A curvilinear, fully implicit, conservative electromagnetic PIC algorithm in multiple dimensions

L. Chacón^{a,*}, G. Chen^a

^a*Los Alamos National Laboratory, Los Alamos, NM 87545*

Abstract

We extend a recently proposed fully implicit PIC algorithm for the Vlasov-Darwin model in multiple dimensions [Chen and Chacón, *Comput. Phys. Comm.*, vol. 197, pp. 73–87 (2015)] to curvilinear geometry. As in the Cartesian case, the approach is based on a potential formulation $(\phi, \mathbf{A})$, and overcomes many difficulties of traditional semi-implicit Darwin PIC algorithms. Conservation theorems for local charge and global energy are derived in curvilinear representation, and then enforced discretely by a careful choice of the discretization of field and particle equations. Additionally, the algorithm conserves canonical-momentum in any ignorable direction, and preserves the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ exactly. An asymptotically well-posed fluid preconditioner allows efficient use of large cell sizes, which are determined by accuracy considerations, not stability, and can be orders of magnitude larger than required in a standard explicit electromagnetic PIC simulation. We demonstrate the accuracy and efficiency properties of the algorithm with numerical experiments in mapped meshes in 1D-3V and 2D-3V.

Keywords: Conservative discretization, Darwin model, fully implicit algorithms, curvilinear meshes

PACS:

1. Introduction

For many laboratory and natural plasma applications of interest (e.g., magnetic fusion, astrophysics, plasma-material interactions, etc.), the ability to perform trustworthy particle-in-cell (PIC) simulations in shaped domains is desired. One option is to use unstructured meshes, but these introduce either significant inefficiencies (if done accurately) or inaccuracies (if done approximately) in the PIC algorithm related to particle tracking in the computational domain. Moreover, the development of modern implicit PIC algorithms for unstructured representations is presently lagging. In the context of structured grids, dealing with such boundaries requires mapped (or boundary-fitted) grids, in which a logical (computational) Cartesian space relates to the physical domain via an invertible map. Generally, such maps result in non-orthogonal grids, which require special treatment of moments, fields, and particles.

*Corresponding author

Email address: chacon@lanl.gov (L. Chacón)

The focus of this study is to generalize a recently proposed fully implicit, energy and charge conserving Vlasov-Darwin electromagnetic PIC algorithm [1] to curvilinear meshes. For this, we will use some of the concepts advanced in the context of electrostatic PIC in Ref. [2]. The use of boundary-fitted grids in the context of PIC is not new. Various approaches have been documented in the literature in non-uniform, curvilinear, or unstructured grids using finite-difference methods [3, 4], finite-volume methods [5, 6], and finite-element methods [7, 8] in many application domains such as microwave modeling [9], plasma propulsion modeling [10], astrophysics [11, 12, 13], and fusion simulations [14, 15]. It should be noted that, to the best of our knowledge, none of these algorithms satisfies the discrete charge continuity equation exactly, or conserves energy or momentum exactly in a non-uniform grid with discrete time-stepping.

One fundamental design issue in curvilinear PIC is how to scatter moments from particles to grid points. In Refs. [16, 17, 18], it was shown that the moment scatter to a curvilinear mesh needs to be corrected to preserve a uniform particle density, while no correction is needed for a Cartesian mesh. However, in those references, such a corrected scatter is motivated in an *ad hoc* manner. In this study, we employ a density-preserving scheme, based on the curvilinear formulation of the continuum Vlasov equation and its underlying conservation properties [19, 2]. The essential difference of our approach is that we collect particle number density in the logical space, while Refs. [16, 17, 18] did it in physical space. In logical space, the conserved quantity is Jf (where J is the Jacobian and f is the distribution function) instead of f [19, 2]. By construction, our formulation automatically takes care of the Jacobian factor as was done, for instance, in the gyrokinetic context in Ref. [20].

Another important design issue in curvilinear PIC is whether particle pushing is performed in physical space or in logical space. Physical-space pushing (PSP) avoids errors stemming from discrete map information [21, 22]. However, PSP may incur inaccuracies related to gather-scatter operations (i.e., interpolation to and from the grid), such as spurious compressibility effects and violation of charge and current density conservation [16, 18, 17]. Furthermore, PSP typically requires expensive particle location-tracking techniques [23, 21] to “relocate” particles in logical cells after each particle push in physical space (although algorithms have been proposed that significantly speed up the particle localization step using a tetrahedral decomposition of hexahedral cells [24]). Logical-space-pushing (LSP) [7, 20, 25] avoids location-tracking and gather-scatter errors, but may incur in particle orbit errors due to discrete map information and the need to account for fictitious inertial forces [25] due to changes in geometry. To avoid these issues, we consider in this study a hybrid particle pushing (HPP) approach [26, 5, 2, 13], which updates logical space positions (thereby inheriting the efficiency of Cartesian PIC in regards to particle location-tracking in the computational domain) and Cartesian velocity components (thereby avoiding fictitious inertial forces). Furthermore, HPP allows one to generalize strict discrete conservation theorems for local charge and global energy to a curvilinear setting [2].

In this study, we present such a generalization for the fully implicit, charge and energy conserving 2D Vlasov-Darwin PIC algorithm introduced in Ref. [1]. We begin by introducing the analytical model and its

properties in Sec. 2. Section 3 introduces its formulation in curvilinear geometry, for both fields and particles. We justify the particle formulation of choice from the curvilinear formulation of the Vlasov equation, and demonstrate that our particle representation indeed solves the corresponding Vlasov equation. The discrete formulation of the field equations (implicit in time, curvilinear in space) is given in Sec. 4, with emphasis on the formulation of strict discrete global energy and local charge conservation theorems. The generalization of the fluid accelerator strategy, proposed in Ref. [1], to curvilinear geometry is outlined in Sec. 5. Finally, we demonstrate the performance of the scheme in Sec. 6, and conclude in Sec. 7.

2. Electromagnetic Vlasov-Darwin model

The minimal set of Vlasov-Darwin equations [27, 28, 29, 30, 31] for a collisionless electromagnetic plasma can be written as [32, 1]:

$$\partial_t f_s + \mathbf{v} \cdot \nabla f_s + \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f_s = 0, \quad (1)$$

$$\frac{1}{\mu_0} \nabla^2 \mathbf{A} + \mathbf{j} - \epsilon_0 \partial_t \nabla \phi = 0, \quad (2)$$

$$\epsilon_0 \partial_t \nabla^2 \phi = \nabla \cdot \mathbf{j}, \quad (3)$$

$$\mathbf{j} = \sum_s q_s \int f_s \mathbf{v} d\mathbf{v}. \quad (4)$$

where $f_s(\mathbf{r}, \mathbf{v})$ is the particle distribution function of species s in phase space, q_s and m_s are the species charge and mass respectively, ϵ_0 and μ_0 are the vacuum permittivity and permeability respectively, ϕ and $\mathbf{A}$ are the scalar and vector potentials, respectively. This set of equations implies two involutions [1], $\nabla \cdot \mathbf{A} = 0$ (Coulomb gauge, required for charge conservation in the Darwin model) and $\epsilon_0 \nabla^2 \phi + \rho = 0$ (Gauss' law). The former is implied by taking the divergence of Eq. 2 and using Eq. 3, which requires that $\nabla \cdot (\nabla^2 \mathbf{A}) = \nabla^2 (\nabla \cdot \mathbf{A}) = 0$, and the boundary conditions be consistent with $\nabla \cdot \mathbf{A} = 0$ [33]. The latter is enforced by Eq. 3 and the first moment of Eq. 1. These two involutions are not redundant, and must be enforced numerically [34, p. 359] to prevent spurious modes from being excited [35]. The set of Darwin equations is closed with the plasma current density, Eq. 4. The electric and magnetic fields are defined uniquely from ϕ , $\mathbf{A}$ as:

$$\mathbf{E} = -\nabla \phi - \partial_t \mathbf{A} ; \mathbf{B} = \nabla \times \mathbf{A}. \quad (5)$$

Equations 1-4, and 5 constitute the Vlasov-Darwin equation set of choice in this study. We emphasize that the main advantage of this set is that the two involutions (Poisson's equation and the solenoidal constraint of $\mathbf{A}$) are built-in, and thus do not need to be enforced or solved explicitly when local charge is strictly conserved. This property, when implemented discretely, will be most advantageous for both accuracy (it avoids spurious modes) and efficiency (it avoids the extra divergence-cleaning step via conventional projection methods [36] or hyperbolic cleaning [37]). Most importantly, this formulation avoids explicitly enforcing the Coulomb gauge [1]. This has been a critical implementation roadblock for the Darwin approximation in multiple dimensions in previous studies [27, 38], which avoided enforcing the Coulomb

gauge by formulating an additional evolution equation for the solenoidal component of the electric field, but it required additional boundary conditions that were not physically motivated [39]. Dealing directly with potential equations poses no such difficulties [29], but carrying the involution enforcement discretely in curvilinear geometry requires a very careful treatment, as will be apparent later in this study.

2.1. Energy conservation theorem of the Vlasov-Darwin model

The Vlasov-Darwin model features an energy conservation theorem. We begin by taking the integral $\sum_s m_s \int d\mathbf{x} \int d\mathbf{v} \frac{v^2}{2}$ of Eq. 1, to find (using Eq. 4):

$$\frac{d}{dt} K_p = \int d\mathbf{x} \mathbf{E} \cdot \mathbf{j},$$

with $K_p = \sum_s m_s \int d\mathbf{x} \int d\mathbf{v} \frac{v^2}{2} f_s$ the total kinetic energy. Using Eq. 5, we have:

$$\int d\mathbf{x} \mathbf{E} \cdot \mathbf{j} = \int d\mathbf{x} \mathbf{j} \cdot [-\nabla\phi - \partial_t \mathbf{A}] = - \int d\mathbf{x} \mathbf{j} \cdot \nabla\phi - \int d\mathbf{x} \mathbf{j} \cdot \partial_t \mathbf{A}.$$

But:

$$\int d\mathbf{x} \mathbf{j} \cdot \nabla\phi = - \int d\mathbf{x} \phi \nabla \cdot \mathbf{j} = -\epsilon_0 \int d\mathbf{x} \phi \partial_t \nabla^2 \phi = \frac{\epsilon_0}{2} \frac{d}{dt} \int d\mathbf{x} |\nabla\phi|^2 = \frac{dW_\phi}{dt},$$

where we have used Eq. 3, and defined the electrostatic energy W_ϕ as:

$$W_\phi = \frac{\epsilon_0}{2} \int d\mathbf{x} |\nabla\phi|^2. \quad (6)$$

Similarly, using Eq. 2, we can show straightforwardly that:

$$\int d\mathbf{x} \mathbf{j} \cdot \partial_t \mathbf{A} = \int d\mathbf{x} \partial_t \mathbf{A} \cdot \left[-\frac{1}{\mu_0} \nabla^2 \mathbf{A} + \epsilon_0 \partial_t \nabla\phi \right] = \frac{dW_B}{dt},$$

where:

$$W_B = -\frac{1}{2\mu_0} \int d\mathbf{x} \mathbf{A} \cdot \nabla^2 \mathbf{A} = \frac{1}{2\mu_0} \int d\mathbf{x} \mathbf{A} \cdot \nabla \times \nabla \times \mathbf{A} = \frac{1}{2\mu_0} \int d\mathbf{x} B^2 \quad (7)$$

is the magnetic field energy, and the displacement current contribution vanishes by virtue of the gauge condition:

$$\int d\mathbf{x} \partial_t \mathbf{A} \cdot \nabla \partial_t \phi = - \int d\mathbf{x} \partial_t \phi \nabla \cdot (\partial_t \mathbf{A}) = 0$$

The energy conservation theorem follows:

$$\frac{d}{dt} [K_p + W_\phi + W_B] = 0.$$

3. Curvilinear formulation of the Vlasov-Darwin model

Given a curvilinear, time-independent map $\mathbf{x}(\xi)$, with contravariant base vectors $\boldsymbol{\alpha} = \nabla \xi^\alpha$, covariant base vectors $\frac{\partial \mathbf{x}}{\partial \xi^\alpha}$, and Jacobian $J = |\partial \mathbf{x} / \partial \xi|$, for a generic vector $\mathbf{S}$, contravariant components are defined as $S^\alpha = \mathbf{S} \cdot \boldsymbol{\alpha}$ and covariant components as $S_\alpha = \mathbf{S} \cdot \frac{\partial \mathbf{x}}{\partial \xi^\alpha}$. The covariant and contravariant components are related by $S_\alpha = g_{\alpha\beta} S^\beta$, with $g_{\alpha\beta}$ the covariant metric tensor components. In what follows, $\partial_\alpha \equiv \partial / \partial \xi^\alpha$.

