(\widetilde{\mathbf{X}(t_n + c_j h)}, \widetilde{\mathbf{V}(t_n + c_j h)}) + \widetilde{\Delta_V^{ni}}, \\ \widetilde{\mathbf{X}(t_n + h)} &= \varphi_0(h M) \widetilde{\mathbf{X}(t_n)} + h \sum_{j=1}^s \bar{b}_j(h M) \mathcal{F} \mathbf{S}^- \widetilde{G}(\widetilde{\mathbf{X}(t_n + c_j h)}, \widetilde{\mathbf{V}(t_n + c_j h)}) + \widetilde{\delta_X^{n+1}}, \\ \widetilde{\mathbf{V}(t_n + h)} &= \varphi_0(h M) \widetilde{\mathbf{V}(t_n)} + h \sum_{j=1}^s \bar{b}_j(h M) \mathcal{F} \mathbf{C}^- \widetilde{G}(\widetilde{\mathbf{X}(t_n + c_j h)}, \widetilde{\mathbf{V}(t_n + c_j h)}) + \widetilde{\delta_V^{n+1}}.\end{aligned}$$

Following the same arguments of Lemma 2.5, the bounds of these remainders are derived as

$$\left\| \widetilde{\Delta_X^{ni}} \right\|_{W_\tau^{1,\infty}} \leq C \epsilon^2 h^r, \quad \left\| \widetilde{\Delta_V^{ni}} \right\|_{W_\tau^{1,\infty}} \leq C \epsilon^2 h^r, \quad \left\| \widetilde{\delta_X^{n+1}} \right\|_{W_\tau^{1,\infty}} \leq C \epsilon^2 h^{r+1}, \quad \left\| \widetilde{\delta_V^{n+1}} \right\|_{W_\tau^{1,\infty}} \leq C \epsilon^2 h^{r+1}.$$

Based on the foregoing estimates, we deduce that

$$\begin{aligned}\left\| e_{\mathcal{M},X}^{n+1} \right\|_{L_\tau^\infty} &\leq \left\| e_{\mathcal{M},X}^n \right\|_{L_\tau^\infty} + h C \sum_{j=1}^s \left\| \widetilde{\Delta f_X^{nj}} \right\|_{L_\tau^\infty} + C \epsilon^2 h^{r+1}, \\ \left\| e_{\mathcal{M},V}^{n+1} \right\|_{L_\tau^\infty} &\leq \left\| e_{\mathcal{M},V}^n \right\|_{L_\tau^\infty} + h C \sum_{j=1}^s \left\| \widetilde{\Delta f_V^{nj}} \right\|_{L_\tau^\infty} + C \epsilon^2 h^{r+1}.\end{aligned}$$

The proof is, then, concluded by using the same arguments as Theorem 2.2. $\square$

4. PRACTICAL INTEGRATORS AND NUMERICAL TESTS

4.1. Some practical integrators

Before the above discretization is applied in practical computations, the coefficients c_i , $\bar{a}_{ij}(h/\epsilon \partial_\tau)$ and $\bar{b}_i(h/\epsilon \partial_\tau)$ appearing in (2.7) should be determined, which is derived in this present section.

Second order integrator. We first consider second order integrators which can be realized by one-stage schemes, *i.e.*, $s = 1$. The first method is obtained by considering

$$c_1 = \frac{1}{2}, \quad \bar{b}_1(h/\epsilon \partial_\tau) = \varphi_1(h/\epsilon \partial_\tau), \quad \bar{a}_{11}(h/\epsilon \partial_\tau) = \varphi_1(c_1 h/\epsilon \partial_\tau),$$

which yields an implicit integrator. We shall refer to it as **IO2**. To get an explicit scheme, we modify the scheme (2.7) of IO2 as

$$X^{n1} = \varphi_0(c_1 h/\epsilon \partial_\tau) X^n - h \bar{a}_{11}(h/\epsilon \partial_\tau) \tau \varphi_1(-\tau J) F(X^n + \tau \varphi_1(\tau J) V^n, \varphi_0(\tau J) V^n),$$

$$\begin{aligned}
V^{n1} &= \varphi_0(c_1 h/\epsilon \partial_\tau) V^n + h \bar{a}_{11}(h/\epsilon \partial_\tau) \varphi_0(-\tau J) F(X^n + \tau \varphi_1(\tau J) V^n, \varphi_0(\tau J) V^n), \\
X^{n+1} &= \varphi_0(h/\epsilon \partial_\tau) X^n - h \bar{b}_1(h/\epsilon \partial_\tau) \tau \varphi_1(-\tau J) F(X^{n1} + \tau \varphi_1(\tau J) V^{n1}, \varphi_0(\tau J) V^{n1}), \\
V^{n+1} &= \varphi_0(h/\epsilon \partial_\tau) V^n + h \bar{b}_1(h/\epsilon \partial_\tau) \varphi_0(-\tau J) F(X^{n1} + \tau \varphi_1(\tau J) V^{n1}, \varphi_0(\tau J) V^{n1}).
\end{aligned}$$

This explicit second order method is denoted by **EO2**. We note that for these two methods, the second order initial data, *i.e.*, (2.6) with $k = 2$, is enough.

