Kinetic Implicit Fluid Methods for Dusty and Relativistic Plasmas

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Abstract

Fully explicit discretizations must resolve all three processes that ideal MHD assumes are instantaneous: oscillations, collisions, and light waves. Asymptotic-preserving discretization requires stepping over these processes. Fully implicit discretization allows stepping not only over these three processes but also over MHD waves, but is expensive because one must repeatedly re-push particles with successive iterations of the implicit field solver. We therefore present semi-implicit discretizations of Maxwell's equations that step over subsets of these processes. Discretizing implicitly in the source term steps over plasma oscillations and collisions and allows asymptotic-preserving agreement with (quasi-)relativistic MHD. Discretizing the flux terms of Maxwell's equations implicitly steps over light waves and allows asymptotic-preserving agreement with classical two-fluid MHD.

To facilitate asymptotic-preserving agreement with fluid models and conservation of physical invariants, we consider kinetic fluid closure.

kinetic-Maxwell (the "truth")

particle evolution:

$$d_t \mathbf{x}_\mathrm{p} = \mathbf{v}_\mathrm{p},$$
$$d_t \mathbf{u}_\mathrm{p} = \tfrac{q_\mathrm{p}}{m_\mathrm{p}}(\mathbf{v}_\mathrm{p}\times\mathbf{B}(\mathbf{x}_\mathrm{p}) + \mathbf{E}(\mathbf{x}_\mathrm{p})),$$
$$\gamma_\mathrm{p}^2 := 1 + (\mathbf{u}_\mathrm{p}/c)^2,$$
$$\mathbf{v}_\mathrm{p} := \mathbf{u}_\mathrm{p}/\gamma_\mathrm{p}.$$

electromagnetic field:

$$\partial_t \mathbf{B} + \nabla\times\mathbf{E} = 0,$$
$$-c^{-2}\partial_t\mathbf{E} + \nabla\times\mathbf{B} = \mu_0\mathbf{J},$$
$$\nabla\cdot\mathbf{B} = 0, \quad c^{-2}\nabla\cdot\mathbf{E} = \mu_0\sigma,$$

where $\sigma(\mathbf{x}) := \sum_p S_p(\mathbf{x}) q_p$ is charge density and $\mathbf{J}(\mathbf{x}) := \sum_p S_p(\mathbf{x}) q_p \mathbf{v}_p$ is current density; here $S_\mathrm{p}(\mathbf{x}) = S(\mathbf{x}-\mathbf{x}_\mathrm{p})$ is the shape function of particle p. To abbreviate, we drop the particle summation index p and the independent variable $\mathbf{x}$ and write

$$\begin{aligned} \sigma &:= \textstyle\sum qS && \text{(charge)},\\ \rho &:= \textstyle\sum mS && \text{(mass)},\\ \mathbf{J} &:= \textstyle\sum \mathbf{v}qS && \text{(current)},\\ \mathbf{M} &:= \textstyle\sum \mathbf{v}mS && \text{(momentum)},\\ \mathcal{E} &:= \textstyle\sum \frac{1}{2}|v|^2 mS && \text{(energy)}. \end{aligned}$$

Modeling and Fluid Moments

Fields evolve in response to charge moments, and mass, momentum, and energy are conserved, motivating the use of fluid models. Kinetic closure allows kinetic algorithms to transition efficiently and smoothly to fluid models.

Moment evolution

Moment definitions are of the form $\sum \chi S$. To derive fluid equations, we differentiate the moment definition with respect to time and use the basic derivatives to the right.

Charge density evolution.

$$\boxed{\partial_t\sigma + \nabla\cdot\mathbf{J} = 0},$$

using $\partial_t\sigma = \sum \dot{q}S + \sum q\partial_t S$, $\partial_t S = -\mathbf{v}\cdot\nabla S$, and $\nabla\mathbf{v} = 0$.

General moment evolution

$$\boxed{\partial_t \sum \chi S + \nabla\cdot\sum \mathbf{v}\chi S = \sum \dot{\chi} S, \quad \dot{\chi} = \frac{\partial\chi}{\partial\mathbf{u}}\cdot\dot{\mathbf{u}} = \frac{\partial\chi}{\partial\mathbf{v}}\cdot\dot{\mathbf{v}}.}$$

Shape motion:

$$\boxed{\partial_t S = -\mathbf{v}\cdot\nabla S}, \tag{1}$$

where we have used the chain rule.