3.1. Curvilinear formulation of the Darwin field equations

To formulate the Darwin field equations in curvilinear geometry, following Ref. [2], we represent the vector potential and electric field in covariant form, and the magnetic field and Ampere's equation (Eq. 2) in contravariant form. There results:

$$\partial_\alpha \left(J g^{\alpha\beta} \partial_\beta \chi \right) = \partial_\alpha (J j^\alpha), \quad (8)$$

$$-\frac{J}{\mu_0} \nabla^2 \mathbf{A}^\alpha = J j^\alpha - J g^{\alpha\beta} \partial_\beta \chi, \quad (9)$$

$$E_\alpha = -\partial_\alpha \phi - \partial_t A_\alpha, \quad (10)$$

$$J B^\alpha = \epsilon_{\alpha\beta\gamma} \partial_\beta A_\gamma, \quad (11)$$

with $\chi = \epsilon_0 \partial_t \phi$ and $\epsilon_{\alpha\beta\gamma}$ the Levi-Civita symbol. Here, $\nabla^2 \mathbf{A}^\alpha$ is the contravariant component of the vector Laplacian.

We show next the energy conservation theorem in curvilinear geometry. We begin with the integral $\int d\mathbf{x} \mathbf{E} \cdot \mathbf{j}$, which in curvilinear representation reads:

$$\int d\mathbf{x} \mathbf{E} \cdot \mathbf{j} = \int d\xi J j^\alpha E_\alpha = - \int d\xi J j^\alpha \partial_\alpha \phi - \int d\xi J j^\alpha \cdot \partial_t A_\alpha.$$

Using Eq. 8, we find:

$$\int d\xi J j^\alpha \partial_\alpha \phi = - \int d\xi \phi \partial_\alpha (J j^\alpha) = -\epsilon_0 \int d\xi \phi \partial_\alpha (J g^{\alpha\beta} \partial_\beta \phi) = \frac{dW_\phi}{dt},$$

where

$$W_\phi = \frac{\epsilon_0}{2} \int d\xi J g^{\alpha\beta} \partial_\alpha \phi \partial_\beta \phi = \frac{\epsilon_0}{2} \int d\mathbf{x} |\nabla \phi|^2 \quad (12)$$

is the curvilinear expression of the electrostatic energy. Similarly, using Eq. 9, we find:

$$\int d\xi J j^\alpha \cdot \partial_t A_\alpha = \int d\xi J \partial_t A_\alpha \left[-\frac{1}{\mu_0} \nabla^2 \mathbf{A}^\alpha + g^{\alpha\beta} \partial_\beta \chi \right] = \frac{dW_B}{dt} - \int d\xi J \underbrace{J^{-1} \partial_\beta (J g^{\beta\alpha} \partial_t A_\alpha)}_{\nabla \cdot \mathbf{A}=0} \chi = \frac{dW_B}{dt},$$

where again we have used that $\nabla \cdot \mathbf{A} = 0$ in the cancellation of the contribution of the displacement current, and we have defined the magnetic field energy as:

$$W_B = -\frac{1}{2\mu_0} \int d\xi J \nabla^2 \mathbf{A}^\alpha A_\alpha = \frac{1}{2\mu_0} \int d\xi J B_\alpha B^\alpha. \quad (13)$$

The energy conservation theorem sought follows.

3.2. Curvilinear formulation of the Vlasov equation and the particle representation

The analysis of the curvilinear formulation of the Vlasov equation is important to motivate the representation of the particle system in curvilinear geometry. We remark that the curvilinear representation is for configuration space only, with the velocity space remaining Cartesian. In curvilinear geometry, Eq. 1 reads:

$$\partial_t f_s + v^\alpha \partial_\alpha f_s + \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = 0, \quad (14)$$

with $v^\alpha = \mathbf{v} \cdot \boldsymbol{\alpha}$. The first observation is that there is a characteristics-based solution of this equation, which makes its representation in terms of particle markers straightforward. However, this equation cannot be readily put in conservative form, since $\partial_\alpha v^\alpha \neq 0$. This implies that f_s is no longer conserved in curvilinear phase space. The correct conserved quantity can be derived by noting that the condition $\nabla \cdot \mathbf{v} = 0$ in curvilinear geometry implies $\partial_\alpha (Jv^\alpha) = 0$. Thus, multiplying Eq. 14 by the (time-independent) Jacobian, we readily find:

$$\partial_t(Jf_s) + \partial_\alpha(v^\alpha Jf_s) + \nabla_{\mathbf{v}} \cdot \left[\frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) Jf_s \right] = 0, \quad (15)$$

which indicates that the conserved quantity in curvilinear phase space is Jf_s (and not f_s) [19, 2].

These observations motivate the particle representation of choice in this study. In particular, we consider the particle representation of Jf_s in curvilinear geometry as [19, 2]:

$$Jf_s \approx \sum_{p \in s} w_p \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)], \quad (16)$$

where the subscript p denotes a particle (or Lagrangian) quantity, and $\boldsymbol{\xi}$ and $\mathbf{v}$ denote logical and velocity coordinates in phase space, respectively, which are Eulerian quantities. Phase-space conservation of Jf_s implies that the particle weight w_p be kept constant during the particle motion along its orbit. Particle orbits are governed by the following equations of motion:

$$\dot{\boldsymbol{\xi}}_p^\alpha = v_p^\alpha = \mathbf{v}_p \cdot \boldsymbol{\alpha}_p, \quad (17)$$

$$\dot{\mathbf{v}}_p = \mathbf{a}_p = \frac{q_p}{m_p} (\mathbf{E}_p + \mathbf{v}_p \times \mathbf{B}_p), \quad (18)$$

These equations update the position in logical space, while velocity is updated in Cartesian representation (so-called hybrid particle pushing [26, 5, 2, 13]).

We prove next that the particle representation in Eqs. 16-18 is a weak solution of Eq. 15, that is, it preserves integral:

$$\frac{d}{dt} \int_{\mathcal{V}} Jf(\boldsymbol{\xi}, \mathbf{v}, t) d\boldsymbol{\xi} = \int_{\mathcal{V}} d\boldsymbol{\xi} \left\{ \partial_t(Jf_s) + \partial_\alpha(v^\alpha Jf_s) + \nabla_{\mathbf{v}} \cdot \left[\frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) Jf_s \right] \right\} = 0,$$

where $\mathcal{V}$ is the phase space volume that follows Eq. 17 and 18. We begin by finding $\partial_t(Jf_s)$ from Eq. 16 as:

$$\partial_t(Jf_s) = \partial_t \left[\sum_{p \in s} w_p \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] \right].$$

Expanding the time derivative, we find:

$$\partial_t(Jf_s) = - \sum_{p \in s} w_p \left(\delta[\mathbf{v} - \mathbf{v}_p(t)] \dot{\boldsymbol{\xi}}_p \cdot \nabla_{\boldsymbol{\xi}} \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] + \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \dot{\mathbf{v}}_p \cdot \nabla_{\mathbf{v}} \delta[\mathbf{v} - \mathbf{v}_p(t)] \right). \quad (19)$$

But, noting that $\boldsymbol{\xi}_p$ and $\mathbf{v}_p$ are unrelated to $\boldsymbol{\xi}, \mathbf{v}$, respectively, we can write:

$$\begin{aligned} \delta[\mathbf{v} - \mathbf{v}_p(t)] \dot{\boldsymbol{\xi}}_p \cdot \nabla_{\boldsymbol{\xi}} \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] &= \partial_\alpha \left(\dot{\boldsymbol{\xi}}_p^\alpha \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] \right), \\ \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \dot{\mathbf{v}}_p \cdot \nabla_{\mathbf{v}} \delta[\mathbf{v} - \mathbf{v}_p(t)] &= \nabla_{\mathbf{v}} \cdot \left(\dot{\mathbf{v}}_p \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] \right). \end{aligned}$$

Figure 1: 2D Yee grid and associated curvilinear vectors and grid metric quantities. An integer index i or j denotes a cell center, and a half index $i + 1/2$ or $j + 1/2$ denotes a cell face. Note that we solve the field equations for the scalar potential ϕ and covariant components of the vector potential $\mathbf{A}$. The discrete map is defined as $\mathbf{x}(\xi_i, \eta_j)$.

Introducing this result in Eq. 19, it follows that:

$$\partial_t(Jf_s) + \partial_\alpha \left(\sum_{p \in s} w_p \dot{\xi}_p^\alpha \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] \right) + \nabla_{\mathbf{v}} \cdot \left(\sum_{p \in s} w_p \dot{\mathbf{v}}_p \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] \right) = 0.$$

This equation becomes Eq. 15 when we note that, from Eqs. 17, 18:

$$\begin{aligned} \sum_{p \in s} w_p \dot{\xi}_p^\alpha \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] &= \sum_{p \in s} w_p v_p^\alpha \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] = v^\alpha Jf_s, \\ \sum_{p \in s} w_p \dot{\mathbf{v}}_p \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] &= \sum_{p \in s} w_p \mathbf{a}(\boldsymbol{\xi}_p, \mathbf{v}_p) \delta[\boldsymbol{\xi} - \boldsymbol{\xi}_p(t)] \delta[\mathbf{v} - \mathbf{v}_p(t)] = \mathbf{a} Jf_s, \end{aligned}$$

where we have used the sifting property of the delta function.

4. Discrete formulation of the curvilinear Vlasov-Darwin model

4.1. Numerical discretization of the field equations in curvilinear geometry

We employ a centered finite-difference method to discretize the 2D-3V Vlasov-Darwin equations on a uniform logical Yee mesh (see Fig. 1). In what follows, we adopt the multidimensional particle gather-scatter and electric field interpolation approach recently put forth in the uniform mesh context in Ref. [1]. We focus on two dimensions (but 3D vector fields), and denote cell centered quantities with integer subindices (i, j) , and face centered quantities by $(i \pm 1/2, j \pm 1/2)$.

The discretization of the curvilinear form of the Darwin field equations, Eqs. 9 and 8, is performed as follows. Equation 8 is discretized at cell centers:

$$\partial_\alpha \left(J g^{\alpha\beta} \partial_\beta \chi^{n+1/2} \right)_{i,j} = \partial_\alpha \left(J \tilde{j}^\alpha \right)_{i,j}^{n+1/2}, \quad (20)$$

by using central differences in space, e.g.:

$$\partial_\alpha \left(J \tilde{j}^\alpha \right)_{i,j} = \frac{(J \tilde{j}^\xi)_{i+1/2,j} - (J \tilde{j}^\xi)_{i-1/2,j}}{\Delta \xi} + \frac{(J \tilde{j}^\eta)_{i,j+1/2} - (J \tilde{j}^\eta)_{i,j-1/2}}{\Delta \eta},$$

and similarly with $\partial_\alpha (J g^{\alpha\beta} \partial_\beta \chi)$. This spatial discretization has the property that it satisfies the identity $\int d\mathbf{x} \mathbf{j} \cdot \nabla \phi = \int d\mathbf{x} \phi \nabla \cdot \mathbf{j}$ discretely, which is needed for the energy conservation theorem proof (Sec. 4.3.2). In Eq. 20, we have used $\tilde{j}^\alpha$ which is an orbit-averaged current density defined later in Eq. 27.

