Computer Physics Communications 185 (2014) 2851–2858

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Application of the phase space action principle to finite-size particle plasma simulations in the drift-kinetic approximation

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ARTICLE INFO

Article history:
Received 19 December 2013
Received in revised form
9 March 2014
Accepted 6 July 2014
Available online 12 July 2014

Keywords:
Numerical
Plasma
Kinetic
Magnetized
Drift-kinetic
Energy conserving
Particle-in-cell

ABSTRACT

We formulate a finite-size particle numerical model of strongly magnetized plasmas in the drift-kinetic approximation. We use the phase space action as an alternative to previous variational formulations based on Low's Lagrangian or on a Hamiltonian with a non-canonical Poisson bracket. The useful property of this variational principle is that it allows independent transformations of particle coordinates and velocities, i.e., transformations in particle phase space. With such transformations, a finite degree-of-freedom drift-kinetic action is obtained through time-averaging of the finite degree-of-freedom fully-kinetic action. Variation of the drift-kinetic Lagrangian density leads to a self-consistent, macro-particles and fields numerical model. Since the computational particles utilize only guiding center coordinates and velocities, there is a large computational advantage in the time integration part of the algorithm. Numerical comparison between the time-averaged fully-kinetic and drift-kinetic charge and current, deposited on a computational grid, offers insight into the range of validity of the model. Being based on a variational principle, the algorithm respects the energy conserving property of the underlying continuous system. The development in this paper serves to further emphasize the advantages of using variational approaches in plasma particle simulations.

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1. Introduction

Finite-size particle algorithms for kinetic plasma simulations have established a strong record of success in a variety of areas [1,2]. Recent work [3] reexamined the variational formulations of these algorithms [4,5] and developed important improvements and generalizations. Two variational formulations were considered in Ref. [3], one based on Low's Lagrangian [6], which generalized previous work and a new one, based on a Hamiltonian functional and a non-canonical Poisson bracket [7,8]. Ref. [3] analyzed in detail the relation between Lagrangian symmetries and conservation properties in the process of reduction from infinite (Vlasov–Poisson or Vlasov–Maxwell system) to finite number of degrees of freedom (DOF), pointing out which approximations led to the retention – or not – of which conserved quantities. It also addressed the relation between force interpolation and particle shape and showed that the particle shape is not the determining factor in an algorithm's overall accuracy; as an illustration, it constructed a charge deposition rule that has a narrow stencil but high smoothness. Energy conservation properties were carefully examined and was shown that in the time-discretized system, energy conservation depends *only* on the time step size; as a comparison, it showed that in the more standard particle-in-cell (PIC) algorithm energy conservation depends on both the time step and the grid spacing. There are many other attractive features of variational formulations, including the ease of change of variables, a consistent way of increasing the overall accuracy (in space and time), etc., which motivate us to seek their further extensions and applications.

The present work has two purposes. First, to offer an alternative formulation to the above two, a formulation based on the phase space action [9,10]. In this variational principle the particle coordinates and velocities are considered independent variables and are varied separately. The physical relations between coordinates and velocities as well as Newton's equations of motion are obtained after performing the variation. The important feature of this approach is that it allows transformation of variables independently for coordinates and velocities, i.e., transformations in *particle phase space* rather than in configuration space only. This property was used by Littlejohn [11], who offered a simplified derivation of the guiding center equations of motion of a point particle in external electric and strong magnetic fields. Thus, the second purpose of the present work is to introduce the guiding center

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http://dx.doi.org/10.1016/j.cpc.2014.07.004
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equations of motion for finite size particles in a self-consistent, particles and fields numerical model. Since this is a variational formulation, the energy conserving property is automatically preserved.

We conduct a brief discussion of related literature to help point out certain novel aspects of our work. The early publication of Lee and Okuda [12] presented a particle model based on drift-kinetic electrons and fully-kinetic ions and used it to simulate the linear and non-linear stages of drift-wave instabilities. An important advantage of such approach was the large reduction in the computational cost due to the larger time step for pushing electrons; another advantage was the ability to use realistic electron-to-ion mass ratio. In a later publication, further computational efficiency was targeted by using gyro-kinetic ions in addition to the drift-kinetic electrons [13,14]. These models were further developed in Refs. [15,16] and were used to study magnetic reconnection [17]. The review article by Garbet et al. [18] provides a summary of other particle-based simulation efforts and available codes.