Lorentz force.

$$\boxed{\dot{\mathbf{u}} = \tfrac{q}{m}(\mathbf{E} + \mathbf{v}\times\mathbf{B})};$$

Energy change.

$$\boxed{\dot{\gamma} = \mathbf{v}\cdot\dot{\mathbf{u}} = \tfrac{q}{m}\mathbf{v}\cdot\mathbf{E}}, \tag{2}$$

because $\gamma^2 = 1 + (\mathbf{u}/c)^2$, so $\gamma\dot{\gamma} = \mathbf{u}\cdot\dot{\mathbf{u}}/c^2$.

Velocity change.

$$\boxed{\dot{\mathbf{v}} = \tfrac{q}{\gamma m}\left(\mathbf{E} - \tfrac{\mathbf{v}\mathbf{v}}{c^2}\cdot\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)},$$

which follows from differentiating $\mathbf{u} = \gamma\mathbf{v}$, to get $\dot{\mathbf{u}} = \dot{\gamma}\mathbf{v} + \gamma\dot{\mathbf{v}}$, i.e. $\gamma\dot{\mathbf{v}} = \dot{\mathbf{u}} - \mathbf{v}\mathbf{v}\cdot\dot{\mathbf{u}}$.

Current evolution (Ohm's law)

Current evolution (Ohm's law, $\chi = q\mathbf{v}$).

$$\boxed{\partial_t\mathbf{J} + \nabla\cdot\mathcal{P} = \sum S\tfrac{q^2}{\gamma m}\left(\mathbb{I} - \tfrac{\mathbf{v}\mathbf{v}}{c^2}\right)\cdot\mathbf{E} + \sum S\tfrac{q^2}{\gamma m}\times\mathbf{B}},$$

where $\mathcal{P} := \sum q\mathbf{v}\mathbf{v}$.

Classical current evolution for species s.

$$\boxed{\partial_t\mathbf{J}_\mathrm{s} + \nabla\cdot\mathcal{P}_\mathrm{s} = \tfrac{q_\mathrm{s}}{m_\mathrm{s}}(\sigma_\mathrm{s}\mathbf{E} + \mathbf{J}_\mathrm{s}\times\mathbf{B})},$$

where $\mathcal{P}_\mathrm{s}$ restricts to species s.

Mass moment evolution

Relativistic case.

Mass density ($\chi = m$).

$$\boxed{\partial_t\rho + \nabla\cdot\sum m\mathbf{v}S = 0.}$$

Momentum density ($\chi = m\mathbf{u}$).

$$\boxed{\partial_t\mathbf{M} + \nabla\cdot\sum m\mathbf{v}\mathbf{u}S = \sigma\mathbf{E} + \mathbf{J}\times\mathbf{B}},$$

Energy density ($\chi = mc^2\gamma$).

$$\boxed{\partial_t\mathcal{E} + \nabla\cdot\mathbf{M} = \mathbf{J}\cdot\mathbf{E}},$$

Classical case.

Mass density ($\chi = m$)

$$\boxed{\partial_t\rho + \nabla\cdot\mathbf{M} = 0},$$

Momentum density ($\chi = m\mathbf{v}$)

$$\boxed{\partial_t\mathbf{M} + \nabla\cdot\sum m\mathbf{v}\mathbf{v}S = \sigma\mathbf{E} + \mathbf{J}\times\mathbf{B}},$$

Energy density ($\chi = \frac{1}{2}m|\mathbf{v}|^2$)

$$\boxed{\partial_t\mathcal{E} + \nabla\cdot\sum\tfrac{1}{2}m\mathbf{v}v^2 S = \mathbf{J}\cdot\mathbf{E}},$$

Semi-implicit methods

Semi-implicit methods are used to step over fast processes such as plasma oscillations (implicit source) and light waves (IMM) without having to step over all processes.