The discretization of Eq. 9 is also conceptually straightforward:

$$-\frac{1}{\mu_0} \left(J \nabla^2 \mathbf{A} \right)_{i+1/2,j}^\xi = (J \tilde{j}^\xi)_{i+1/2,j} - (J g^{\xi\xi} \partial_\xi \chi + J g^{\xi\eta} \partial_\eta \chi)_{i+1/2,j}, \quad (21)$$

$$-\frac{1}{\mu_0} \left(J \nabla^2 \mathbf{A} \right)_{i,j+1/2}^\eta = (J \tilde{j}^\eta)_{i,j+1/2} - (J g^{\eta\xi} \partial_\xi \chi + J g^{\eta\eta} \partial_\eta \chi)_{i,j+1/2}, \quad (22)$$

$$-\frac{1}{\mu_0} \left(J \nabla^2 \mathbf{A} \right)_{i,j}^\zeta = (J \tilde{j}^\zeta)_{i,j}. \quad (23)$$

All quantities here are at $n + 1/2$, with:

$$\mathbf{A}^{n+1/2} = \frac{\mathbf{A}^{n+1} + \mathbf{A}^n}{2}; \quad \chi^{n+1/2} = \epsilon_0 \frac{\phi^{n+1} - \phi^n}{\Delta t}.$$

The critical requirements of the discretization of the Darwin field equations are that 1) the Laplacian fluxes $J g^{\alpha\beta} \partial_\beta \chi$ that appear in Eq. 20, 21 and 22 are discretized self-adjointly at faces, and 2) the discretization of the components of $J \nabla^2 \mathbf{A}$ at faces is self-adjoint and allows the commutative property $\nabla \cdot \nabla^2 \mathbf{A} = \nabla^2 \nabla \cdot \mathbf{A}$. Both requirements ensure that proper discrete energy measures exist, and that a proper discrete measure of $\nabla \cdot \mathbf{A}$ (to be defined later) vanishes. A suitable self-adjoint discretization of the fluxes of the curvilinear Laplacian, $(J g^{\alpha\beta} \partial_\beta \phi)$, which meets these requirements, is the following:

$$\begin{aligned} \left[J g^{\xi\xi} \partial_\xi \phi + J g^{\xi\eta} \partial_\eta \phi \right]_{i+1/2,j} &\approx J g^{\xi\xi} \Big|_{i+1/2,j} \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta \xi} \\ &+ \left[J g^{\xi\eta} \Big|_{i+1/2,j+1/2} \frac{\phi_{i+1,j+1} - \phi_{i+1,j} + \phi_{i,j+1} - \phi_{i,j}}{4\Delta \eta} \right. \\ &\quad \left. J g^{\xi\eta} \Big|_{i+1/2,j-1/2} \frac{\phi_{i+1,j} - \phi_{i+1,j-1} + \phi_{i,j} - \phi_{i,j-1}}{4\Delta \eta} \right], \end{aligned} \quad (24)$$

and similarly with the other set of fluxes at $(i, j + 1/2)$.

The details of a self-adjoint numerical discretization of the components of $J \nabla^2 \mathbf{A}$ at faces are considered later in this study.

4.2. Numerical discretization of particle equations and quantities in curvilinear geometry

Particle orbits are subcycled for accuracy. The particles equations of motion (Eqs. 17, 18) are discretized using a Crank-Nicolson scheme at $\nu + 1/2$ (with ν the timestep subcycling index) according to:

$$\frac{\tilde{\zeta}_p^{\alpha, \nu+1} - \tilde{\zeta}_p^{\alpha, \nu}}{\Delta t} = \mathbf{v}_p^{\nu+1/2} \cdot \boldsymbol{\alpha}_p^{\nu+1/2}, \quad (25)$$

$$\frac{\mathbf{v}_p^{\nu+1} - \mathbf{v}_p^{\nu}}{\Delta t} = \frac{q_p}{m_p} E_{\alpha, p}^{\nu+1/2} \boldsymbol{\alpha}_p^{\nu+1/2} + \mathbf{v}_p^{\nu+1/2} \times (B_p^\alpha \partial_\alpha \mathbf{x}|_p)^{\nu+1/2}. \quad (26)$$

Summation over repeated α indices is implied. Here, $\mathbf{v}_p^{\nu+1/2} = (\mathbf{v}_p^{\nu+1} + \mathbf{v}_p^{\nu})/2$.

The current density $\bar{\mathbf{j}}$ in Eqs. 20, 21-23 is obtained from particles by orbit-averaging the individual current contributions [40, 41, 42, 2, 32, 1],

$$\bar{\mathbf{j}}^{n+1/2} = \frac{1}{\Delta t} \sum_p \sum_{\nu=0}^{N_\nu-1} \mathbf{j}_p^{\nu+1/2} \Delta \tau_p^\nu, \quad (27)$$

where $\Delta \tau_p^\nu$ is the substep, and N_ν denotes the number of substeps. Particle substeps satisfy $\sum_{\nu=0}^{N_\nu-1} \Delta \tau_p^\nu = \Delta t$. The individual *contravariant* current components are scattered on the mesh (see Fig. 1) from particles at every particle substep according to:

$$(J \tilde{\zeta}_p^{\xi})_{i+1/2, j}^{\nu+1/2} = \frac{q_p}{\Delta \tilde{\zeta} \Delta \eta} \mathbf{v}_p^{\nu+1/2} \cdot (\nabla \tilde{\zeta})_p \mathbf{S}_{12}^{\nu+1/2}, \quad (28)$$

$$(J \tilde{\eta}_p^{\eta})_{i, j+1/2}^{\nu+1/2} = \frac{q_p}{\Delta \tilde{\zeta} \Delta \eta} \mathbf{v}_p^{\nu+1/2} \cdot (\nabla \eta)_p \mathbf{S}_{21}^{\nu+1/2}, \quad (29)$$

$$(J \tilde{\zeta}_p^{\zeta})_{i, j}^{\nu+1/2} = \frac{q_p}{\Delta \tilde{\zeta} \Delta \eta} \mathbf{v}_p^{\nu+1/2} \cdot (\nabla \zeta)_p \left[\mathbf{S}_{22}^{\nu+1/2} + \Delta \mathbf{S}_{22}^{\nu+1/2} \right]. \quad (30)$$

Here:

$$\begin{aligned} \mathbf{S}_{21}^{\nu+1/2} &\equiv \mathbf{S}_2^{\nu+1/2} (\tilde{\zeta}_p - \tilde{\zeta}_i) \mathbf{S}_1(\eta_p^{\nu+1/2} - \eta_{j+1/2}), \\ \mathbf{S}_{12}^{\nu+1/2} &\equiv \mathbf{S}_1(\tilde{\zeta}_p^{\nu+1/2} - \tilde{\zeta}_{i+1/2}) \mathbf{S}_2^{\nu+1/2} (\eta_p - \eta_j), \\ \mathbf{S}_{22}^{\nu+1/2} &\equiv \mathbf{S}_2^{\nu+1/2} (\tilde{\zeta}_p - \tilde{\zeta}_j) \mathbf{S}_2^{\nu+1/2} (\eta_p - \eta_j), \end{aligned} \quad (31)$$

$$\Delta \mathbf{S}_{22}^{\nu+1/2} \equiv \frac{\mathbf{S}_2(\tilde{\zeta}_p^{\nu+1} - \tilde{\zeta}_i) - \mathbf{S}_2(\tilde{\zeta}_p^\nu - \tilde{\zeta}_i)}{2} \frac{\mathbf{S}_2(\eta_p^{\nu+1} - \eta_j) - \mathbf{S}_2(\eta_p^\nu - \eta_j)}{2}, \quad (32)$$

where:

$$\mathbf{S}_2^{\nu+1/2} (\tilde{\zeta}_p - \tilde{\zeta}_i) \equiv \left[\mathbf{S}_2(\tilde{\zeta}_p^{\nu+1} - \tilde{\zeta}_i) + \mathbf{S}_2(\tilde{\zeta}_p^\nu - \tilde{\zeta}_i) \right] / 2. \quad (33)$$

Note that, in these definitions, the half-time first-order splines are always evaluated on the half mesh and at the half-time particle position, whereas the half-time second-order splines are always evaluated on the integer mesh and integer-time particle positions, and averaged as indicated in Eq. 33. The B-spline shape functions are defined as:

$$\mathbf{S}_1(\tilde{\zeta}_p - \tilde{\zeta}_{i-1/2}) = 1 - \frac{\tilde{\zeta}_p - \tilde{\zeta}_{i-1/2}}{\Delta \tilde{\zeta}}, \quad (34)$$

$$S_1(\xi_p - \xi_{i+1/2}) = \frac{\xi_p - \xi_{i-1/2}}{\Delta \xi}, \quad (35)$$

$$S_2(\xi_p - \xi_i) = \frac{3}{4} - \left(\frac{\xi_p - \xi_i}{\Delta \xi} \right)^2, \quad (36)$$

$$S_2(\xi_p - \xi_{i\pm 1}) = \frac{1}{2} \left(\frac{1}{2} \pm \frac{\xi_p - \xi_i}{\Delta \xi} \right)^2. \quad (37)$$

The additional Jacobian factor in the left hand side of Eqs. 28-30 stems from our choice of particle representation, Eq. 16. This prescription will ensure charge conservation when each substep of a particle orbit lies within a cell (Sec. 4.4). Note that interpolations are done in logical space, and that the shape functions used here are dimensionless quantities. The interpolation for $j_z = \tilde{j}_p^\zeta$ features a small truncation error correction, $\Delta S_{22}^{v+1/2}$, which originates in the electric-field gather to ensure canonical momentum conservation in the ignorable direction [1], and is needed in the current for exact energy conservation (Sec. 4.3).

The magnetic field contravariant components $(B_p^\zeta, B_p^\eta, B_p^\zeta)^{v+1/2}$ are gathered from the mesh covariant vector potential components as described in Sec. 4.5. The covariant electric field components $(E_\zeta, E_\eta, E_\zeta)$ on the mesh are computed at faces from ϕ and $\mathbf{A}$ according to Eq. 5 as:

$$E_{\zeta,i+1/2,j}^{n+1/2} = -\frac{\phi_{i+1,j}^{n+1/2} - \phi_{i,j}^{n+1/2}}{\Delta \xi_i} - \frac{A_{\zeta,i+1/2,j}^{n+1} - A_{\zeta,i+1/2,j}^n}{\Delta t}, \quad (38)$$

$$E_{\eta,i,j+1/2}^{n+1/2} = -\frac{\phi_{i,j+1}^{n+1/2} - \phi_{i,j}^{n+1/2}}{\Delta \eta_j} - \frac{A_{\eta,i,j+1/2}^{n+1} - A_{\eta,i,j+1/2}^n}{\Delta t}, \quad (39)$$

$$E_{\zeta,i,j}^{n+1/2} = -\frac{A_{\zeta,i,j}^{n+1} - A_{\zeta,i,j}^n}{\Delta t}. \quad (40)$$

Here, $\phi^{n+1/2} = (\phi^{n+1} + \phi^n)/2$. The covariant electric field components are gathered to particles as:

$$E_{\zeta,p}^{v+1/2} = \sum_{i,j} E_{\zeta,i+1/2,j}^{n+1/2} S_{12}^{v+1/2}, \quad (41)$$

$$E_{\eta,p}^{v+1/2} = \sum_{i,j} E_{\eta,i,j+1/2}^{n+1/2} S_{21}^{v+1/2}, \quad (42)$$

$$E_{\zeta,p}^{v+1/2} = \sum_{i,j} E_{\zeta,i,j}^{n+1/2} \left[S_{22}^{v+1/2} + \Delta S_{22}^{v+1/2} \right]. \quad (43)$$

Note that, on the right hand sides, the mesh electric field is evaluated at $n + 1/2$, while shape functions are evaluated at $v + 1/2$. These definitions are in analogy to the corresponding current components. This is so to ensure energy conservation, as discussed next.

4.3. Discrete energy conservation theorem in curvilinear geometry

We show that the discretization chosen features a numerically exact global energy conservation theorem in a doubly-periodic system.