Fourth order integrator. We now turn to the fourth order integrators with the fourth order initial data which is obtained by (2.6) with $k = 4$. This can be achieved by three-stage implicit integrators. Solving $\psi_i(h/\epsilon \partial_\tau) = 0$ and $\psi_{j,i}(h/\epsilon \partial_\tau) = 0$ for $i, j = 1, 2, 3$, and choosing $c_1 = 1$, $c_2 = 1/2$, $c_3 = 0$ yields

$$\begin{aligned}
\bar{a}_{31}(\Upsilon) &= \bar{a}_{32}(\Upsilon) = \bar{a}_{33}(\Upsilon) = 0, & \bar{a}_{21}(\Upsilon) &= -\frac{1}{4}\varphi_2(c_2\Upsilon) + \frac{1}{2}\varphi_3(c_2\Upsilon), \\
\bar{a}_{22}(\Upsilon) &= \varphi_2(c_2\Upsilon) - \varphi_3(c_2\Upsilon), & \bar{a}_{23}(\Upsilon) &= \frac{1}{2}\varphi_1(c_2\Upsilon) - \frac{3}{4}\varphi_2(c_2\Upsilon) + \frac{1}{2}\varphi_3(\Upsilon), \\
\bar{a}_{11}(\Upsilon) &= \bar{b}_1(\Upsilon) = 4\varphi_3(\Upsilon) - \varphi_2(\Upsilon), & \bar{a}_{12}(\Upsilon) &= \bar{b}_2(\Upsilon) = 4\varphi_2(\Upsilon) - 8\varphi_3(\Upsilon), \\
\bar{a}_{13}(\Upsilon) &= \bar{b}_3(\Upsilon) = \varphi_1(\Upsilon) - 3\varphi_2(\Upsilon) + 4\varphi_3(\Upsilon),
\end{aligned}$$

with $\Upsilon = h/\epsilon \partial_\tau$. It can be checked that these coefficients satisfy all the fourth stiff order conditions presented in Table 1. This implicit integrator of order four is referred as **IO4**. For explicit examples, we need to consider $s = 5$ and choose the coefficients [31]

$$\begin{aligned}
c_1 &= 0, & c_2 &= c_3 = c_5 = \frac{1}{2}, & c_4 &= 1, \\
a_{2,1} &= \frac{1}{2}\varphi_{1,2}, & a_{3,1} &= \frac{1}{2}\varphi_{1,3} - \varphi_{2,3}, & a_{3,2} &= \varphi_{2,3}, \\
a_{4,1} &= \varphi_{1,4} - 2\varphi_{2,4}, & a_{4,2} &= a_{4,3} = \varphi_{2,4}, & a_{5,1} &= \frac{1}{2}\varphi_{1,5} - 2a_{5,2} - a_{5,4}, \\
a_{5,2} &= \frac{1}{2}\varphi_{2,5} - \varphi_{3,4} + \frac{1}{2}\varphi_{2,4} - \frac{1}{2}\varphi_{3,5}, & a_{5,3} &= a_{5,2}, & a_{5,4} &= \frac{1}{2}\varphi_{2,5} - \varphi_{5,2}, \\
b_1 &= \varphi_1 - 3\varphi_2 + 4\varphi_3, & b_2 &= b_3 = 0, & b_4 &= -\varphi_2 + 4\varphi_3, \quad b_5 = 4\varphi_2 - 8\varphi_3,
\end{aligned}$$

where $\varphi_{i,j} = \varphi_{i,j}(\Upsilon) = \varphi_i(c_j \Upsilon)$. This integrator is referred as **EO4**.

The above two kinds of methods, *i.e.*, explicit and implicit schemes, are presented to show that the improved accuracy proposed in the paper can be obtained by these methods. Moreover, we end this section by noting that, with the definition of symmetric methods [27], it can be verified that the above two explicit schemes (EO2 and EO4) are not symmetric but the implicit ones (IO2 and IO4) are symmetric. Thus IO2 and IO4 are hoped to have long term conservation in the conserved quantity of the CPD and this issue will be researched in our next work.

4.2. Numerical experiment

Let us illustrate the performance of our schemes with a single particle in two space dimensions under a strong magnetic field [13]:

$$\dot{x}(t) = v(t), \quad \dot{v}(t) = \frac{b(x)}{\varepsilon} Jv(t) + g(x(t)), \quad t > 0,$$

where $g(x) = (\cos(q(1)/2) \sin(q(2))/2, \sin(q(1)/2) \cos(q(2)))^\top$ and $b(x) = 1 + \sin(q(1)) \sin(q(2))$. This is a reduced model from the three dimensional CPD case when the external magnetic field has a fixed direction and is homogenous in space. We choose the initial value $x(0) = (0.1, 0.1)^\top$, $v(0) = (0.2, 0.1)^\top$, and fix $N_\tau = 2^6$ in the computations. For comparison, we choose the well known Boris method (with second-order accuracy) denoted by Boris and a Runge-Kutta method (the fourth order Gauss-Legendre method) denoted by RK4. In the