Field discretizations

The Implicit Moment Method is an example of a semi-implicit method. For plasma simulations, one of four types of discretization is generally used:

Discretization	must resolve...	must iterate...
1. Explicit	plasma period [everything]	[no iteration]
2. Implicit Source	light waves	classical: no iteration relativistic: source iteration
3. Implicit Moment (IMM)	electron sound waves	iterate fields
4. Fully implicit	[no restriction]	iterate particles [everything]

The Implicit Source discretization naturally suits an asymptotic-preserving transition to relativistic MHD, since ideal relativistic MHD takes the electron charge (gyrofrequency) to infinity. The Implicit Moment Method naturally suits an asymptotic-preserving transition to two-fluid MHD, which takes light speed to infinity.

Explicit discretization

Start with the basic equations:

$$\partial_t\mathbf{B} + \nabla\times\mathbf{E} = 0,$$
$$\partial_t\mathbf{E} - c^2\nabla\times\mathbf{B} = -\mathbf{J}/\epsilon_0,$$
$$\partial_t\mathbf{x}_\mathrm{p} = \mathbf{v}_\mathrm{p},$$
$$\partial_t\mathbf{u}_\mathrm{p} = \tfrac{q_\mathrm{p}}{m_\mathrm{p}}(\mathbf{E}(\mathbf{x}_\mathrm{p}) + \mathbf{v}_\mathrm{p}\times\mathbf{B}(\mathbf{x}_\mathrm{p})).$$

For a second-order discretization, use a leapfrog discretization, and time-split velocity update for a symplectic method:

$$\mathbf{B}^2 = \mathbf{B}^0 - \Delta t\nabla\times\mathbf{E}^1,$$
$$\mathbf{E}^1 = \mathbf{E}^{-1} + \Delta t c^2\nabla\times\mathbf{B}^0 - \mathbf{J}^0/\epsilon_0,$$
$$\mathbf{u}_\mathrm{p}^* = \mathbf{u}_\mathrm{p}^0 + \frac{q_\mathrm{p}}{2m_\mathrm{p}\gamma_\mathrm{p}^0}(\mathbf{u}_\mathrm{p}^* + \mathbf{u}_\mathrm{p}^0)\times\bar{\mathbf{B}}^1(\mathbf{x}_\mathrm{p}^1),$$
$$\mathbf{u}_\mathrm{p}^2 = \mathbf{u}_\mathrm{p}^* + \tfrac{q_\mathrm{p}}{m_\mathrm{p}}\mathbf{E}^1(\mathbf{x}_\mathrm{p}^1),$$

where $\bar{\mathbf{B}}^1 := \frac{1}{2}\mathbf{B}^0 + \frac{1}{2}\mathbf{B}^2$.

Fully implicit method

Modify the IMM discretization by making all terms implicit:

$$\partial_t\mathbf{B} + \nabla\times\bar{\mathbf{E}} = 0$$
$$\partial_t\mathbf{E} - c^2\nabla\times\bar{\mathbf{B}} = -\bar{\mathbf{J}}/\epsilon_0$$
$$\partial_t\mathbf{u}_\mathrm{p} = \tfrac{q_\mathrm{p}}{m_\mathrm{p}}\left(\bar{\sigma}_\mathrm{p}\bar{\mathbf{E}}(\bar{\mathbf{x}}_p) + \bar{\mathbf{v}}_\mathrm{p}\times\bar{\mathbf{B}}(\bar{\mathbf{x}}_\mathrm{p})\right),$$
$$\partial_t\mathbf{x}_\mathrm{p} = \bar{\mathbf{v}}_\mathrm{p},$$
$$\partial_t\sigma_\mathrm{s} + \nabla\cdot\bar{\mathbf{J}}_\mathrm{s} = 0,$$
$$\partial_t\mathbf{J}_\mathrm{s} + \nabla\cdot\mathcal{P}_\mathrm{s} = \tfrac{q_\mathrm{s}}{m_\mathrm{s}}\left(\bar{\sigma}_\mathrm{s}\bar{\mathbf{E}} + \bar{\mathbf{J}}_\mathrm{s}\times\bar{\mathbf{B}}\right).$$

Remarks.

- Particle advance must be redone with successive iterations of the field solver.
- This discretization is fully symmetric in time, so by Noether's theorem conserves energy if iterated to convergence.