4.3.1. Particle kinetic energy

We begin by dotting Eq. 26 by $m_p \mathbf{v}_p^{v+1/2}$ and summing over all particles and subimesteps to find [2, 32, 1] (using Eqs. 27-30):

$$\frac{K_p^{n+1} - K_p^n}{\Delta t} = \sum_{i,j} \Delta \xi \Delta \eta \left[\left(J j^{\xi} E_{\xi} \right)_{i+1/2,j}^{n+1/2} + \left(J j^{\eta} E_{\eta} \right)_{i,j+1/2}^{n+1/2} + \left(J j^{\zeta} E_{\zeta} \right)_{i,j}^{n+1/2} \right],$$

where the $\mathbf{v} \times \mathbf{B}$ term has vanished exactly. Introducing Eqs. 38-40, we find:

$$\begin{aligned} \frac{K_p^{n+1} - K_p^n}{\Delta t} &= - \sum_{i,j} \Delta \xi \Delta \eta \left[\left(J j^{\xi} \partial_{\xi} \phi \right)_{i+1/2,j}^{n+1/2} + \left(J j^{\eta} \partial_{\eta} \phi \right)_{i,j+1/2}^{n+1/2} \right] \\ &\quad - \sum_{i,j} \Delta \xi \Delta \eta \left[\left(J j^{\xi} \partial_t A_{\xi} \right)_{i+1/2,j}^{n+1/2} + \left(J j^{\eta} \partial_t A_{\eta} \right)_{i,j+1/2}^{n+1/2} + \left(J j^{\zeta} \partial_t A_{\zeta} \right)_{i,j}^{n+1/2} \right] \\ &= \sum_{i,j} \Delta \xi \Delta \eta \phi_{i,j}^{n+1/2} \partial_{\alpha} \left(J j^{\alpha} \right)_{i,j}^{n+1/2} \\ &\quad + \sum_{i,j} \Delta \xi \Delta \eta \left[\left(\partial_t A_{\xi} \right) \left(-\frac{1}{\mu_0} \left(J \nabla^2 \mathbf{A} \right)^{\xi} \right) + \left(J g^{\xi \xi} \partial_{\xi} \chi + J g^{\xi \eta} \partial_{\eta} \chi \right) \right]_{i+1/2,j}^{n+1/2} \\ &\quad + \sum_{i,j} \Delta \xi \Delta \eta \left[\left(\partial_t A_{\eta} \right) \left(-\frac{1}{\mu_0} \left(J \nabla^2 \mathbf{A} \right)^{\eta} \right) + \left(J g^{\eta \xi} \partial_{\xi} \chi + J g^{\eta \eta} \partial_{\eta} \chi \right) \right]_{i,j+1/2}^{n+1/2} \\ &\quad + \sum_{i,j} \Delta \xi \Delta \eta \left[\left(\partial_t A_{\zeta} \right) \left(-\frac{1}{\mu_0} \left(J \nabla^2 \mathbf{A} \right)^{\zeta} \right) \right]_{i,j}^{n+1/2} \\ &= - \frac{\left(\hat{W}_{\phi}^{n+1} + \hat{W}_B^{n+1} \right) - \left(\hat{W}_{\phi}^n + \hat{W}_B^n \right)}{\Delta t}, \end{aligned} \quad (44)$$

where:

$$\hat{W}_{\phi} = \frac{\epsilon_0}{2} \sum_{i,j} \Delta \xi \Delta \eta \left[\left(J g^{\xi \xi} (\partial_{\xi} \phi)^2 \right)_{i+1/2,j} + 2 \left(J g^{\eta \xi} \partial_{\xi} \phi \partial_{\eta} \phi \right)_{i+1/2,j+1/2} + \left(J g^{\eta \eta} (\partial_{\eta} \phi)^2 \right)_{i,j+1/2} \right], \quad (45)$$

and:

$$\hat{W}_B = \sum_{i,j} \Delta \xi \Delta \eta \left[\left(J g^{\xi \xi} (\partial_{\xi} A_z)^2 \right)_{i+1/2,j} + 2 \left(J g^{\eta \xi} \partial_{\xi} A_z \partial_{\eta} A_z \right)_{i+1/2,j+1/2} + \left(J g^{\eta \eta} (\partial_{\eta} A_z)^2 \right)_{i,j+1/2} + \left(J \frac{B_{\zeta} B_{\zeta}}{2} \right)_{i+1/2,j+1/2} \right].$$

In the second step of Eq. 44, we have used Eqs. 21-23. We detail the last step in what follows.

4.3.2. Electrostatic energy

The first term $\sum_{i,j} \Delta \xi \Delta \eta \phi_{i,j}^{n+1/2} \partial_{\alpha} \left(J j^{\alpha} \right)_{i,j}^{n+1/2}$ in Eq. 44 is a discrete measure of the rate of change of the electrostatic energy W_{ϕ} . This can be shown by using Eqs. 20 and 24, to find:

$$\begin{aligned} \sum_{i,j} \Delta \xi \Delta \eta \phi_{i,j}^{n+1/2} \partial_{\alpha} \left(J j^{\alpha} \right)_{i,j}^{n+1/2} &= \epsilon_0 \sum_{i,j} \Delta \xi \Delta \eta \phi_{i,j}^{n+1/2} \partial_{\alpha} \left(J g^{\alpha \beta} \partial_{\beta} \phi \right)_{i,j}^{n+1/2} \\ &= -\epsilon_0 \sum_{i,j} \Delta \xi \Delta \eta \left[\left(J g^{\xi \xi} \partial_t (\partial_{\xi} \phi) \partial_{\xi} \phi \right)_{i+1/2,j}^{n+1/2} \right. \\ &\quad \left. + \left(J g^{\eta \xi} [\partial_t (\partial_{\xi} \phi) \partial_{\eta} \phi + \partial_t (\partial_{\eta} \phi) \partial_{\xi} \phi] \right)_{i+1/2,j+1/2}^{n+1/2} \right] \end{aligned}$$

$$\begin{aligned}
& + (Jg^{\eta\eta}\partial_t(\partial_\eta\phi)\partial_\eta\phi)_{i,j+1/2}^{n+1/2} \Big] \\
& = -\frac{\epsilon_0}{\Delta t} \sum_{i,j} \Delta\zeta\Delta\eta \left[\left(\frac{Jg^{\zeta\zeta}}{2} [(\partial_\zeta\phi)_{n+1}^2 - (\partial_\zeta\phi)_n^2] \right)_{i+1/2,j} \right. \\
& \quad + \left(Jg^{\eta\zeta} [(\partial_\zeta\phi\partial_\eta\phi)^{n+1} - (\partial_\eta\phi\partial_\zeta\phi)^n] \right)_{i+1/2,j+1/2} \\
& \quad \left. + \left(\frac{Jg^{\eta\eta}}{2} [(\partial_\eta\phi)_{n+1}^2 - (\partial_\eta\phi)_n^2] \right)_{i,j+1/2} \right] \\
& = -\frac{(\hat{W}_\phi^{n+1} - \hat{W}_\phi^n)}{\Delta t},
\end{aligned}$$

where is a suitable discrete measure of the electrostatic energy in Eq. 6.

4.3.3. Cancellation of displacement current contribution to the energy measure: discrete definition of $\nabla \cdot \mathbf{A}$

The terms $(Jg^{\zeta\zeta}\partial_\zeta\chi + Jg^{\zeta\eta}\partial_\eta\chi)_{i+1/2,j}$ and $(Jg^{\eta\zeta}\partial_\zeta\chi + Jg^{\eta\eta}\partial_\eta\chi)_{i,j+1/2}$ in the previous equations must be discretized *exactly* as in Eq. 24. Exact conservation of energy requires that these terms vanish when summed over the whole mesh, which in turn requires that $\nabla \cdot \mathbf{A} = 0$ numerically. We derive the discretization of $\nabla \cdot \mathbf{A}$ that ensures this property. We begin by introducing the discrete form of the fluxes in Eq. 44. It follows that:

$$\begin{aligned}
\sum_{i,j} \Delta\zeta\Delta\eta \left[(\partial_t A_\zeta) \left(Jg^{\zeta\zeta}\partial_\zeta\chi + Jg^{\zeta\eta}\partial_\eta\chi \right) \right]_{i+1/2,j}^{n+1/2} &= \sum_{i,j} \Delta\zeta\Delta\eta \left[Jg^{\zeta\zeta} \Big|_{i+1/2,j} \frac{\chi_{i+1,j} - \chi_{i,j}}{\Delta\zeta} \right] (\partial_t A_\zeta)_{i+1/2,j} \\
&+ \sum_{i,j} \Delta\zeta\Delta\eta \left[Jg^{\zeta\eta} \Big|_{i+1/2,j+1/2} \frac{\chi_{i+1,j+1} - \chi_{i+1,j} + \chi_{i,j+1} - \chi_{i,j}}{4\Delta\eta} \right. \\
&+ \left. Jg^{\zeta\eta} \Big|_{i+1/2,j-1/2} \frac{\chi_{i+1,j} - \chi_{i+1,j-1} + \chi_{i,j} - \chi_{i,j-1}}{4\Delta\eta} \right] (\partial_t A_\zeta)_{i+1/2,j} \\
&= -\sum_{i,j} \Delta\zeta\Delta\eta \chi_{i,j} \left[\partial_\zeta (Jg^{\zeta\zeta}\partial_t A_\zeta)_{i,j} + \frac{1}{2} \left(\partial_\eta (Jg^{\eta\zeta}\partial_t A_\zeta)_{i+1/2,j} + \partial_\eta (Jg^{\eta\zeta}\partial_t A_\zeta)_{i-1/2,j} \right) \right],
\end{aligned}$$

where $\partial_\zeta (Jg^{\zeta\zeta}\partial_t A_\zeta)_{i,j}$ is discretized using central differences in a standard way, and:

$$\begin{aligned}
\partial_\eta (Jg^{\zeta\eta}\partial_t A_\zeta)_{i+1/2,j} &= \frac{Jg^{\zeta\eta} \Big|_{i+1/2,j+1/2} \left[(\partial_t A_\zeta)_{i+1/2,j} + (\partial_t A_\zeta)_{i+1/2,j+1} \right]}{2\Delta\eta} \\
&- \frac{Jg^{\zeta\eta} \Big|_{i+1/2,j-1/2} \left[(\partial_t A_\zeta)_{i+1/2,j} + (\partial_t A_\zeta)_{i+1/2,j-1} \right]}{2\Delta\eta}.
\end{aligned} \tag{46}$$

Similarly:

$$\begin{aligned}
\sum_{i,j} \Delta\zeta\Delta\eta \left[(\partial_t A_\eta) \left(Jg^{\eta\zeta}\partial_\zeta\chi + Jg^{\eta\eta}\partial_\eta\chi \right) \right]_{i,j+1/2}^{n+1/2} &= \\
&= -\sum_{i,j} \Delta\zeta\Delta\eta \chi_{i,j} \left[\partial_\eta (Jg^{\eta\eta}\partial_t A_\eta)_{i,j} + \frac{1}{2} \left(\partial_\zeta (Jg^{\zeta\eta}\partial_t A_\eta)_{i,j+1/2} + \partial_\zeta (Jg^{\zeta\eta}\partial_t A_\eta)_{i,j-1/2} \right) \right].
\end{aligned}$$

It follows that:

$$\sum_{i,j} \Delta\zeta\Delta\eta \left[\left[(\partial_t A_\zeta) \left(Jg^{\zeta\zeta}\partial_\zeta\chi + Jg^{\zeta\eta}\partial_\eta\chi \right) \right]_{i+1/2,j}^{n+1/2} + \left[(\partial_t A_\eta) \left(Jg^{\eta\zeta}\partial_\zeta\chi + Jg^{\eta\eta}\partial_\eta\chi \right) \right]_{i,j+1/2}^{n+1/2} \right]$$

$$\begin{aligned}
&= - \sum_{i,j} \Delta \xi \Delta \eta \chi_{i,j} \left[\partial_\eta (J g^{\eta\eta} \partial_t A_\eta)_{i,j} + \frac{1}{2} \left(\partial_\xi (J g^{\xi\eta} \partial_t A_\eta)_{i,j+1/2} + \partial_\xi (J g^{\xi\eta} \partial_t A_\eta)_{i,j-1/2} \right) \right] \\
&\quad - \sum_{i,j} \Delta \xi \Delta \eta \chi_{i,j} \left[\partial_\xi (J g^{\xi\xi} \partial_t A_\xi)_{i,j} + \frac{1}{2} \left(\partial_\eta (J g^{\eta\xi} \partial_t A_\xi)_{i+1/2,j} + \partial_\eta (J g^{\eta\xi} \partial_t A_\xi)_{i-1/2,j} \right) \right] \\
&= - \sum_{i,j} \Delta \xi \Delta \eta \chi_{i,j} J (\nabla \cdot \partial_t \mathbf{A})_{i,j}^{n+1/2},
\end{aligned}$$

and therefore the discrete definition of $\nabla \cdot \mathbf{A}$ is given by:

$$\begin{aligned}
J (\nabla \cdot \mathbf{A})_{i,j} &= \partial_\xi (J g^{\xi\xi} A_\xi)_{i,j} + \partial_\eta (J g^{\eta\eta} A_\eta)_{i,j} \\
&\quad + \frac{1}{2} \left(\partial_\eta (J g^{\eta\xi} A_\xi)_{i+1/2,j} + \partial_\eta (J g^{\eta\xi} A_\xi)_{i-1/2,j} \right) \\
&\quad + \frac{1}{2} \left(\partial_\xi (J g^{\xi\eta} A_\eta)_{i,j+1/2} + \partial_\xi (J g^{\xi\eta} A_\eta)_{i,j-1/2} \right).
\end{aligned} \tag{47}$$

Here, cross terms are discretized as in Eq. 46. Note that this definition couples covariant components of $\mathbf{A}$ at faces within a 9-point stencil, and is therefore compact. One can write Eq. 47 in terms of the contravariant components of $\mathbf{A}$ as:

$$J (\nabla \cdot \mathbf{A})_{i,j} = \partial_\alpha (J A^\alpha)_{i,j}, \tag{48}$$

where:

$$\begin{aligned}
(J A^\xi)_{i+1/2,j} &= (J g^{\xi\xi} A_\xi)_{i+1/2,j} \\
&\quad + \frac{1}{4} \left[(J g^{\xi\eta})_{i+1/2,j+1/2} (A_{\eta,i,j+1/2} + A_{\eta,i+1,j+1/2}) + (J g^{\xi\eta})_{i+1/2,j-1/2} (A_{\eta,i,j-1/2} + A_{\eta,i+1,j-1/2}) \right],
\end{aligned}$$

and similarly for the $(J A^\eta)_{i,j+1/2}$ contravariant component. Equation 48 defines a suitable discrete transformation rule from staggered covariant to contravariant that is consistent with the divergence definition in Eq. 47.