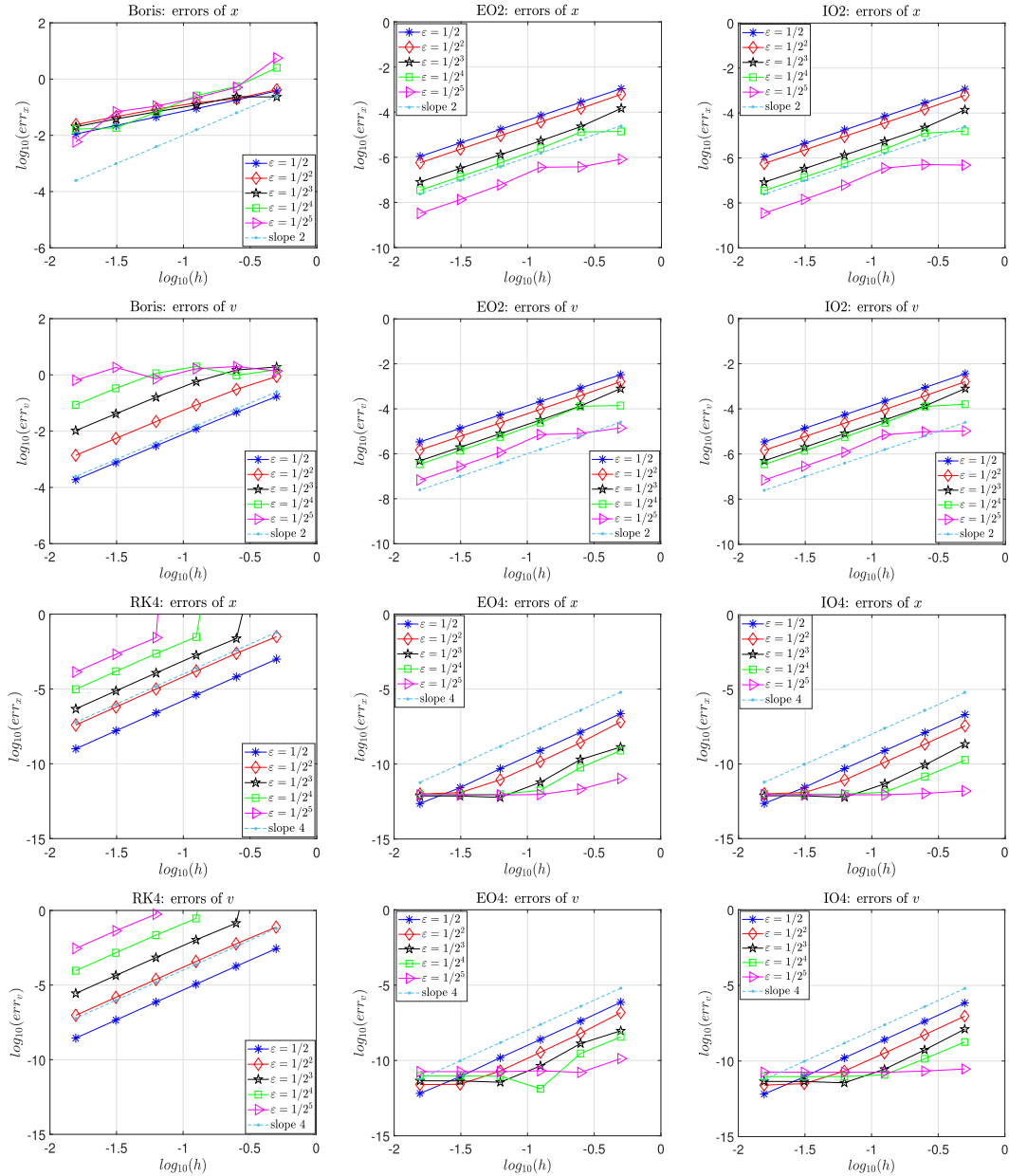


FIGURE 1. The errors (4.1) at $t = 1$ of the second-order schemes (top two rows) and fourth-order schemes (below two rows) with $h = 1/2^k$ for $k = 1, 2, \dots, 6$ under different ε .

computations of implicit methods, we apply a fixed point iteration with the error tolerance and the maximum number of each iteration set as 10^{-12} and 100, respectively. The initial condition is chosen by the first two formulae of (2.14). Figure 1 displays the numerical errors

$$\text{err}_x := \frac{\|x^n - x(t_n)\|}{\|x(t_n)\|}, \quad \text{err}_v := \frac{\|v^n - v(t_n)\|}{\|v(t_n)\|}. \quad (4.1)$$