The main method followed by the above authors in obtaining a finite DOF system, i.e., a numerical model, was to first time- or gyro-phase average the fully-kinetic continuous equations to obtain drift- or gyro-kinetic continuous equations and *then* apply specific spatial and time descretizations. This is similar to the approach used in the PIC method. In doing so, existing conservation laws in the continuous system do not automatically transfer to the resulting numerical model. For example, the loss of energy conservation is due to errors of order higher than the discretization accuracy. It is known that nonphysical numerical artifacts occur in so-discretized systems [19,20]. In contrast, our starting point is a finite DOF fully-kinetic system, i.e., a reduced Maxwell–Vlasov system described by finite-size particles and spatially discretized fields (with continuous time). To this reduced system, we then apply a time-averaging procedure to directly obtain a numerical model with finite-size particles and spatially discretized fields in the drift kinetic approximation (the gyro-kinetic approximation lies outside the scope of the present work). All steps, including those leading to the reduced fully-kinetic system and its time-averaging, are performed within the Lagrangian framework, which permits to preserve to the fullest the existing symmetries of the original continuous system; in particular, the energy-conserving property is preserved. Additional conservation laws may be respected depending on the specifics of the discretization [3]. In following this approach, we construct discretization schemes, in which discretization errors cancel out exactly to make the conservation of certain quantities possible. The Lagrangian framework is not mandatory in deriving such discretizations, however alternatively, one would be faced with the difficult task of tracking unbalanced errors and modifying discretizations to achieve the same effect.

The energy-conserving deficiency in the PIC model was addressed recently in two publications [21,22]. In addition, a novel implicit technique was introduced that projects large computational advantage. Only fully-kinetic plasmas were addressed in these works.

Recent variational finite-size particle formulations were reported by several authors [23–26]. These models were restricted to fully-kinetic electrostatic or electromagnetic plasmas. Another difference with the present work is that these authors use time and space discretized action vs. our use of continuous time and spatially discretized Lagrangian; in fact, our keeping time continuous is crucial in order to apply the time-averaging procedure to the fully-kinetic Lagrangian equation (Appendix A). The equations of our formulation are most suited to time-explicit schemes while those in the cited references result, as a rule, in time-implicit schemes [27] (e.g., when magnetic field is included or when higher than second order time integration is desired).

The rest of the paper is organized as follows. Section 2 describes an alternative formulation of finite-size particle algorithms based on the phase–space action. Section 3 describes the drift-kinetic approximation of the phase space action and the drift-kinetic numerical model. Section 4 provides numerical comparison between the fully-kinetic and the drift-kinetic models. Section 5 discusses the results and concludes.

2. Phase space variational principle

Our starting point is the phase space Lagrangian density (or simply Lagrangian) for the fully-kinetic system of particles and fields in Coulomb gauge [9,10], reduced to a finite number of degrees of freedom [3]:

$$\begin{aligned}\mathscr{L}_{\mathrm{FK}} = &\sum_{\alpha=1}^{N_\mathrm{p}} w_\alpha \left[\mathtt{m}\mathbf{v}_\alpha + \mathtt{q}\mathbf{A}(\mathbf{x}_\alpha, t)\right]\cdot\dot{\mathbf{x}}_\alpha \\ &- \sum_{\alpha=1}^{N_\mathrm{p}} w_\alpha \left[\frac{1}{2}\mathtt{m}\mathbf{v}_\alpha^2 + \mathtt{q}\varphi(\mathbf{x}_\alpha, t)\right] \\ &+ h_x h_y h_z \left\{-\frac{\epsilon_0}{2}\sum_{\mathbf{m},\mathbf{n}} \varphi_\mathbf{m}(t)\nabla^2_{\mathbf{mn}}\varphi_\mathbf{n}(t)\right. \\ &\left. + \frac{\epsilon_0}{2}\sum_{\mathbf{m}} \dot{\mathbf{A}}_\mathbf{m}(t)\cdot\dot{\mathbf{A}}_\mathbf{m}(t) + \frac{1}{2\mu_0}\sum_{\mathbf{m},\mathbf{n}} \mathbf{A}_\mathbf{m}(t)\cdot\nabla^2_{\mathbf{mn}}\mathbf{A}_\mathbf{n}(t)\right\}, \quad (1)\end{aligned}$$