4.3.4. Magnetic energy: Discrete definition of $\nabla^2 \mathbf{A}$

There are several constraints that the discrete form of $\nabla^2 \mathbf{A}$ must satisfy. Firstly, it must lead to a suitable discrete measure of the magnetic energy, $\hat{W}_B$. Secondly, it must ensure that the operators $\nabla \cdot$ and ∇^2 commute discretely:

$$\nabla \cdot \nabla^2 \mathbf{A} = \nabla^2 \nabla \cdot \mathbf{A} = 0, \tag{49}$$

such that the Coulomb gauge involution is implied automatically by the discretization, consistently with the definition of $\nabla \cdot \mathbf{A}$ from the last section (Eq. 47). To achieve this, we consider the identity:

$$\nabla^2 \mathbf{A} = \nabla (\nabla \cdot \mathbf{A}) - \nabla \times \nabla \times \mathbf{A}, \tag{50}$$

and do *not* use the Coulomb gauge condition to simplify this expression. We have kept the divergence term, which will be critical for the well-posedness of the resulting discretization in a multigrid context (as required in our preconditioning approach, Sec. 5). It is trivial to show that Eq. 49 follows automatically from Eq. 50 as long as $\nabla \cdot \nabla \times = 0$ discretely.

We consider next the discretization of the contravariant components of $\nabla^2 \mathbf{A}$ at faces (for ζ and η) and cell centers (for ξ). We begin by expressing the contravariant components of $\nabla^2 \mathbf{A}$ from Eq. 50 as:

$$J \nabla^2 \mathbf{A} \Big|^\xi = J g^{\xi\alpha} \partial_\alpha (\nabla \cdot \mathbf{A}) - \epsilon_{\xi\alpha\beta} \partial_\alpha B_\beta, \quad (51)$$

and similarly with the η and ζ components. Here, B_β are the covariant components of the magnetic field. We specialize this result for a 2D domain with a Cartesian ignorable direction $z = \zeta$. For this case, $A^\zeta = A_z$ (and similarly for B_ζ), and $\partial_\zeta = \partial_z = 0$. There results:

$$J \nabla^2 \mathbf{A} \Big|_{i+1/2,j}^\xi = -\partial_\eta B_\zeta \Big|_{i+1/2,j} + J g^{\xi\alpha} \partial_\alpha (\nabla \cdot \mathbf{A}) \Big|_{i+1/2,j}, \quad (52)$$

$$J \nabla^2 \mathbf{A} \Big|_{i,j+1/2}^\eta = \partial_\xi B_\zeta \Big|_{i,j+1/2} + J g^{\eta\alpha} \partial_\alpha (\nabla \cdot \mathbf{A}) \Big|_{i,j+1/2}, \quad (53)$$

$$J \nabla^2 \mathbf{A} \Big|_{i,j}^\zeta = J \nabla^2 A_z \Big|_{i,j}. \quad (54)$$

The last term in the right hand side of the ξ and η components is discretized as outlined in Eq. 24, with $\nabla \cdot \mathbf{A}$ discretized as given in Eq. 47.

Regarding the derivatives of B_ζ (which is the covariant ζ -component of the magnetic field), we first express B_ζ at vertices from the vector potential components (following from $\mathbf{B} = \nabla \times \mathbf{A}$) as:

$$B_{\zeta,i+1/2,j+1/2} = B_{\zeta,i+1/2,j+1/2}^\zeta = \frac{1}{J_{i+1/2,j+1/2}} \left[\frac{(A_\eta)_{i+1,j+1/2} - (A_\eta)_{i,j+1/2}}{\Delta \xi} - \frac{(A_\xi)_{i+1/2,j+1} - (A_\xi)_{i+1/2,j}}{\Delta \eta} \right]. \quad (55)$$

Taking derivatives at faces, we find:

$$\begin{aligned} \partial_\eta B_\zeta \Big|_{i+1/2,j} &= \frac{1}{J_{i+1/2,j+1/2} \Delta \eta} \left[\frac{(A_\eta)_{i+1,j+1/2} - (A_\eta)_{i,j+1/2}}{\Delta \xi} - \frac{(A_\xi)_{i+1/2,j+1} - (A_\xi)_{i+1/2,j}}{\Delta \eta} \right] \\ &\quad - \frac{1}{J_{i+1/2,j-1/2} \Delta \eta} \left[\frac{(A_\eta)_{i+1,j-1/2} - (A_\eta)_{i,j-1/2}}{\Delta \xi} - \frac{(A_\xi)_{i+1/2,j} - (A_\xi)_{i+1/2,j-1}}{\Delta \eta} \right], \end{aligned} \quad (56)$$

$$\begin{aligned} \partial_\xi B_\zeta \Big|_{i,j+1/2} &= \frac{1}{J_{i+1/2,j+1/2} \Delta \xi} \left[\frac{(A_\eta)_{i+1,j+1/2} - (A_\eta)_{i,j+1/2}}{\Delta \xi} - \frac{(A_\xi)_{i+1/2,j+1} - (A_\xi)_{i+1/2,j}}{\Delta \eta} \right] \\ &\quad - \frac{1}{J_{i-1/2,j+1/2} \Delta \xi} \left[\frac{(A_\eta)_{i,j+1/2} - (A_\eta)_{i-1,j+1/2}}{\Delta \xi} - \frac{(A_\xi)_{i-1/2,j+1} - (A_\xi)_{i-1/2,j}}{\Delta \eta} \right]. \end{aligned} \quad (57)$$

These forms trivially satisfy $\nabla \cdot \nabla \times = 0$ discretely, with the discrete divergence given in Eq. 48. Equations 56 and 57 can then be substituted in Eqs. 53, 52 to obtain the discrete form of the vector Laplacian operator sought.

We show next that the discretization above recovers the corresponding discrete magnetic energy, given by:

$$\begin{aligned} \hat{W}_B &= -\sum_{i,j} \Delta \xi \Delta \eta \left\{ \left[A_\zeta \left(J \nabla^2 \mathbf{A} \Big|^\xi \right) \right]_{i+1/2,j} + \left[A_\eta \left(J \nabla^2 \mathbf{A} \Big|^\eta \right) \right]_{i,j+1/2} + \left[A_\zeta \left(J \nabla^2 \mathbf{A} \Big|^\zeta \right) \right]_{i,j} \right\} \\ &= \sum_{i,j} \Delta \xi \Delta \eta J_{i+1/2,j+1/2} \left(\frac{B_\xi B^\xi + B_\eta B^\eta + B_\zeta B^\zeta}{2} \right)_{i+1/2,j+1/2}. \end{aligned} \quad (58)$$

We first consider the z-component. Note that the scalar Laplacian operator in Eq. 54 is discretized the same way as that of the electrical potential. As a result, the z-component trivially gives a quadratic form owing to the self-adjointness of the Laplacian operator, which approximates the contribution

$$^{1/2} \sum_{i,j} \Delta \xi \Delta \eta J_{i+1/2,j+1/2} \left(B_{\xi} B^{\xi} + B_{\eta} B^{\eta} \right)_{i+1/2,j+1/2}.$$

To see that the contributions from the ξ and η components of $\nabla^2 \mathbf{A}$ result in the B^{ξ} contribution to the energy principle, it is convenient to rewrite Eqs. 52 and 53 as (using that $\nabla \cdot \mathbf{A} = 0$ discretely upon convergence):

$$\begin{aligned} (J \nabla^2 \mathbf{A})_{i+1/2,j}^{\xi} &= - \frac{(B_{\xi})_{i+1/2,j+1/2} - (B_{\xi})_{i+1/2,j-1/2}}{\Delta \eta}, \\ (J \nabla^2 \mathbf{A})_{i,j+1/2}^{\eta} &= \frac{(B_{\xi})_{i+1/2,j+1/2} - (B_{\xi})_{i-1/2,j+1/2}}{\Delta \xi}. \end{aligned}$$

It follows that the associated terms in the discrete energy principle, Eq. 58, yield, after telescoping the sums:

$$\begin{aligned} \sum_{i,j} \Delta \xi \Delta \eta \left\{ \left[A_{\xi} (J \nabla^2 \mathbf{A})_{i+1/2,j}^{\xi} \right] + \left[A_{\eta} (J \nabla^2 \mathbf{A})_{i,j+1/2}^{\eta} \right] \right\} &= \\ - \sum_{i,j} \Delta \xi \Delta \eta \left[\frac{A_{\eta,i+1,j+1/2} - A_{\eta,i,j+1/2}}{\Delta \xi} - \frac{A_{\xi,i+1/2,j+1} - A_{\xi,i+1/2,j}}{\Delta \eta} \right] B_{\xi,i+1/2,j+1/2} &= \\ - \sum_{i,j} \Delta \xi \Delta \eta (J B^{\xi})_{i+1/2,j+1/2} B_{\xi,i+1/2,j+1/2} &, \end{aligned}$$

as desired.

4.4. Discrete charge conservation theorem

Discrete charge conservation is enforced by the particle mover in multiple dimensions [1] by ensuring that the continuity equation,

$$\frac{\partial J \rho}{\partial t} + \frac{\partial (J j^{\alpha})}{\partial \xi^{\alpha}} = 0, \quad (59)$$

is satisfied per particle per substep, such that, in 2D:

$$\frac{(J \rho_p)_{i,j}^{v+1} - (J \rho_p)_{i,j}^{v+1}}{\Delta \tau} + \frac{(J j_p^{\xi})_{i+1/2,j}^{v+1/2} - (J j_p^{\xi})_{i-1/2,j}^{v+1/2}}{\Delta \xi} + \frac{(J j_p^{\eta})_{i,j+1/2}^{v+1/2} - (J j_p^{\eta})_{i,j-1/2}^{v+1/2}}{\Delta \eta} = 0. \quad (60)$$

Here, $(J \rho_p)_{i,j}^v = \frac{q_p}{\Delta \xi \Delta \eta} S_2(\xi_p^v - \xi_i) S_2(\eta_p^v - \eta_j)$, and $J j_p^{\xi}$ and $J j_p^{\eta}$ are defined in Eqs. 28, 29.