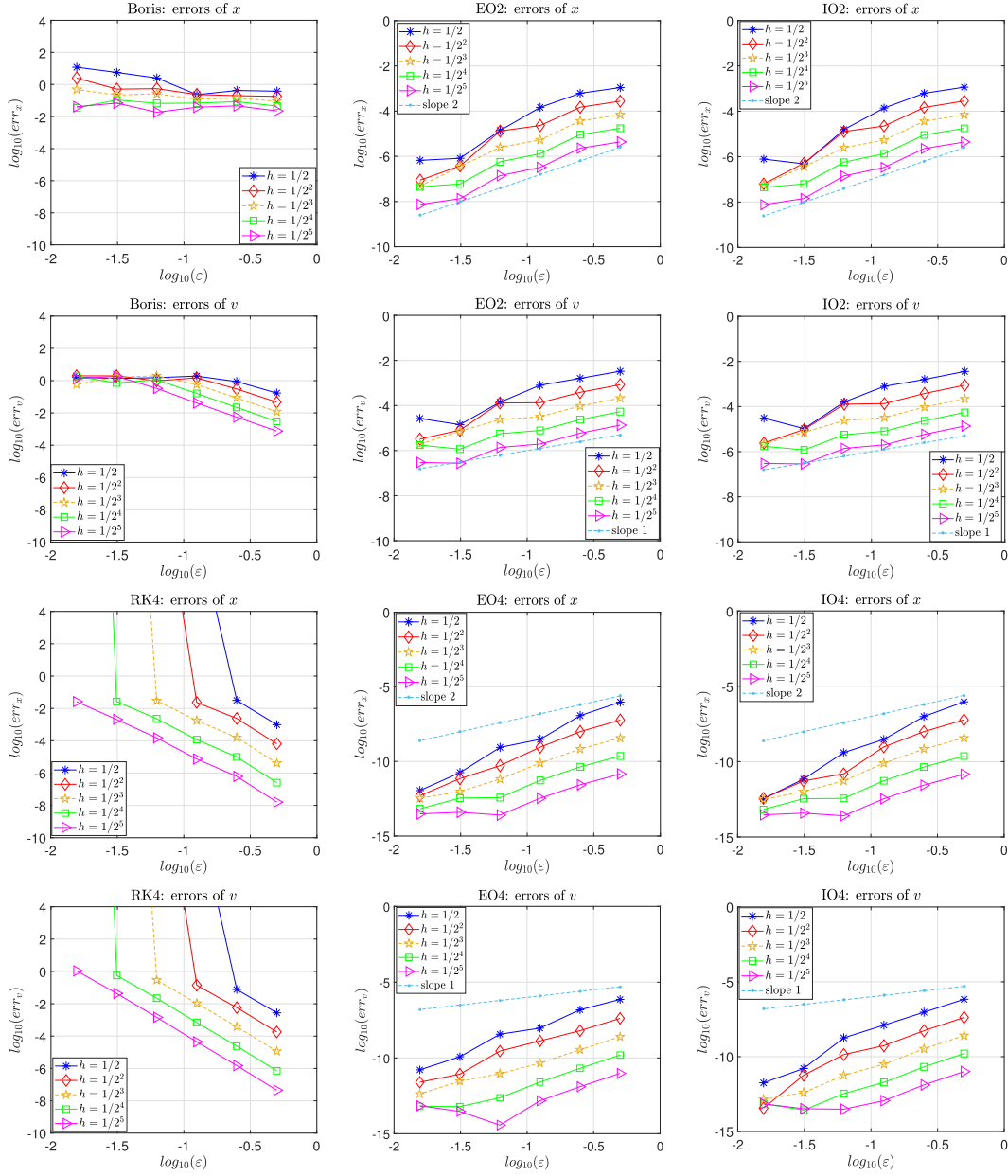


FIGURE 2. The errors (4.1) at $t = 1$ of the second-order schemes (top two rows) and fourth-order schemes (below two rows) with $\varepsilon = 1/2^k$ for $k = 1, 2, \dots, 6$ under different h .

against h for different ε . These results show that Boris, EO2, IO2 perform second order and RK4, EO4, IO4 display fourth order. In order to show the influence of ε on the accuracy, we present the errors err_x and err_v against ε for different h in Figure 2. In the light of these results, we have the following observations. The four integrators formulated in this paper have improved uniformly high accuracy in both position and velocity, and

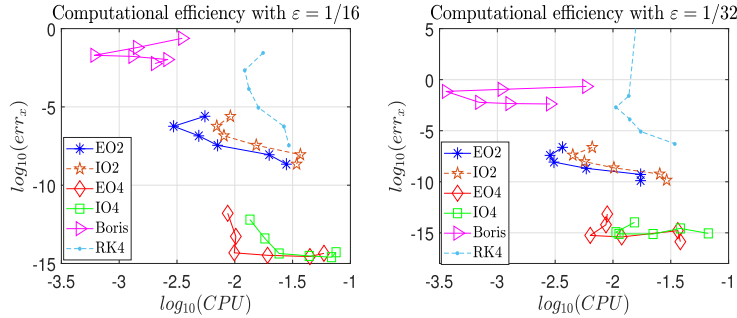


FIGURE 3. The log–log plot of the temporal error err_x at $t = 1$ against CPU time, where $h = 1/2^k$ with $k = 2, 3, \dots, 7$.

when ε decreases, the accuracy is improved. However, for the methods Boris and RK4, they do not have such improved accuracy. The accuracy of these two methods becomes worse as ε decreases.

Compared with the methods Boris and RK4 which are directly applied to the ODEs (1.4), the scheme of our integrators is given for the PDEs (2.4). For the computational efficiency², we solve this problem on $[0, 1]$ and the results are shown in Figure 3. It can be seen that our integrators have nice efficiency even compared with Boris and RK4 applied to the ODEs (1.4) directly. The reason is that when ε is small, Boris and RK4 need small stepsizes $\mathcal{O}(\varepsilon)$ in the time simulation to keep their accuracy but our methods only need $\mathcal{O}(1)$ stepsizes.

5. APPLICATION TO THE THREE DIMENSIONAL CPD

For the three dimensional CPD (1.4), it is noted that we cannot take the approach given for the two dimensional case, since in that way, $s\varphi_1(sB(x(0)))$ is no longer periodic and thus two-scale exponential integrator cannot be used. For the uniformly accurate (UA) methods for solving three dimensional CPD, some novel algorithms have been recently proposed in [14]. Based on the approach given in this paper for the two dimensional case, we can formulate a kind of UA methods with more simple scheme for the three dimensional CPD (1.4) in maximal ordering case. We state the application as follows.

For the three dimensional CPD (1.4) in maximal ordering case [6, 28, 38], *i.e.*, $B = B(\varepsilon x) := (b_1(\varepsilon x), b_2(\varepsilon x), b_3(\varepsilon x))^T \in \mathbb{R}^3$, we first rewrite it as

$$\dot{x}(t) = v(t), \quad \dot{v}(t) = \frac{\widehat{B}_0}{\varepsilon} v(t) + F(x(t), v(t)), \quad 0 < t \leq T, \quad x(0) = x_0 \in \mathbb{R}^3, \quad v(0) = v_0 \in \mathbb{R}^3, \quad (5.1)$$

where $\widehat{B}_0 = \widehat{B}(\varepsilon x(0))$ with $\widehat{B}(\varepsilon x) = \begin{pmatrix} 0 & b_3(\varepsilon x) & -b_2(\varepsilon x) \\ -b_3(\varepsilon x) & 0 & b_1(\varepsilon x) \\ b_2(\varepsilon x) & -b_1(\varepsilon x) & 0 \end{pmatrix}$ and $F(x(t), v(t)) = \frac{\widehat{B}(\varepsilon x(t)) - \widehat{B}_0}{\varepsilon} v(t) + E(x(t))$.