Implicit Source discretization [KumarMishra11]

Use initial values for flux terms. Use implicit values in stiff source term.

$$\partial_t\mathbf{B} + \nabla\times\mathbf{E} = 0,$$
$$\partial_t\mathbf{E} - c^2\nabla\times\mathbf{B} = -\bar{\mathbf{J}}/\epsilon_0,$$
$$\partial_t\mathbf{u}_\mathrm{p} = \tfrac{q_\mathrm{p}}{m_\mathrm{p}}\left(\bar{\mathbf{E}}(\mathbf{x}_\mathrm{p}) + \bar{\mathbf{v}}_\mathrm{p}\times\bar{\mathbf{B}}(\mathbf{x}_\mathrm{p})\right),$$
$$\partial_t\mathbf{x}_\mathrm{p} = \bar{\mathbf{v}}_\mathrm{p},$$
$$\partial_t\sigma_\mathrm{s} + \nabla\cdot\mathbf{J}_\mathrm{s} = 0,$$
$$\partial_t\mathbf{J}_\mathrm{s} + \nabla\cdot\mathcal{P}_\mathrm{s} = \tfrac{q_\mathrm{s}}{m_\mathrm{s}}\left(\bar{\sigma}_\mathrm{s}\bar{\mathbf{E}} + \bar{\mathbf{J}}_\mathrm{s}\times\bar{\mathbf{B}}\right).$$

Time discretization is

$$\partial_t Q \to (Q^1 - Q^0)/\Delta t,$$
$$\nabla F \to F^0,$$
$$\bar{\mathbf{X}} = X^1$$

Classical case: No source term iteration happens to be needed, because $\bar{\mathbf{v}}$ is linear in $\bar{\mathbf{E}}$. Can sum the response over all particles to eliminate $\bar{\mathbf{J}} = \widehat{\mathbf{J}} + \mathbb{A}\cdot\bar{\mathbf{E}}$ in favor of $\bar{\mathbf{E}}$.

Relativistic case: Must iterate particle velocity advance, but positions need not be advanced, so iterative solve involves no communication between mesh cells.

High-order accuracy: Use an IMEX Runge-Kutta solver.

IMM (implicit moment method) [VuBrackbill92]

Modify the Implicit Source discretization by using implicit flux for electromagnetic field advance, but keep the particle position advance explicit.

$$\partial_t\mathbf{B} + \nabla\times\bar{\mathbf{E}} = 0$$
$$\partial_t\mathbf{E} - c^2\nabla\times\bar{\mathbf{B}} = -\bar{\mathbf{J}}/\epsilon_0,$$
$$\partial_t\mathbf{u}_\mathrm{p} = \tfrac{q_\mathrm{p}}{m_\mathrm{p}}\left(\bar{\mathbf{E}}(\mathbf{x}_p) + \bar{\mathbf{v}}_\mathrm{p}\times\mathbf{B}'(\mathbf{x}_\mathrm{p})\right),$$
$$\partial_t\mathbf{x}_\mathrm{p} = \bar{\mathbf{v}}_\mathrm{p},$$
$$\partial_t\sigma_\mathrm{s} + \nabla\cdot\bar{\mathbf{J}}_\mathrm{s} = 0,$$
$$\partial_t\mathbf{J}_\mathrm{s} + \nabla\cdot\mathcal{P}_\mathrm{s} = \tfrac{q_\mathrm{s}}{m_\mathrm{s}}\left(\sigma_\mathrm{s}'\bar{\mathbf{E}} + \bar{\mathbf{J}}_\mathrm{s}\times\mathbf{B}'\right)$$

For second-order accuracy in relevant terms, use time averages for the implicit terms:

$$\partial_t Q \to (Q^1 - Q^0)/\Delta t,$$
$$\nabla F \to F^0, \bar{\mathbf{X}} = \tfrac{1}{2}X^0 + \tfrac{1}{2}X^1,$$
$$\bar{\mathbf{v}} = \tfrac{1}{2}\mathbf{v}^0 + \tfrac{1}{2}\mathbf{v}^1,$$
$$\bar{\mathbf{J}} = \tfrac{1}{2}\mathbf{J}^0 + \tfrac{1}{2}\mathbf{J}^1,$$
$$\bar{\mathbf{E}} = \tfrac{1}{2}\mathbf{E}^0 + \tfrac{1}{2}\mathbf{E}^1.$$