To prove the discrete local charge conservation theorem (i.e, to satisfy Eq. 60), we first note that, upon substitution of the current components and the charge density definitions, it is sufficient that:

$$\begin{aligned} & \frac{S_2(\xi_p^{v+1} - \xi_i) S_2(\eta_p^{v+1} - \eta_j) - S_2(\xi_p^v - \xi_i) S_2(\eta_p^v - \eta_j)}{\Delta \tau} + \\ & + v_p^{\xi,v+1/2} \frac{S_1(\xi_p^{v+1/2} - \xi_{i+1/2}) - S_1(\xi_p^{v+1/2} - \xi_{i-1/2})}{\Delta \xi} S_2^{v+1/2}(\eta_p - \eta_j) + \\ & + v_p^{\eta,v+1/2} \frac{S_1(\eta_p^{v+1/2} - \eta_{j+1/2}) - S_1(\eta_p^{v+1/2} - \eta_{j-1/2})}{\Delta \eta} S_2^{v+1/2}(\xi_p - \xi_j) = 0, \end{aligned} \quad (61)$$

where $S_2^{\nu+1/2}$ has been defined in Eq. 33, and this can be proved by some straightforward algebra. The derivation makes use of the identity:

$$\begin{aligned} & \frac{S_2(\xi_p^{\nu+1} - \xi_i)S_2(\eta_p^{\nu+1} - \eta_j) - S_2(\xi_p^\nu - \xi_i)S_2(\eta_p^\nu - \eta_j)}{\Delta\tau} \\ &= \frac{S_2(\xi_p^{\nu+1} - \xi_i) - S_2(\xi_p^\nu - \xi_i)}{\Delta\tau} S_2^{\nu+1/2}(\eta_p - \eta_j) \\ &+ \frac{S_2(\eta_p^{\nu+1} - \eta_j) - S_2(\eta_p^\nu - \eta_j)}{\Delta\tau} S_2^{\nu+1/2}(\xi_p - \xi_i). \end{aligned} \quad (62)$$

By properties of the B-splines, we have:

$$\left. \frac{\partial S_m(\xi_i - \xi_p)}{\partial \xi_p} \right|_{\xi_p^{\nu+1/2}} = \frac{S_{m-1}(\xi_{i+1/2} - \xi_p^{\nu+1/2}) - S_{m-1}(\xi_{i-1/2} - \xi_p^{\nu+1/2})}{\Delta\xi},$$

and by Taylor expansion (for $m \leq 2$ [41, 1]):

$$S_m(\xi_i - \xi_p^{\nu+1}) - S_m(\xi_i - \xi_p^\nu) = \left. \frac{\partial S_m(\xi_i - \xi_p)}{\partial \xi_p} \right|_{\xi_p^{\nu+1/2}} (\xi_p^{\nu+1} - \xi_p^\nu).$$

Together with similar expressions for the η direction, and using that $v_p^{\xi, \nu+1/2} = (\xi_p^{\nu+1} - \xi_p^\nu)/\Delta\tau^\nu$ and $v_p^{\eta, \nu+1/2} = (\eta_p^{\nu+1} - \eta_p^\nu)/\Delta\tau^\nu$, Eq. 61 vanishes exactly as long as the particle travels within the cell identified by ξ_i .

The charge conserving scheme therefore requires an additional component, namely, to ensure that particle substeps are always taken within a given cell. For this, we force particles to land at cell faces along their orbits whenever they try to cross a cell. This approach is the same as the one proposed in Refs. [41, 32, 1].

4.5. Magnetic field gathering formulas for exact conservation of particle canonical momentum

We begin with the equation of the canonical momentum conservation in the third dimension (namely, z or ξ):

$$m_p \dot{v}_{p,z} + q_p \dot{A}_{z,p} = 0, \quad (63)$$

where, consistently with the z -component of the electric field:

$$A_{z,p} \equiv \sum_{i,j} A_{z,i,j} S_2(\xi_p - \xi_i) S_2(\eta_p - \eta_j). \quad (64)$$

Equation 63 can be rewritten discretely per particle substep as:

$$\frac{v_{p,z}^{\nu+1} - v_{p,z}^\nu}{\Delta\tau} = -\frac{q_p}{m_p} \sum_{i,j} \frac{A_{z,i,j}^{\nu+1} S_2(\xi_p^{\nu+1} - \xi_i) S_2(\eta_p^{\nu+1} - \eta_j) - A_{z,i,j}^\nu S_2(\xi_p^\nu - \xi_i) S_2(\eta_p^\nu - \eta_j)}{\Delta\tau}. \quad (65)$$

We cast this equation in the form of Eq. 26 by using the B-splines identities in the previous section and Taylor-expanding around $\nu + 1/2$, to find:

$$\frac{A_{z,i,j}^{\nu+1} S_2(\xi_p^{\nu+1} - \xi_i) S_2(\eta_p^{\nu+1} - \eta_j) - A_{z,i,j}^\nu S_2(\xi_p^\nu - \xi_i) S_2(\eta_p^\nu - \eta_j)}{\Delta\tau} =$$

$$\begin{aligned}
& \frac{A_{z,i,j}^{v+1} - A_{z,i,j}^v}{\Delta\tau} (S_{22}^{v+1/2} + \Delta S_{22}^{v+1/2}) + \frac{S_2(\xi_p^{v+1} - \xi_i) - S_2(\xi_p^v - \xi_i)}{\Delta\tau} S_2^{v+1/2} (\eta_p - \eta_j) A_{z,i,j}^{v+1/2} \\
& + \frac{S_2(\eta_p^{v+1} - \eta_j) - S_2(\eta_p^v - \eta_j)}{\Delta\tau} S_2^{v+1/2} (\xi_p - \xi_j) A_{z,i,j}^{v+1/2} = \\
& \frac{A_{z,i,j}^{v+1} - A_{z,i,j}^v}{\Delta\tau} (S_{22}^{v+1/2} + \Delta S_{22}^{v+1/2}) + v_p^{\xi,v+1/2} \left. \frac{\partial S_2}{\partial \xi} \right|_{\xi_p^{v+1/2}} S_2^{v+1/2} (\eta_p - \eta_j) A_{z,i,j}^{v+1/2} \\
& v_p^{\eta,v+1/2} \left. \frac{\partial S_2}{\partial \eta} \right|_{\eta_p^{v+1/2}} S_2^{v+1/2} (\xi_p - \xi_j) A_{z,i,j}^{v+1/2}, \tag{66}
\end{aligned}$$

with S_{22} and ΔS_{22} defined in Eqs. 31 and 32, respectively. It follows that,

$$\frac{v_{p,z}^{v+1} - v_{p,z}^v}{\Delta\tau} = \frac{q_p}{m_p} \sum_{i,j} \left[E_{z,i,j}^{n+1/2} (S_{22}^{v+1/2} + \Delta S_{22}^{v+1/2}) + \frac{q_p}{m_p} \left(v_p^{\xi,v+1/2} (JB^\eta)_p^{v+1/2} - v_p^{\eta,v+1/2} (JB^\xi)_p^{v+1/2} \right) \right]. \tag{67}$$

where the in-plane magnetic field contravariant components B^ξ and B^η at the particle position are given by:

$$(JB^\eta)_p^{v+1/2} = - \sum_{i,j} A_{z,i,j}^{v+1/2} \left. \frac{\partial S_2}{\partial \xi} \right|_{\xi_p^{v+1/2}} S_2^{v+1/2} (\eta_p - \eta_j), \tag{68}$$

$$(JB^\xi)_p^{v+1/2} = \sum_{i,j} A_{z,i,j}^{v+1/2} \left. \frac{\partial S_2}{\partial \eta} \right|_{\eta_p^{v+1/2}} S_2^{v+1/2} (\xi_p - \xi_j). \tag{69}$$

Here, we have assumed that each micro-step satisfies:

$$- \frac{A_{z,i,j}^{v+1} - A_{z,i,j}^v}{\Delta\tau} = - \frac{A_{z,i,j}^{n+1} - A_{z,i,j}^n}{\Delta t} = E_{z,i,j}^{n+1/2},$$

and

$$A_{z,i,j}^{v+1/2} = \frac{A_{z,i,j}^{v+1} + A_{z,i,j}^v}{2}.$$

Regarding the magnetic field component in the ignorable direction, we define the in-plane components of the vector potential in analogy with the in-plane electric field components (Eqs. 38, 39) as:

$$A_{\xi,p}^{v+1/2} \equiv \sum_{i,j} A_{\xi,i+1/2,j}^{v+1/2} S_{12}^{v+1/2}; \quad A_{\eta,p}^{v+1/2} \equiv \sum_{i,j} A_{\eta,i,j+1/2}^{v+1/2} S_{21}^{v+1/2}.$$

The magnetic field component in the ignorable direction follows from $\mathbf{B} = \nabla \times \mathbf{A}$ as:

$$(JB^\xi)_p^{v+1/2} = \sum_{i,j} \left[A_{\eta,i,j}^{v+1/2} \partial_\xi S_{21}^{v+1/2} - A_{\xi,i,j}^{v+1/2} \partial_\eta S_{12}^{v+1/2} \right]$$

The Cartesian magnetic field components at the particle position are recovered as $\mathbf{B}_p = (JB^\alpha)_p (J^{-1} \partial_\alpha \mathbf{x})_p$. Here we use second-order B-spline local interpolations to find the Jacobian matrix and its determinant at the particle locations.

5. Fluid Preconditioning

We follow the formulation of the fluid preconditioner for moderately magnetized plasmas outlined in Ref. [1], which consists of solving a linear momentum equation for δn , a Poisson equation for $\delta\phi$, and a

vector elliptic equation for $\delta\mathbf{A}$, which is then followed by a divergence cleaning solve (so that $\nabla \cdot \delta\mathbf{A} \approx 0$). The implementation of the preconditioner is as follows. We begin by solving for the electrostatic response, which is decoupled from the electromagnetic one owing to the moderately magnetized assumption. For this, we invert the coupled linear operators:

$$\frac{\epsilon_0}{\Delta t} \nabla^2 \delta\phi - \nabla \cdot \delta\bar{\mathbf{j}}_\phi = -R_\phi, \quad (70)$$

$$\frac{\delta n_s}{\Delta t} + \nabla \cdot \delta\bar{\mathbf{\Gamma}}_{\phi,s} = 0, \quad (71)$$

with:

$$\delta\mathbf{F}_{\phi,s}^- = -n_s \nabla \delta\phi - \delta n_s \nabla \phi - \frac{\nabla(T_s \delta n_s)}{2q_s}. \quad (72)$$

$$\delta\bar{\mathbf{\Gamma}}_{\phi,s} = \alpha_s \frac{\delta\mathbf{F}_{\phi,s}^- + [\alpha_s \delta\mathbf{F}_{\phi,s}^- \times \mathbf{B}_0 + \alpha_s^2 (\delta\mathbf{F}_{\phi,s}^- \cdot \mathbf{B}_0) \mathbf{B}_0]}{1 + (\alpha_s B_0)^2} \quad (73)$$

$$\delta\bar{\mathbf{j}}_\phi = \sum_s q_s \delta\bar{\mathbf{\Gamma}}_{\phi,s}, \quad (74)$$

where $\alpha_s = \Delta t q_s / 2m_s$, and the subscript s indicates the species. Once $\delta\phi$, δn_s are found, we solve for the electromagnetic response $\delta\mathbf{A}$ from:

$$\frac{1}{2\mu_0} \nabla^2 \delta\mathbf{A} + \delta\bar{\mathbf{j}}_\mathbf{A} = -R_\mathbf{A} + \epsilon_0 \frac{\nabla \delta\phi}{\Delta t} - \delta\bar{\mathbf{j}}_\phi, \quad (75)$$

with:

$$\delta\bar{\mathbf{j}}_\mathbf{A} = \sum_s q_s \alpha_s \delta\bar{\mathbf{\Gamma}}_{\mathbf{A},s}, \quad (76)$$

$$\delta\bar{\mathbf{\Gamma}}_{\mathbf{A},s} = \frac{\delta\mathbf{F}_{\mathbf{A},s}^- + [\alpha_s \delta\mathbf{F}_{\mathbf{A},s}^- \times \mathbf{B}_0 + \alpha_s^2 (\delta\mathbf{F}_{\mathbf{A},s}^- \cdot \mathbf{B}_0) \mathbf{B}_0]}{1 + (\alpha_s B_0)^2}, \quad (77)$$

$$\delta\mathbf{F}_{\mathbf{A},s}^- = -n_s \frac{\delta\mathbf{A}}{\Delta t} + \bar{\mathbf{\Gamma}}_s \times \nabla \times \delta\mathbf{A}. \quad (78)$$

In these equations, T_s and $\bar{\mathbf{\Gamma}}_s$ are scattered on the mesh from particles at the current Newton state.