With the maximal ordering property, it is worth noticing that $F(x(t), v(t))$ is uniformly bounded w.r.t. ε . It is noted that the constant case $B \equiv C$ also ensures the uniform boundedness of F and the methods as well as their analysis of this section are applicable to this case. We introduce the filtered variable $w(t) = \varphi_0(-t\widehat{B}_0/\varepsilon)v(t)$, then (5.1) reads:

$$\dot{x}(t) = \varphi_0\left(t\widehat{B}_0/\varepsilon\right)w(t), \quad \dot{w}(t) = \varphi_0\left(-t\widehat{B}_0/\varepsilon\right)F\left(x(t), \varphi_0\left(t\widehat{B}_0/\varepsilon\right)w(t)\right), \quad x(0) = x_0, \quad w(0) = v_0. \quad (5.2)$$

²This test is conducted in a sequential program in MATLAB R2020b on a laptop ThinkPad X1 nano (CPU: i7-1160G7 @ 1.20 GHz 2.11 GHz, Memory: 16 GB, Os: Microsoft Windows 10 with 64bit).

With the help of $\widehat{B}_0$, $e^{\pm t\widehat{B}_0/\varepsilon}$ is periodic in t/ε on $[0, 2\pi]$. By isolating the fast time variable t/ε as another variable τ and denoting $X(t, \tau) = x(t)$, $W(t, \tau) = w(t)$, the two-scale system of (5.2) takes the form

$$\begin{cases} \partial_t X(t, \tau) + \frac{1}{\varepsilon} \partial_\tau X(t, \tau) = \varphi_0(\tau \widehat{B}_0) W(t, \tau), \\ \partial_t W(t, \tau) + \frac{1}{\varepsilon} \partial_\tau W(t, \tau) = \varphi_0(-\tau \widehat{B}_0) F(X(t, \tau), \varphi_0(\tau \widehat{B}_0) W(t, \tau)). \end{cases} \quad (5.3)$$

The initial data $[X^0; W^0] := [X(0, \tau); W(0, \tau)]$ for (5.3) is obtained by (2.6) with the replacement f_τ (2.5) of

$$f_\tau([X; W]) = \begin{pmatrix} \varphi_0(\tau \widehat{B}_0) W \\ \varphi_0(-\tau \widehat{B}_0) F(X, \varphi_0(\tau \widehat{B}_0) W) \end{pmatrix}.$$

We now obtain the semi-discretization of the three dimensional CPD (1.4) in maximal ordering case.

Definition 5.1. For the three dimensional CPD (1.4) in maximal ordering case, choose a time step h . Then for solving the equation (5.3) with the initial value $[X^0; W^0]$, consider an s -stage two-scale exponential integrator

$$\begin{aligned} X^{ni} &= \varphi_0(c_i h/\varepsilon \partial_\tau) X^n + h \sum_{j=1}^s \bar{a}_{ij}(h/\varepsilon \partial_\tau) \varphi_0(\tau \widehat{B}_0) W^{nj}, & i = 1, 2, \dots, s, \\ W^{ni} &= \varphi_0(c_i h/\varepsilon \partial_\tau) W^n + h \sum_{j=1}^s \bar{a}_{ij}(h/\varepsilon \partial_\tau) \varphi_0(-\tau \widehat{B}_0) F(X^{nj}, \varphi_0(\tau \widehat{B}_0) W^{nj}), & i = 1, 2, \dots, s, \\ X^{n+1} &= \varphi_0(h/\varepsilon \partial_\tau) X^n + h \sum_{j=1}^s \bar{b}_j(h/\varepsilon \partial_\tau) \varphi_0(\tau \widehat{B}_0) W^{nj}, \\ W^{n+1} &= \varphi_0(h/\varepsilon \partial_\tau) W^n + h \sum_{j=1}^s \bar{b}_j(h/\varepsilon \partial_\tau) \varphi_0(-\tau \widehat{B}_0) F(X^{nj}, \varphi_0(\tau \widehat{B}_0) W^{nj}), \end{aligned}$$

with the coefficients $c_i \in [0, 1]$, $\bar{a}_{ij}(h/\varepsilon \partial_\tau)$ and $\bar{b}_j(h/\varepsilon \partial_\tau)$. The numerical solution $x^{n+1} \approx x(t_{n+1})$ and $v^{n+1} \approx v(t_{n+1})$ of (1.4) is given by

$$x^{n+1} = X^{n+1}, \quad v^{n+1} = \varphi_0(t_{n+1} \widehat{B}_0/\varepsilon) W^{n+1}.$$

Based on the Fourier pseudospectral method in τ , the full-discretization can be formulated by using the same way as that of two dimensional CPD. For simplicity, we do not go further on this point here. For the semi-discretization, it has a uniform accuracy and we state it as follows.

Theorem 5.2. Under the conditions of Theorem 2.2, for the final numerical solution x^n, v^n produced by the method given in Definition 5.1, the global error is

$$\|x^n - x(t_n)\| + \|v^n - v(t_n)\| \leq Ch^r, \quad 0 \leq n \leq T/h,$$

where C is independent of n, h, ε .

Remark 5.3. It is noted that for the three dimensional CPD, the function $F(X(t, \tau), \varphi_0(\tau \widehat{B}_0) W(t, \tau))$ appeared in (5.3) only has the boundedness $O(1)$ while in the two dimensional case that $F(X(t, \tau) + \tau \varphi_1(\tau J) V(t, \tau), \varphi_0(\tau J) V(t, \tau))$ is bounded by $O(\varepsilon)$ (see (2.12)). This difference makes that Lemma 2.5 does not hold for the solution of (5.3). More specifically, the solution of (5.3) are bounded by

$$\|\partial_t^k X(t, \tau)\|_{L_t^\infty(W_\tau^{1,\infty})} \leq C, \quad \|\partial_t^k W(t, \tau)\|_{L_t^\infty(W_\tau^{1,\infty})} \leq C, \quad k = 0, 1, \dots, r.$$

With this result and the same arguments proposed in Section 2, Theorem 5.2 can be proved and we skip it for brevity.