Observe that in this discretization,

$$\partial_t X = 2(\bar{\mathbf{X}} - X^0)/\Delta t.$$

Divergence constraints. Eliminating $\mathbf{B}$ from this field discretization and assuming mimetic operators, the field solve is exactly equivalent to

$$c^{-2}\partial_t\mathbf{E} = (\tfrac{1}{2}\Delta t)\left(\nabla^2\bar{\mathbf{E}} - \nabla(\nabla\cdot\bar{\mathbf{E}})\right) + \left(\nabla\times\mathbf{B}^0 - \mu_0\bar{\mathbf{J}}\right);$$

following [RicciLapentaBrackbill02], to ensure the divergence constraint error is damped, substitute $(\nabla\cdot\bar{\mathbf{E}}) \to (\mu_0 c^2\bar{\sigma})$.

Classical case. No iteration is needed, because $\bar{\mathbf{v}}$ is linear in $\bar{\mathbf{E}}$. Can sum the response over all particles to eliminate $\bar{\mathbf{J}} = \widehat{\mathbf{J}} + \mathbb{A}\cdot\bar{\mathbf{E}}$ in favor of $\bar{\mathbf{E}}$. IMM in literature uses $\mathbf{B}' = \mathbf{B}^0$ and $\sigma_\mathrm{s}' = \sigma_\mathrm{s}^0$, but $\mathbf{B}' = \mathbf{B}^0 - \Delta t\nabla\times\mathbf{E}^0$ and $\sigma_\mathrm{s}' = \sigma_\mathrm{s}^0 - \Delta t\nabla\cdot\mathbf{J}^0$ would yield full second-order accuracy in time.

Relativistic case. Implicit Source seems preferable to IMM for the relativistic case:

- Why step over light waves but not over relativistic sound waves or fluid speed? An IMEX time step is much cheaper and involves no long-distance communication.
- The source term system responds nonlinearly to $\bar{\mathbf{E}}$ and is not closed, so an implicit particle velocity advance must be repeated with successive iterations of the field solve.

Implicit particle mover (classical)

Particle position and velocity are differenced as

$$\mathbf{x}_\mathrm{p}^1 = \mathbf{x}_\mathrm{p}^0 + \bar{\mathbf{v}}_\mathrm{p}\Delta t, \quad \bar{\mathbf{v}}_\mathrm{p} := \tfrac{1}{2}\mathbf{v}_\mathrm{p}^1 + \tfrac{1}{2}\mathbf{v}_\mathrm{p}^0,$$
$$\mathbf{v}_\mathrm{p}^1 = \mathbf{v}_\mathrm{p}^0 + 2\beta_\mathrm{p}\left(\mathbf{E}_\mathrm{p}^\theta + \bar{\mathbf{v}}_\mathrm{p}\times\mathbf{B}_\mathrm{p}^\vartheta\right),$$

where ϑ might equal θ or 0 and

$$\beta_\mathrm{p} := \frac{q_\mathrm{p}\Delta t}{2m_\mathrm{p}}.$$

Choosing $\mathbf{B}_\mathrm{p}^\vartheta := \mathbf{B}^\vartheta(\mathbf{x}_\mathrm{p}^0)$ yields an explicit particle advance. Choosing $\mathbf{B}_\mathrm{p}^\vartheta := \mathbf{B}^\vartheta(\bar{\mathbf{x}}_\mathrm{p})$ and $\mathbf{E}_\mathrm{p}^\theta := \mathbf{E}^\theta(\bar{\mathbf{x}}_\mathrm{p})$, where

$$\bar{\mathbf{x}}_\mathrm{p} := \tfrac{1}{2}\mathbf{x}_\mathrm{p}^1 + \tfrac{1}{2}\mathbf{x}_\mathrm{p}^0,$$

defines an implicit particle advance. Use 2 iterations starting with an explicit advance for 2nd-order accuracy. Eliminating $\mathbf{v}_\mathrm{p}^1$ in favor of $\bar{\mathbf{v}}_\mathrm{p}$,

$$\bar{\mathbf{v}}_\mathrm{p} = \mathbf{v}_\mathrm{p}^0 + \beta_\mathrm{p}\left(\mathbf{E}_\mathrm{p}^\theta + \bar{\mathbf{v}}_\mathrm{p}\times\mathbf{B}_\mathrm{p}^\vartheta\right).$$