These equations are formulated in curvilinear geometry as follows. Divergence operators and scalar and vector Laplacian operators are formulated as outlined earlier in this study. All vectors are staggered. To avoid as many vector transformations as possible, the vectors $\delta\mathbf{F}_A^-$ and $\delta\mathbf{F}_\phi^-$ are formulated in the covariant representation, δF_α^- , while the vectors $\bar{\mathbf{\Gamma}}$, $\delta\bar{\mathbf{\Gamma}}$, and $\delta\bar{\mathbf{j}}$ are formulated in contravariant representation, $\bar{\Gamma}^\alpha$, $\delta\bar{\Gamma}^\alpha$, and $\delta\bar{j}^\alpha$. The vector $\mathbf{B}_0$ is considered in both representations, as needed. It follows that, for each species s :

$$(\delta F_{s,\alpha})_\phi^- = -n_s \partial_\alpha \delta\phi - \delta n_s \partial_\alpha \phi - \frac{\partial_\alpha (T_s \delta n_s)}{2q_s},$$

$$(\delta F_{s,\alpha})_\mathbf{A}^- = -n_s \frac{\delta A_\alpha}{\Delta t} + \bar{\Gamma}_s^\beta \partial_\alpha \delta A_\beta - \bar{\Gamma}_s^\beta \partial_\beta \delta A_\alpha,$$

and, for both ϕ and $\mathbf{A}$:

$$\delta\bar{\Gamma}_s^\alpha = \frac{g^{\alpha\beta} \delta F_{s,\beta}^- + [\alpha_s \epsilon_{\alpha\beta\gamma} \delta F_{s,\beta}^- B_{0,\gamma} / J + \alpha_s^2 (\delta F_{s,\gamma}^- B_0^\gamma) B_0^\alpha]}{1 + \alpha_s^2 B_0^\gamma B_{0,\gamma}}.$$

These system of equations are solved using an approximate multigrid solver that renders the algorithm scalable with grid refinement. For more details on the basic formulation of the preconditioner and its performance, see Ref. [1].

6. Numerical results

We consider two test cases to demonstrate the properties of the proposed curvilinear algorithm. The first one is a piston-driven 1D slow magnetosonic wave shock problem, with a grid packed near the piston. Unlike earlier studies in implicit PIC algorithms [41, 43, 32, 1], this example features an open system with non-periodic boundary conditions (inflow and perfect conductor). The second one is a 2D Weibel instability on a fully curvilinear grid based on a sinusoidal map deformation.

6.1. Slow-shock problem

We employ the so-called piston method to simulate a slow magneto-sonic wave switch-off shock in a 1D domain [44, 45, 46]. The piston sits on the right of the simulation domain and provides the boundary conditions. The simulation domain is in the frame that the piston is stationary, and a left-to-right flow in the x direction is reflected off the piston. The inflow velocity is greater than the slow magnetosonic wave speed and smaller than the intermediate wave speed. The boundary conditions on the piston are that the transverse magnetic field switches off, and particles are reflected off the boundary [44]. The open boundary conditions are that the magnetic field is constant, and an inflow of particles that keep the particle density of first cell near the boundary constant.

The particles are initially loaded as a drift Maxwellian with an inflow $V_0 = 0.00856 c$, where c is the speed of light. The plasma consists of Maxwellian electrons with $v_{eT} = \sqrt{T_e/m_e} = 0.0745$ and $\beta_e = 0.1$, and Maxwellian ions with $v_{iT} = \sqrt{T_i/m_i} = 0.0149$ and $\beta_i = 0.1$. The mass ratio is $m_i/m_e = 25$ [44, 45, 46]. The simulation domain is $L_x = 50 (d_i)$. The magnetic field is set to be $B_0 = 0.0667$, and 75 degrees with respect to the x direction. Note that for this problem $\omega_{pe}/\omega_{ce} = 3$. The timestep is $\Delta t = 0.1 \omega_{pi}^{-1}$. We consider a uniform grid with 512 mesh points, and a non-uniform one with 64. The grid spacing at the piston is comparable in both grids. Both simulations start with 500 particles per cell. The Jacobian of the grid (which shows mesh compression towards the piston on the right) is shown in Fig. 2.

Figure 3 shows some comparisons between simulations with uniform and non-uniform grids. At the early time (e.g. $t = 10$), there is an immediate pile up of plasma density near the piston. Leading the wave-front is a fast wave (perturbations in density and magnetic field have the same sign). This fast wave expands and becomes weaker and weaker as it propagates. The agreement between the two simulations at the early stages is excellent. The agreement at later times ($t = 120$) remains excellent despite large resolution changes in the adaptive simulation. We see that a small jump in density develops at in both simulations, but the jump is slightly sharper in the uniform-grid simulation owing to the fact that the non-uniform mesh is becoming quite coarse. The density jump corresponds to a wave perturbation seen in B_x at the same location, which is also slightly sharper in the uniform-grid simulation. The development of a

Figure 2: The Jacobian ($dx/d\xi$) of the 1D non-uniform grid using 64 grid-points.

Table 1: Solver performance for uniform and non-uniform grid simulations. The measurements are averaged over 20 timesteps. For these tests, we have converged the nonlinear residual to a relative tolerance of 10^{-4} .

	uniform grid	non-uniform grid
Newton	4	4
GMRES	1	4.2
CPU(s)	51.6	17.1

shock front is clearly captured in both simulations. The oscillatory signal developed right near the piston, a signature of switch-off slow shock [47], is seen in both simulations. The phase of the oscillation is in good agreement between the two, although the B_x magnitude of the non-uniform grid simulation is slightly lower than the uniform-grid one. Overall, we see very good agreement between uniform and non-uniform grid simulations despite the resolution differences. We note that getting this kind of agreement between uniform and adaptive solutions in the slow-shock problem has not been straightforward, and represents a stringent test of our numerics.

It is interesting to look at the CPU speedup of the non-uniform grid vs. the uniform one. We provide solver and CPU performance numbers for both uniform and non-uniform grid simulations in Table 1. We find that, while the number of Newton iterations remains unchanged, there is a slight loss of performance in the GMRES solve between uniform and non-uniform simulations. This loss of performance is expected, and originates in the degradation of performance of our multigrid solver in the presence of strongly varying mesh resolution. In addition, the particle mover in the non-uniform case is significantly more expensive than in the uniform one owing to the required interpolations of mesh metrics to the particle orbit. As a result, Table 1 only shows a speedup of a factor of 3 instead of the maximum possible speedup of 8 (which is the mesh size ratio). This lower-than-optimal speedup from increasing particle and solver costs in the non-uniform mesh case is of marginal concern, however, as a reliable, accurate curvilinear PIC simulation capability may enable simulations that are not possible otherwise.

Figure 3: Comparisons of plasma density and magnetic field profiles using uniform (512 points) and non-uniform (64 points) grids at $t = 10$ and $t = 120$ (ω_{pi}^{-1}).

Figure 4: The curvilinear grid created by the map given in Eq. 80, and used for the 2D Weibel instability test problem.

6.2. 2D Weibel instability problem

The 2D Weibel instability test case setup is similar to that used in Ref. [1], except for the curvilinear mesh and some minor differences in parameters. In particular, both electrons and ions are initialized with an anisotropic Maxwell distribution with $T_{ey,z}/T_{ex} = 4$, and the thermal velocity parallel to the wave vector is $v_{eTx} \equiv \sqrt{T_{ex}/m} = 0.1$. We employ a quasi-quiet (or non-random) start [48], and the initial plasma is neutral. The timestep is taken to be $\Delta t = 1 (\omega_{pe}^{-1})$, which is about 14 times larger than the explicit CFL ($\sim \lambda_D/c\sqrt{2}$). The simulated domain has $L_x \times L_y = 20(d_e) \times 20(d_e)$, with 32×32 uniform cells and doubly periodic boundary conditions. The average number of particles per cell of each species is 400. A δ -function-like perturbation is introduced by shifting the velocity of all the electrons in one cell (in the middle of the domain) by a small amount:

$$v_p = v_{p0} + a \quad (79)$$

where v_{p0} is particle velocity sampled from the Maxwellian distribution, and $a = 10^{-2}$ is the perturbation level.

Figure 4 shows the sinusoidally perturbed map in physical space, which is given by:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \xi + \varepsilon_g \sin(2\pi\xi/L_x) \sin(2\pi\eta/L_y) \\ \eta + \varepsilon_g \sin(2\pi\xi/L_x) \sin(2\pi\eta/L_y) \\ \xi \end{pmatrix}, \quad (80)$$

where $\varepsilon_g = 0.2$ provides a significant sinusoidal perturbation to the grid. The mesh is non-orthogonal.

Figure 5: Time history of the magnetic field energy evolving from an electron Weibel instability. Very good agreement is found between uniform grid and curvilinear grid simulations.

Figure 5 shows the evolution of the magnetic field energy using both Cartesian and curvilinear grids. We see only small differences between the two in either linear or nonlinear regimes. The time history of conserved quantities (e.g., charge, energy, momentum, canonical momenta, and $\nabla \cdot \mathbf{A}$) is depicted in Fig. 6, for both uniform and curvilinear meshes. We see that charge conservation is preserved at round-off level in both cases. Energy conservation is also comparable, as is expected given that it is essentially controlled by the JFNK nonlinear convergence tolerance (a relative tolerance of 10^{-5} is used in this study). The canonical momentum in the ignorable direction (z) is also comparable, and consistent with the Picard tolerance for the Crank-Nicolson orbit integration scheme (an absolute tolerance of 10^{-10} is used). As in earlier studies [41], the total particle momentum in the x -direction is not conserved exactly, but the relative error is small, even in the curvilinear grid. Finally, also as expected, $\nabla \cdot \mathbf{A}$ is well conserved in both simulations, with the error level consistent with the JFNK nonlinear tolerance. These results confirm the effectiveness of our curvilinear discretization approach in preserving conserved quantities and involutions.

7. Conclusions

We have formulated and demonstrated a fully implicit, curvilinear, conservative discretization for the Vlasov-Darwin model in multiple dimensions. Our approach extends recent work [32, 1] on the 1D-3V and 2D-3V treatment of the Vlasov-Darwin system in uniform meshes. The approach conserves local charge, global energy, and canonical momenta in ignorable directions. It also preserves involutions –Gauss’ law and the Coulomb gauge of the vector potential– exactly (in practice, to nonlinear tolerance). Momentum is

Figure 6: Time histories of conserved quantities and involutions for the electron Weibel instability. Charge conservation is measured as the root-mean-square (rms) of the continuity equation, numerically evaluated at grid cells as $\sqrt{\sum_{i,j=1}^{N_g} J_{i,j} \Delta \xi \Delta \eta (\rho_{i,j}^{n+1} - \rho_{i,j}^n + \Delta t [\nabla \cdot \mathbf{j}]_{i,j})^2}$, where N_g is the number of grid-points. Energy conservation is measured as the accumulated change in the total energy (c.f. Eq. 58) with respect to the initial one. Momentum conservation in the x direction is measured as $\sum_p m_p v_{p,x} / \sum_p m_p v_{th,x}$, with p the particle index respectively. The maximum error in the conservation of canonical momenta in the z -direction for all particles is measured as $\max_p (|m_p v_{z,p}^{n+1} + q_p A_{z,p}^{n+1} - m_p v_{z,p}^n - q_p A_{z,p}^n|)$. Finally, the rms of $\nabla \cdot \mathbf{A}$ is found as $\sqrt{\sum_{i,j=1}^{N_g} J_{i,j} \Delta \xi \Delta \eta [\nabla \cdot \mathbf{A}]_{i,j}^2}$.

not exactly conserved, but numerical errors are kept small by particle subcycling. Key to the approach is the use of a hybrid particle pusher (motivated by the curvilinear formulation of the Vlasov equation), and the judicious choice of discretization of various operators, and in particular of the particle velocity equation in the ignorable direction (to conserve canonical momentum) and the vector Laplacian operator for the vector potential, $\mathbf{A}$ (to preserve the Coulomb gauge).