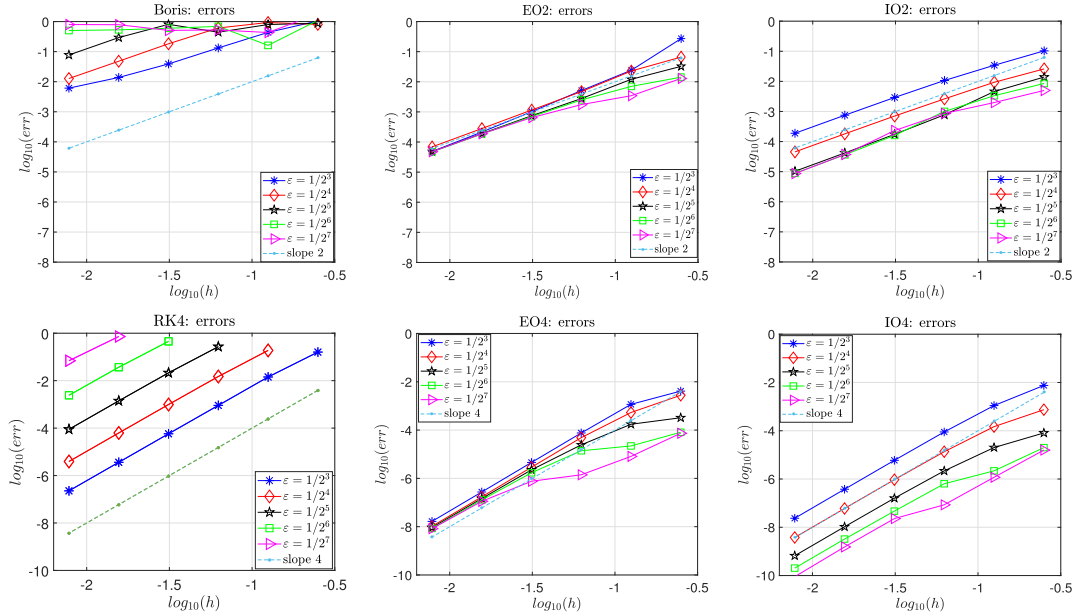


FIGURE 4. The errors (5.4) at $t = 1$ of the second-order schemes (*top row*) and fourth-order schemes (*below row*) with $h = 1/2^k$ for $k = 1, 2, \dots, 6$ under different ε .

Numerical test. As an illustrative numerical experiment, we consider the three dimensional CPD (1.4) with a strong magnetic field [28]

$$B(x, t) = \nabla \times \frac{1}{\varepsilon} \begin{pmatrix} 0 \\ x_1 \\ 0 \end{pmatrix} + \nabla \times \begin{pmatrix} 0 \\ x_1 x_3 \\ 0 \end{pmatrix} = \frac{1}{\varepsilon} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} -x_1 \\ 0 \\ x_3 \end{pmatrix},$$

and $E(x, t) = -\nabla_x U(x)$ with the potential $U(x) = \frac{1}{\sqrt{x_1^2 + x_2^2}}$. The initial values are chosen as $x(0) = (\frac{1}{3}, \frac{1}{4}, \frac{1}{2})^\top$ and $v(0) = (\frac{2}{5}, \frac{2}{3}, 1)^\top$. We solve this problem on $[0, 1]$ by the same methods of Section 4.2 combined with the Fourier pseudospectral method ($N_\tau = 2^6$). The errors of all the methods

$$\text{err} := \frac{\|x^n - x(t_n)\|}{\|x(t_n)\|} + \frac{\|v^n - v(t_n)\|}{\|v(t_n)\|} \quad (5.4)$$

are displayed in Figures 4 and 5. From these results, it follows that EO2 and IO2 show uniform second order accuracy, EO4 and IO4 have uniform fourth order accuracy, but Boris and RK4 do not have such uniform accuracy. We remark here that in Figure 4, the errors from IO2 and IO4 are better than expected. When ε becomes small, it seems that the errors are improved. This behaviour may come from the symmetry of IO2 and IO4 or other reasons that are currently not clear. This issue will be researched further in future.

6. CONCLUSION

In this paper, we formulated and studied the numerical solution of the charged-particle dynamics (CPD) in a strong nonuniform magnetic field. The system involves a small parameter $0 < \varepsilon \ll 1$ inversely proportional to the strength of the external magnetic field. Firstly, a novel class of semi-discretization and full-discretization was presented for the two dimensional CPD and an improved accuracy was rigorously derived. It was shown that