This is of the form

$$\mathbf{U} = \mathbf{V} + \mathbf{U}\times\boldsymbol{\Omega}, \text{ i.e.,} \tag{3}$$
$$(\mathbb{I} + \boldsymbol{\Omega}\times\mathbb{I})\cdot\mathbf{U} = \mathbf{V}, \tag{4}$$

where $\mathbf{U} = \bar{\mathbf{v}}_\mathrm{p}$, $\mathbf{V} = \mathbf{v}_\mathrm{p}^0 + \beta_\mathrm{p}\mathbf{E}_\mathrm{p}^\theta$, and $\boldsymbol{\Omega} = \beta_\mathrm{p}\mathbf{B}_\mathrm{p}^\vartheta$. To solve for $\mathbf{U}$, cross and dot both sides with $\boldsymbol{\Omega}$:

$$\mathbf{U}\times\boldsymbol{\Omega} = \mathbf{V}\times\boldsymbol{\Omega} + \boldsymbol{\Omega}\boldsymbol{\Omega}\cdot\mathbf{U} - |\boldsymbol{\Omega}|^2\mathbf{U}, \text{ and}$$
$$\mathbf{U}\cdot\boldsymbol{\Omega} = \mathbf{V}\cdot\boldsymbol{\Omega}, \text{ so eliminating } \mathbf{U}\times\boldsymbol{\Omega} \text{ in (3)},$$
$$\mathbf{U}(1 + |\boldsymbol{\Omega}|^2) = (\mathbb{I} - \boldsymbol{\Omega}\times\mathbb{I} + \boldsymbol{\Omega}\boldsymbol{\Omega})\cdot\mathbf{V}, \text{ i.e.,}$$
$$\mathbf{U} = (1 + |\boldsymbol{\Omega}|^2)^{-1}(\mathbb{I} - \boldsymbol{\Omega}\times\mathbb{I} + \boldsymbol{\Omega}\boldsymbol{\Omega})\cdot\mathbf{V};$$

from this and (4), we infer that

$$\boxed{(\mathbb{I} + \boldsymbol{\Omega}\times\mathbb{I})^{-1} = (1 + |\boldsymbol{\Omega}|^2)^{-1}(\mathbb{I} - \boldsymbol{\Omega}\times\mathbb{I} + \boldsymbol{\Omega}\boldsymbol{\Omega}).}$$

Thus,

$$\boxed{\bar{\mathbf{v}}_\mathrm{p} = \Pi_\mathrm{p}^\vartheta\cdot(\mathbf{v}_\mathrm{p}^0 + \beta_\mathrm{p}\mathbf{E}_\mathrm{p}^\theta), \text{ where } \Pi_\mathrm{p}^\vartheta := (\mathbb{I} - \mathbb{I}\times\boldsymbol{\Omega}_\mathrm{p})^{-1} \text{ and } \boldsymbol{\Omega}_\mathrm{p} := \beta_\mathrm{p}\mathbf{B}_\mathrm{p}^\vartheta.}$$

Observe that $|\boldsymbol{\Omega}_\mathrm{p}|$ is half the gyrofrequency for particle p. Note that $\vartheta \in \{0, \theta\}$ is chosen based on whether the updated magnetic field is already known. A first-order-accurate field predictor allows for a fully second-order-accurate solve with $\vartheta = \theta = \frac{1}{2}$.

Conforming fluid-Maxwell

The Implicit Moment Method may be criticized, because although it exactly maintains $\nabla\cdot\mathbf{B} = 0$ and damps $\nabla\cdot\mathbf{E} - \sigma/\epsilon_0$, it is not exactly conforming and does not conserve momentum and energy. This can be remedied, however, with a predictor-corrector approach, where particle distributions are tweaked to match evolved, slaved fluid quantities.

Divergence constraints: consistency of fields with fluid moments

A predictor-corrector strategy can be used to maintain the divergence constraints to machine precision while maintaining order of accuracy for arbitrarily high order:

1. Evolve the fields with sufficient accuracy.
2. Evolve face-normal field fluxes using the evolved fields.
3. Enforce consistency of the evolved fields with the evolved face-normal field fluxes.