where N_p is the number of simulation particles; w_α is their computational weight; $\mathtt{m}$ and $\mathtt{q}$ are the physical mass and charge of the plasma species (we do not show explicitly a sum over particle species but such can be trivially added); ϵ_0 and μ_0 are the permittivity and permeability of vacuum; $\varphi_\mathbf{m}$ and $\mathbf{A}_\mathbf{m}$ denote the collection of grid (or nodal) values of the electric and magnetic vector potential, respectively, on a three-dimensional grid with $\mathbf{m} \equiv (m_x, m_y, m_z)$; the grid is assumed uniform with grid spacings h_x, h_y, and h_z; sums in $\mathbf{m}$, $\mathbf{n}$ range over all grid points; $\mathbf{x}_\alpha$ is the computational particle's coordinate and $\dot{\mathbf{x}}_\alpha$ its time derivative; $\mathbf{v}_\alpha$ is the particle's velocity, which at this point is considered an independent variable, i.e., unrelated to $\dot{\mathbf{x}}_\alpha$. The abbreviated notations $\varphi(\mathbf{x}_\alpha, t)$ and $\mathbf{A}(\mathbf{x}_\alpha, t)$ have been used to denote interpolated values of the electric and magnetic vector potential from the computational grid to the particle location:

$$\varphi(\mathbf{x}_\alpha, t) = \sum_\mathbf{m} \rho_\mathbf{m}(\mathbf{x}_\alpha)\varphi_\mathbf{m}(t), \quad (2)$$

$$\mathbf{A}(\mathbf{x}_\alpha, t) = \sum_\mathbf{m} \rho_\mathbf{m}(\mathbf{x}_\alpha)\mathbf{A}_\mathbf{m}(t). \quad (3)$$

$\rho_\mathbf{m}(\mathbf{x}_\alpha)$ is a charge deposition rule of choice; $\rho_\mathbf{m}(\mathbf{x}_\alpha)$ could either be chosen from some of the well known rules in the particle-in-cell method [1,2] or from the more general ones described in [3]. The operator $\nabla^2_{\mathbf{mn}}$ denotes the appropriately discretized Laplacian operator, e.g., by central differences. Additionally, we introduce the following notation (which becomes apparent in deriving equations (6)–(9)):

$$\mathbf{B}(\mathbf{x}_\alpha, t) = \nabla\times\mathbf{A}(\mathbf{x}_\alpha, t) = \sum_\mathbf{m} \frac{\partial\rho_\mathbf{m}(\mathbf{x}_\alpha)}{\partial\mathbf{x}_\alpha}\times\mathbf{A}_\mathbf{m}(t), \quad (4)$$

$$\nabla\varphi(\mathbf{x}_\alpha, t) = \sum_\mathbf{m} \frac{\partial\rho_\mathbf{m}(\mathbf{x}_\alpha)}{\partial\mathbf{x}_\alpha}\varphi_\mathbf{m}(t),$$

$$\frac{\partial A(\mathbf{x}_\alpha, t)}{\partial t} = \sum_\mathbf{m} \rho_\mathbf{m}(\mathbf{x}_\alpha)\frac{\mathrm{d}\mathbf{A}_\mathbf{m}(t)}{\mathrm{d}t},$$

$$\mathbf{E}(\mathbf{x}_\alpha, t) = -\nabla\varphi(\mathbf{x}_\alpha, t) - \frac{\partial A(\mathbf{x}_\alpha, t)}{\partial t}. \quad (5)$$

In the following part of the paper, where we do not show explicitly the arguments of field variables, we assume definitions similar

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