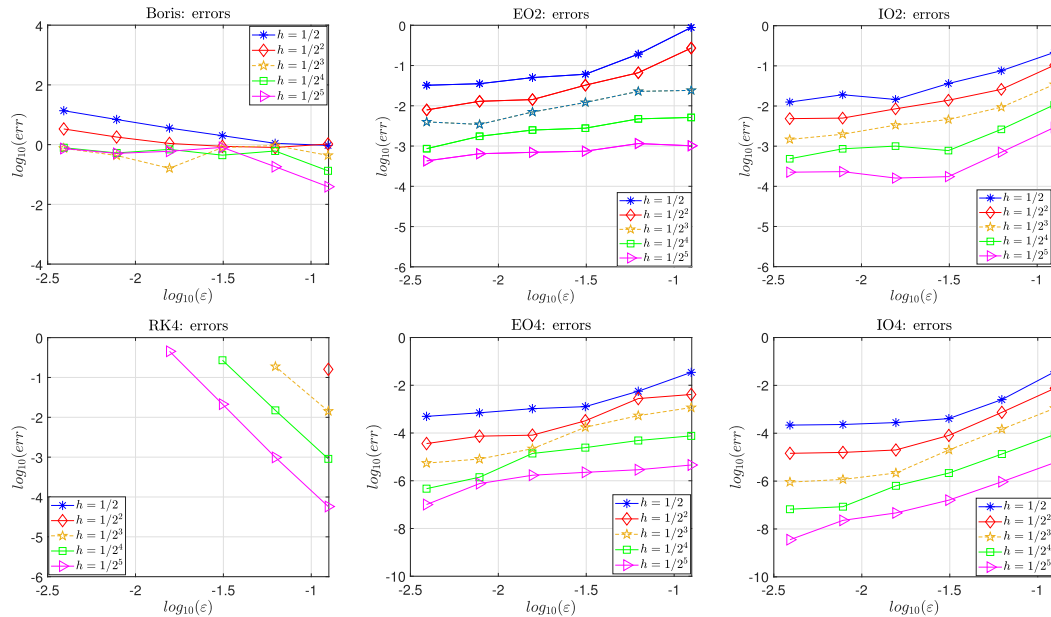


FIGURE 5. The errors (5.4) at $t = 1$ of the second-order schemes (*top row*) and fourth-order schemes (*below row*) with $\varepsilon = 1/2^k$ for $k = 3, 4, \dots, 8$ under different h .

the accuracy of those discretizations is improved in the position and in the velocity when ε becomes smaller. Then based on the approach given for the two dimensional case, a kind of uniformly accurate methods with simple scheme was formulated for the three dimensional CPD in maximal ordering case. The improved accuracy of the obtained discretizations was illustrated by some numerical tests.

Finally, it is remarked that higher-order algorithms with improved accuracy would be an issue for future exploration. Another object of future study could be the structure-preserving methods with improved accuracy.

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REFERENCES

- [1] V.I. Arnold, V.V. Kozlov and A.I. Neishtadt, *Mathematical Aspects of Classical and Celestial Mechanics*. Springer, Berlin (1997).
- [2] W. Bao and X. Ruan, Computing ground states of Bose–Einstein Condensates with higher order interaction via a regularized density function formulation. *SIAM J. Sci. Comput.* **41** (2019) B1284–B1309.
- [3] G. Benettin and P. Sempio, Adiabatic invariants and trapping of a point charge in a strong nonuniform magnetic field. *Nonlinearity* **7** (1994) 281–304.
- [4] C.K. Birdsall and A.B. Langdon, *Plasma Physics Via Computer Simulation*. *Series in Plasma Physics*. Taylor & Francis, New York (2005).
- [5] J.P. Boris, Relativistic plasma simulation-optimization of a hybrid code, in *Proceeding of Fourth Conference on Numerical Simulations of Plasmas* (1970) 3–67.
- [6] A.J. Brizard and T.S. Hahm, Foundations of nonlinear gyrokinetic theory. *Rev. Modern Phys.* **79** (2007) 421–468.
- [7] L. Brugnano, J.I. Montijano and L. Rándz, High-order energy-conserving line integral methods for charged particle dynamics. *J. Comput. Phys.* **396** (2019) 209–227.
- [8] L. Brugnano, F. Iavernaro and R. Zhang, Arbitrarily high-order energy-preserving methods for simulating the gyrocenter dynamics of charged particles. *J. Comput. Appl. Math.* **380** (2020) 112994.