Enforcing $\nabla\cdot\mathbf{B} = 0$:

Integrating magnetic field evolution over a time step and over a mesh cell face A gives

$$\int_A \widehat{\mathbf{n}}\cdot\mathbf{B}^1 = \int_A \widehat{\mathbf{n}}\cdot\mathbf{B}^0 - \Delta t\oint_{\partial A}\widehat{\tau}\cdot\bar{\mathbf{E}},$$

where $\bar{\mathbf{E}}$ is the time-averaged value of the the electric field on the edges of the face. A predictor step can be used to supply high-order-accurate values of the average value of the parallel component of $\mathbf{E}$ along each edge, giving a high-order-accurate update of the total magnetic flux perpendicular to each face. For any order of accuracy, there is at least enough freedom to enforce that the magnetic field representation satisfies these constraints, and when extra freedom is available one can do so so as to minimize a norm.

Enforcing $\nabla\cdot\mathbf{E} = \sigma/\epsilon_0$:

Integrating electric field evolution over a time step and over a mesh cell face A gives

$$\int_A \widehat{\mathbf{n}}\cdot\mathbf{E}^1 = \int_A \widehat{\mathbf{n}}\cdot\mathbf{E}^0 + c^2\Delta t\oint_{\partial A}\widehat{\tau}\cdot\bar{\mathbf{B}} - \Delta t\int_A \widehat{\mathbf{n}}\cdot\bar{\mathbf{J}}/\epsilon_0;$$

to maintain consistency, define $\bar{\mathbf{J}}$ using the flux of charge across face A, update the face-normal electric field flux accordingly, and modify the electric field representation to enforce consistency.

Conservation framework

To enforce exact conservation of momentum and energy, use Maxwell's equations to put evolution in conservation form.

Conservation of momentum.

To put momentum equation in conservation form, rewrite the source term as the sum of a time derivative and a spatial derivative:

$$-(\sigma\mathbf{E} + \mathbf{J}\times\mathbf{B})/\epsilon_0 = \partial_t(\mathbf{E}\times\mathbf{B}) + \tfrac{1}{2}\nabla(E^2 + c^2B^2) - \nabla\cdot(\mathbf{E}\mathbf{E} + c^2\mathbf{B}\mathbf{B}),$$

where we have used all four Maxwell's equations and a vector product rule.

Conservation of energy.

To put energy evolution in conservation form, rewrite the source term as

$$-\mathbf{J}\cdot\mathbf{E}/\epsilon_0 = \tfrac{1}{2}\partial_t(E^2 + c^2B^2) + \nabla\cdot(\mathbf{E}\times\mathbf{B}),$$

where we have used Maxwell's evolution equations and the identity $\mathbf{E}\cdot\nabla\times\mathbf{B} = \mathbf{B}\cdot\nabla\times\mathbf{E} - \nabla\cdot(\mathbf{E}\times\mathbf{B})$.

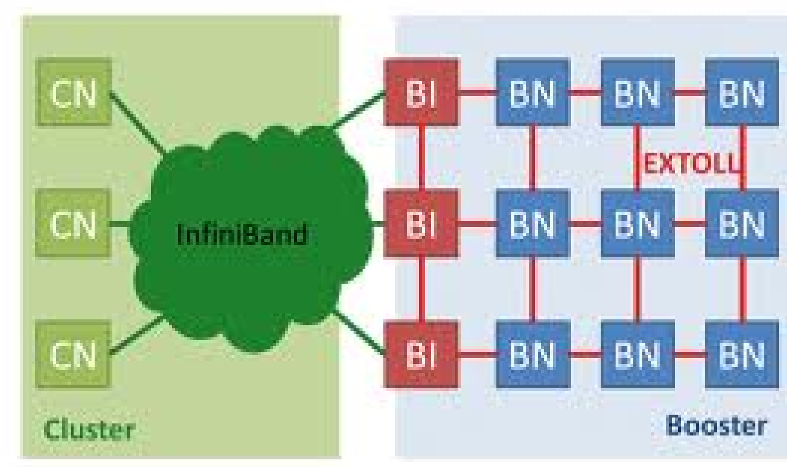
Positivity.