We have demonstrated the potential of the approach with two examples: a slow shock in 1D, and the Weibel instability in 2D. The first example has been well studied by many authors [49, 50, 44, 45, 46]. It is an open system, and brings to the fore boundary-condition complexity in the presence of one-dimensional non-uniform meshes. The second example is a doubly periodic, curvilinear multidimensional example, which truly tests the advertised multidimensional features of the scheme. We have found that the solution is virtually unchanged by the introduction of a sinusoidal map deformation of the Cartesian mesh up to 20%.

Future work will involve the generalization of the scheme to 3D. The only expected substantial change to the study documented here is the discretization of the vector Laplacian from the energy principle (Sec. 4.3.4), which in 3D will require the consideration of all three contributions to the energy measure in a similar fashion. All the other details of the algorithm will remain virtually unchanged.

Acknowledgments

This work was partially sponsored by the Los Alamos National Laboratory Directed Research and Development program (LDRD) and by the Office of Applied Scientific Computing Research of the US Department of Energy (DOE). This work was performed under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory, managed by LANS, LLC under contract DE-AC52-06NA25396.

- [1] G. Chen and L. Chacón, "A multi-dimensional, energy- and charge-conserving, nonlinearly implicit, electromagnetic vlasov-darwin particle-in-cell algorithm," *Comput. Phys. Commun.*, vol. 197, pp. 73–87, 2015.
- [2] L. Chacón, G. Chen, and D. C. Barnes, "A charge- and energy-conserving implicit, electrostatic particle-in-cell algorithm on mapped computational meshes," *J. Comput. Phys.*, vol. 233, pp. 1–9, 2013.
- [3] S. E. Parker, A. Friedman, S. L. Ray, and C. K. Birdsall, "Bounded multi-scale plasma simulation: Application to sheath problems," *J. Comput. Phys.*, vol. 107, pp. 388 – 402, 1993.
- [4] R. Fonseca, L. Silva, F. Tsung, V. Decyk, W. Lu, C. Ren, W. Mori, S. Deng, S. Lee, T. Katsouleas, *et al.*, "Osiris: a three-dimensional, fully relativistic particle in cell code for modeling plasma based accelerators," *Lecture Notes in Computational Science*, pp. 342–351, 2002.
- [5] J. Wang, D. Kondrashov, P. C. Liewer, and S. R. Karmesin, "Three-dimensional deformable-grid electromagnetic particle-in-cell for parallel computers," *J. Plasma Phys.*, vol. 61, pp. 367 – 389, 1999.
- [6] C. Munz, R. Schneider, E. Sonnendrücker, E. Stein, U. Voss, and T. Westermann, "A finite-volume particle-in-cell method for the numerical treatment of Maxwell-Lorentz equations on boundary-fitted meshes," *International journal for numerical methods in engineering*, vol. 44, no. 4, pp. 461–487, 1999.
- [7] J. W. Eastwood, W. Arter, N. J. Brealey, and R. W. Hockney, "Body-fitted electromagnetic PIC software for use on parallel computers," *Comput. Phys. Commun.*, vol. 87, no. 1-2, pp. 155 – 78, 1995.
- [8] G. Jacobs and J. Hesthaven, "High-order nodal discontinuous galerkin particle-in-cell method on unstructured grids," *Journal of Computational Physics*, vol. 214, no. 1, pp. 96–121, 2006.
- [9] A. Stock, J. Neudorfer, M. Riedlinger, G. Pirrung, G. Gassner, R. Schneider, S. Roller, and C. Munz, "Three-dimensional numerical simulation of a 30-GHz gyrotron resonator with an explicit high-order discontinuous-galerkin-based parallel particle-in-cell method," *IEEE Transactions on Plasma Science*, vol. 40, pp. 1860–1870, 2012.
- [10] J. Wang, O. Chang, and Y. Cao, "Electron-ion coupling in mesothermal plasma beam emission: Full particle pic simulations," *IEEE Transactions on Plasma Science*, vol. 40, no. 2, pp. 230–236, 2012.
- [11] T. Bagdonat and U. Motschmann, "3d hybrid simulation code using curvilinear coordinates," *Journal of Computational Physics*, vol. 183, no. 2, pp. 470–485, 2002.
- [12] K. Fujimoto and R. Sydora, "Electromagnetic particle-in-cell simulations on magnetic reconnection with adaptive mesh refinement," *Computer Physics Communications*, vol. 178, no. 12, pp. 915–923, 2008.
- [13] G. L. Delzanno, E. Camporeale, J. D. Moulton, J. E. Borovsky, E. MacDonald, M. F. Thomsen, *et al.*, "CPIC: A curvilinear particle-in-cell code for plasma-material interaction studies," *IEEE Transactions on Plasma Science*, vol. 41, no. 12, pp. 3577–3587, 2013.

- [14] Z. Lin, T. Hahm, W. Lee, W. Tang, and R. White, "Turbulent transport reduction by zonal flows: Massively parallel simulations," *Science*, vol. 281, no. 5384, pp. 1835–1837, 1998.
- [15] J. L. Vay, A. Friedman, and D. P. Grote, "Application of adaptive mesh refinement to PIC simulations in heavy ion fusion," *Nuclear instruments & methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment*, vol. 544, no. 1-2, pp. 347 – 52, 2005.
- [16] W. M. Ruyten, "Density-conserving shape factors for particle simulations in cylindrical and spherical coordinates," *J. Comput. Phys.*, vol. 105, no. 2, pp. 224 – 32, 1993.
- [17] J. P. Verboncoeur, "Symmetric spline weighting for charge and current density in particle simulation," *J. Comput. Phys.*, vol. 174, no. 1, pp. 421 – 7, 2001.
- [18] D. J. Larson, D. W. Hewett, and A. B. Langdon, "Correction factors for PIC accumulation on radial grids," *Comput. Phys. Commun.*, vol. 90, no. 2-3, pp. 260 – 6, 1995.
- [19] A. Y. Aydemir, "A unified monte carlo interpretation of particle simulations and applications to non-neutral plasmas," *Physics of Plasmas (1994-present)*, vol. 1, no. 4, pp. 822–831, 1994.
- [20] Y. Chen and S. E. Parker, "Electromagnetic gyrokinetic δf particle-in-cell turbulence simulation with realistic equilibrium profiles and geometry," *Journal of Computational Physics*, vol. 220, no. 2, pp. 839–855, 2007.
- [21] T. Westermann, "Localization schemes in 2D-boundary-fitted grids," *J. Comput. Phys.*, vol. 101, no. 2, pp. 307 – 313, 1992.
- [22] T. Westermann, "Particle-in-cell simulations with moving boundaries-adaptive mesh generation," *J. Comput. Phys.*, vol. 114, no. 2, pp. 161 – 75, 1994.
- [23] D. Seldner and T. Westermann, "Algorithms for interpolation and localization in irregular 2D-meshes," *J. Comput. Phys.*, vol. 79, no. 1, pp. 1 – 11, 1988.
- [24] D. N. Kenwright and D. A. Lane, "Optimization of time-dependent particle tracing using tetrahedral decomposition," in *Proceedings of the 6th conference on Visualization'95*, p. 321, IEEE Computer Society, 1995.
- [25] C. Fichtl, J. Finn, and K. Cartwright, "An arbitrary curvilinear-coordinate method for particle-in-cell modeling," *Computational Science & Discovery*, vol. 5, no. 1, p. 014011, 2012.
- [26] D. Swift, "Use of a hybrid code for global-scale plasma simulation," *J. Comput. Phys.*, vol. 126, no. 1, pp. 109–121, 1996.
- [27] C. W. Nielson and H. R. Lewis, "Particle-code models in the nonradiative limit," *Methods in Computational Physics*, vol. 16, pp. 367–388, 1976.

- [28] D. W. Hewett, "Elimination of electromagnetic radiation in plasma simulation: The Darwin or magnetoinductive approximation," *Space Science Reviews*, vol. 42, pp. 29–40, 1985.
- [29] P. Degond and P.-A. Raviart, "An analysis of the Darwin model of approximation to Maxwell's equations," *Forum Math*, vol. 4, no. 4, pp. 13–44, 1992.
- [30] P.-A. Raviart and E. Sonnendrücker, "A hierarchy of approximate models for the Maxwell equations," *Numerische Mathematik*, vol. 73, no. 3, pp. 329–372, 1996.
- [31] T. B. Krause, A. Apte, and P. Morrison, "A unified approach to the Darwin approximation," *Physics of Plasmas*, vol. 14, p. 102112, 2007.
- [32] G. Chen and L. Chacón, "An energy- and charge-conserving, nonlinearly implicit, electromagnetic 1D-3V Vlasov-Darwin particle-in-cell algorithm," *Comput. Phys. Commun.*, vol. 185, no. 10, pp. 2391–2402, 2014.
- [33] A. Hasegawa and H. Okuda, "One-dimensional plasma model in the presence of a magnetic field," *Physics of Fluids*, vol. 11, p. 1995, 1968.
- [34] C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation*. New York: McGraw-Hill, 2005.
- [35] B.-N. Jiang, J. Wu, and L. A. Povinelli, "The origin of spurious solutions in computational electromagnetics," *Journal of computational physics*, vol. 125, no. 1, pp. 104–123, 1996.
- [36] J. Boris, "Relativistic plasma simulation-optimization of a hybrid code," in *Proc. Fourth Conf. Num. Sim. Plasmas, Naval Res. Lab, Wash. DC*, pp. 3–67, 1970.
- [37] C.-D. Munz, P. Omnes, R. Schneider, E. Sonnendrücker, and U. Voss, "Divergence correction techniques for maxwell solvers based on a hyperbolic model," *Journal of Computational Physics*, vol. 161, no. 2, pp. 484–511, 2000.
- [38] D. Hewett, "Low-frequency electromagnetic (Darwin) applications in plasma simulation," *Computer physics communications*, vol. 84, no. 1, pp. 243–277, 1994.
- [39] H. Weitzner and W. S. Lawson, "Boundary conditions for the Darwin model," *Physics of Fluids B: Plasma Physics*, vol. 1, p. 1953, 1989.
- [40] B. I. Cohen, R. P. Freis, and V. Thomas, "Orbit-averaged implicit particle codes," *J. Comput. Phys.*, vol. 45, no. 3, pp. 345–366, 1982.
- [41] G. Chen, L. Chacón, and D. C. Barnes, "An energy- and charge-conserving, implicit, electrostatic particle-in-cell algorithm," *J. Comput. Phys.*, vol. 230, pp. 7018–7036, 2011.

- [42] G. Chen, L. Chacón, and D. C. Barnes, "An efficient mixed-precision, hybrid CPU-GPU implementation of a nonlinearly implicit one-dimensional particle-in-cell algorithm," *J. Comput. Phys.*, vol. 231, no. 16, pp. 5374–5388, 2012.
- [43] G. Chen, L. Chacon, C. A. Leibs, D. A. Knoll, and W. Taitano, "Fluid preconditioning for Newton-Krylov-based, fully implicit, electrostatic particle-in-cell simulations," *Journal of computational physics*, vol. 258, p. 555, 2014.
- [44] W. Daughton, D. Winske, L. Yin, and S. P. Gary, "Role of electron physics in slow mode shocks," *Journal of Geophysical Research: Space Physics (1978–2012)*, vol. 106, no. A11, pp. 25031–25039, 2001.
- [45] L. Yin, D. Winske, W. Daughton, and F. Coroniti, "Dissipation in oblique slow shocks," *Journal of Geophysical Research: Space Physics (1978–2012)*, vol. 110, no. A9, 2005.
- [46] L. Yin, D. Winske, and W. Daughton, "Kinetic alfvén waves and electron physics. ii. oblique slow shocks," *Physics of Plasmas (1994-present)*, vol. 14, no. 6, p. 062105, 2007.
- [47] F. Coroniti, "Laminar wave-train structure of collisionless magnetic slow shocks," *Nuclear Fusion*, vol. 11, no. 3, p. 261, 1971.
- [48] J. Denavit and J. Walsh, "Nonrandom initializations of particle codes," *Comments Plasma Phys. Controlled Fusion*, vol. 6, p. 209, 1981.
- [49] D. Winske, E. K. Stover, and S. P. Gary, "The structure and evolution of slow mode shocks," *Geophysical research letters*, vol. 12, no. 5, pp. 295–298, 1985.
- [50] J. Brackbill and H. Vu, "Electron kinetic effects in switch-off slow shocks," *Geophysical research letters*, vol. 20, no. 19, pp. 2015–2018, 1993.