- [9] J.R. Cary and A.J. Brizard, Hamiltonian theory of guiding-center motion. *Rev. Modern Phys.* **81** (2009) 693–738.
- [10] P. Chartier, N. Crouseilles, M. Lemou and F. Méhats, Uniformly accurate numerical schemes for highly oscillatory Klein–Gordon and nonlinear Schrödinger equations. *Numer. Math.* **129** (2015) 211–250.
- [11] P. Chartier, F. Méhats, M. Thalhammer and Y. Zhang, Improved error estimates for splitting methods applied to highly-oscillatory nonlinear Schrödinger equations. *Math. Comput.* **85** (2016) 2863–2885.
- [12] P. Chartier, N. Crouseilles and X. Zhao, Numerical methods for the two-dimensional Vlasov–Poisson equation in the finite Larmor radius approximation regime. *J. Comput. Phys.* **375** (2018) 619–640.
- [13] P. Chartier, N. Crouseilles, M. Lemou, F. Méhats and X. Zhao, Uniformly accurate methods for Vlasov equations with non-homogeneous strong magnetic field. *Math. Comput.* **88** (2019) 2697–2736.
- [14] P. Chartier, N. Crouseilles, M. Lemou, F. Méhats and X. Zhao, Uniformly accurate methods for three dimensional Vlasov equations under strong magnetic field with varying direction. *SIAM J. Sci. Comput.* **42** (2020) B520–B547.
- [15] N. Crouseilles, M. Lemou, F. Méhats and X. Zhao, Uniformly accurate Particle-In-Cell method for the long time two-dimensional Vlasov–Poisson equation with uniform strong magnetic field. *J. Comput. Phys.* **346** (2017) 172–190.
- [16] N. Crouseilles, S. Jin and M. Lemou, Nonlinear geometric optics method based multi-scale numerical schemes for highly-oscillatory transport equations. *Math. Mod. Meth. App. Sci.* **27** (2017) 2031–2070.
- [17] N. Crouseilles, S.A. Hirstoaga and X. Zhao, Multiscale Particle-In-Cell methods and comparisons for the long-time two-dimensional Vlasov–Poisson equation with strong magnetic field. *Comput. Phys. Comm.* **222** (2018) 136–151.
- [18] F. Filbet and M. Rodrigues, Asymptotically stable Particle-In-Cell methods for the Vlasov–Poisson system with a strong external magnetic field. *SIAM J. Numer. Anal.* **54** (2016) 1120–1146.
- [19] F. Filbet and M. Rodrigues, Asymptotically preserving Particle-In-Cell methods for inhomogeneous strongly magnetized plasmas. *SIAM J. Numer. Anal.* **55** (2017) 2416–2443.
- [20] F. Filbet, T. Xiong and E. Sonnendrücker, On the Vlasov–Maxwell system with a strong magnetic field. *SIAM J. Appl. Math.* **78** (2018) 1030–1055.
- [21] F. Filbet, M. Rodrigues and H. Zakerzadeh, Convergence analysis of asymptotic preserving schemes for strongly magnetized plasmas. *Numer. Math.* **149** (2021) 549–593.
- [22] E. Frénod, F. Salvarani and E. Sonnendrücker, Long time simulation of a beam in a periodic focusing channel via a two-scale PIC-method. *Math. Models Methods Appl. Sci.* **19** (2009) 175–197.
- [23] E. Frénod, S. Hirstoaga, M. Lutz and E. Sonnendrücker, Long time behavior of an exponential integrator for a Vlasov–Poisson system with strong magnetic field. *Commun. Comput. Phys.* **18** (2015) 263–296.
- [24] E. Hairer and C. Lubich, Energy behaviour of the Boris method for charged-particle dynamics. *BIT* **58** (2018) 969–979.
- [25] E. Hairer and C. Lubich, Symmetric multistep methods for charged-particle dynamics. *SMAI J. Comput. Math.* **3** (2017) 205–218.
- [26] E. Hairer and C. Lubich, Long-term analysis of a variational integrator for charged-particle dynamics in a strong magnetic field. *Numer. Math.* **144** (2020) 699–728.
- [27] E. Hairer, C. Lubich and G. Wanner, Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations, 2nd edition. Springer-Verlag, Berlin, Heidelberg (2006).
- [28] E. Hairer, C. Lubich and B. Wang, A filtered Boris algorithm for charged-particle dynamics in a strong magnetic field. *Numer. Math.* **144** (2020) 787–809.
- [29] Y. He, Y. Sun, J. Liu and H. Qin, Volume-preserving algorithms for charged particle dynamics. *J. Comput. Phys.* **281** (2015) 135–147.
- [30] Y. He, Z. Zhou, Y. Sun, J. Liu and H. Qin, Explicit K-symplectic algorithms for charged particle dynamics. *Phys. Lett. A* **381** (2017) 568–573.
- [31] M. Hochbruck and A. Ostermann, Explicit exponential Runge–Kutta methods for semilinear parabolic problems. *SIAM J. Numer. Anal.* **43** (2006) 1069–1090.
- [32] M. Hochbruck and A. Ostermann, Exponential integrators. *Acta Numer.* **19** (2010) 209–286.
- [33] C. Knapp, A. Kendl, A. Koskela and A. Ostermann, Splitting methods for time integration of trajectories in combined electric and magnetic fields. *Phys. Rev. E* **92** (2015) 063310.
- [34] M. Kraus, K. Kormann, P. Morrison and E. Sonnendrücker, GEMPIC: geometric electromagnetic particle in cell methods. *J. Plasma Phys.* **4** (2017) 83.
- [35] W.W. Lee, Gyrokinetic approach in particle simulation. *Phys. Fluids* **26** (1983) 556–562.
- [36] T. Li and B. Wang, Efficient energy-preserving methods for charged-particle dynamics. *Appl. Math. Comput.* **361** (2019) 703–714.
- [37] T.G. Northrop, The adiabatic motion of charged particles, in Interscience Tracts on Physics and Astronomy. Vol. 21. Interscience Publishers John Wiley and Sons New York-London-Sydney (1963).
- [38] S. Possanner, Gyrokinetics from variational averaging: existence and error bounds. *J. Math. Phys.* **59** (2018) 082702.
- [39] H. Qin and X. Guan, Variational symplectic integrator for long-time simulations of the guiding-center motion of charged particles in general magnetic fields. *Phys. Rev. Lett.* **100** (2008) 035006.
- [40] H. Qin, S. Zhang, J. Xiao, J. Liu, Y. Sun and W. Tang, Why is Boris algorithm so good? *Phys. Plasmas* **20** (2013) 084503.
- [41] L.F. Ricketson and L. Chacón, An energy-conserving and asymptotic-preserving charged-particle orbit implicit time integrator for arbitrary electromagnetic fields. *J. Comput. Phys.* **418** (2020) 109639.
- [42] J. Shen, T. Tang and L. Wang, Spectral Methods: Algorithms, Analysis, Applications. Springer, Berlin (2011).

- [43] E. Sonnendrücker, Numerical methods for Vlasov equations. Lecture notes (2016).
- [44] M. Tao, Explicit high-order symplectic integrators for charged particles in general electromagnetic fields. *J. Comput. Phys.* **327** (2016) 245–251.
- [45] B. Wang, Exponential energy-preserving methods for charged-particle dynamics in a strong and constant magnetic field. *J. Comput. Appl. Math.* **387** (2021) 112617.
- [46] B. Wang and X. Zhao, Error estimates of some splitting schemes for charged-particle dynamics under strong magnetic field. *SIAM J. Numer. Anal.* **59** (2021) 2075–2105.
- [47] B. Wang and X. Zhao, Geometric two-scale integrators for highly oscillatory system: uniform accuracy and near conservations. *SIAM J. Numer. Anal.* **61** (2023) 1246–1277.
- [48] S.D. Webb, Symplectic integration of magnetic systems. *J. Comput. Phys.* **270** (2014) 570–576.
- [49] R. Zhang, H. Qin, Y. Tang, J. Liu, Y. He and J. Xiao, Explicit symplectic algorithms based on generating functions for charged particle dynamics. *Phys. Rev. E* **94** (2016) 013205.



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