Conservation form allows an explicit fluid code to enforce positivity using the framework of *Outflow Positivity Limiting*, as described in [JoRo12]. Here we assume that the thermal energy, defined as the gas-dynamic energy in the reference frame in which the gas-dynamic momentum is zero, is a concave function of the conserved state variables $(\rho, \widetilde{\mathbf{M}}, \widetilde{\mathcal{E}}, \mathbf{B}, \mathbf{E})$, where $\widetilde{\mathcal{E}} := \mathcal{E} + \frac{1}{2}(E^2 + c^2B^2)$ is defined to be the total energy and $\widetilde{\mathbf{M}} := \mathbf{M} + \mathbf{E}\times\mathbf{B}$ is defined to be the total momentum.

Porting of iPic3D to DEEP

We are porting iPic3D to the Dynamic Exascale Entry Platform (DEEP). DEEP is an Exascale project funded by the EU 7th framework programme.

DEEP: Cluster attached to Booster



The architecture of DEEP consists of a 128-node, 21.3 teraflop **Cluster** of 16-core 2.7 GHz Intel Xeon processors connected to an infiniband network and will be augmented with a a 512-node, 590 teraflop **Booster** each of whose nodes is a 1.2 GHz 60-core Xeon Phi MIC (Many Integrated Core) accelerators.

The DEEP architecture was developed with the idea of accelerating codes that run on the cluster by making it easy to offload computationally intensive parts of the code to the booster while leaving complex, communication-intensive code on the cluster.

FieldSolver on Cluster, ParticleSolver on Booster

iPic3D implements the implicit moment method and consists of a cycle of three steps:

1. (ParticleSolver): Sum moments $\widehat{\mathbf{J}}^0$, σ^0, and σ_s^0 of particles. Communicate moments to FieldSolver.
2. (FieldSolver): Advance the electromagnetic field, $\mathbf{E}^0 \to \mathbf{E}^1$, using moments. Communicate fields to ParticleSolver.
3. (ParticleSolver): Advance the particles using the already advanced fields.

Due to its implicit nature, the FieldSolver makes many all-to-all communications and naturally is best suited to the Cluster.

In contrast, since particles can be pushed in parallel, the ParticleSolver only needs to communicate particles to neighboring processors in the torus.

To increase resolution and demonstrate converged solutions, the number of particles per mesh cell must increase. Therefore, in the high resolution limit, computing particles increasingly dominates PIC codes. The port of iPic3D to DEEP aims for unprecedented resolution of turbulent reconnection on long time scales in the classical regime.

A beneficial side-effect of the DEEP port is the clean separation of the particle solver and the field solver. This allows replacing one or the other as appropriate:

- The FieldSolver could be replaced with an Implicit Source field solver or could be iterated to yield a fully implicit discretization.
- The ParticleSolver could be replaced with a fluid model or a gyrokinetic or relativistic mover.

References

The following paper describes a general framework to enforce positivity in a fluid model.

[JoRo12] E.A. Johnson and J.A. Rossmanith, *Outflow positivity limiting: Part 1, framework and recipe.* `http://arxiv.org/abs/1212.4695`

[KumarMishra11] Harish Kumar and Siddartha Mishra, *Entropy stable numerical schemes for two-fluid plasma equations*, J. Sci. Comput. (2012), `http://dx.doi.org/10.1007/s10915-011-9554-7`.

The following describes a clearer formulation of the implicit moment method, viewed as solving the momentum evolution equations for each species with kinetic closure in conjunction with Maxwell's equations.

[MarkidisHLRHML13] Stefano Markidis, Pierre Henri, Giovanni Lapenta, Kjell Rönnmark, Maria Hamrin, Zakaria Meliani, Erwin Laure. *The Fluid-Kinetic Particle-in-Cell Solver for Plasma Simulations.* Submitted to Journal of Computational Physics (2013). `http://arxiv.org/abs/1306.1089`.

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The following article derives the implicit Maxwell scheme.

[RicciLapentaBrackbill02] Paolo Ricci, Giovanni Lapenta, and J.U. Brackbill. *A simplified implicit Maxwell solver.* Journal of Computational Physics **183**, 117–141 (2002).

The following article derives an approximation for $\bar{\mathbf{J}}$ using a Taylor expansion.

[VuBrackbill92] H.X. Vu and J.U. Brackbill. *CELEST1D: an implicit, fully kinetic model for low-frequency, electromagnetic plasma simulation.* Computer Physics Communications 69 (1992) 253–276.

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