Fully implicit particle in cell algorithm for electromagnetic plasma simulations

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Outline

- Particle-in-cell (PIC) methods for plasmas
- Explicit vs. implicit PIC
- ES implicit PIC:
  - Charge and energy conservation
  - Moment-based acceleration (NEW)
- Generalization to EM PIC (NEW)
  - Review and motivation for Darwin model
  - Conservation properties (energy, charge, and canonical momenta)
- Some comments on algorithm co-design

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Introduction
Particle-in-cell (PIC) methods for kinetic plasma simulation

\[ \partial_t f + \mathbf{v} \cdot \nabla f + \frac{F}{m} \cdot \nabla_v f = 0 \]

- **Lagrangian solution by the method of characteristics:**

\[ f(x, v, t) = f_0 \left( x - \int_0^t dv \mathbf{v}, v - \frac{1}{m} \int_0^t dtF \right) ; \quad x(t = 0) = x_0 ; \quad v(t = 0) = v_0 \]

- **PIC approach follows characteristics employing macroparticles** (volumes in phase space)

\[ f(x, v, t) = \sum_p \delta(x - x_p)\delta(v - v_p) \]

\[ \begin{align*}
\dot{x}_p &= \mathbf{v}_p \\
\dot{\mathbf{v}}_p &= \frac{q_p}{m_p} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \\
\partial_t \mathbf{B} + \nabla \times \mathbf{E} &= 0 \\
-\mu_0 \varepsilon_0 \partial_t \mathbf{E} + \nabla \times \mathbf{B} &= \mu_0 \mathbf{j} \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \cdot \mathbf{E} &= \frac{e(n_i - n_e)}{\varepsilon_0} 
\end{align*} \]

\[ \delta(x - x_p) \rightarrow S(x - x_p) ; \quad E_p = \sum_i E_i S(x_i - x_p) ; \quad j_i = \sum_p j_p S(x_i - x_p) \]

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State-of-the-art classical PIC algorithm is explicit

- Classical explicit PIC approach “leap-frogs” particle positions and velocities, solves for fields after position update:

Severe performance limitations:
- $\Delta x < \lambda_{Debye}$ (finite-grid instability: enforces a minimum spatial resolution)
- $\omega_{pe}\Delta t < 1$ (CFL-type instability: enforces a minimum temporal resolution)
- Inefficient for long-time, large-scale integrations

In the presence of strong magnetic fields, gyro-averaging the Vlasov-Maxwell model can significantly ameliorate these limitations, but there are other issues (e.g. not asymptotic preserving, required order of expansion to capture some physical effects, treatment of nonlinear terms)

We focus on electrostatic PIC as a proof of principle

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What about implicit PIC?

- Implicit PIC holds the promise of overcoming the difficulties and inefficiencies of explicit methods for long time-scale simulations
- Exploration of implicit PIC started in the 1980s
  - Moment method [Mason, 1981; Brackbill, 1982]
  - Direct method [Friedman, Langdon, Cohen, 1981]
- Early approaches used linearized, semi-implicit formulations:
  - Lack of nonlinear convergence
  - Inconsistencies between particles and moments
  - Inaccuracies! → Plasma self-heating/cooling [Cohen, 1989]

Our goal is to explore the viability of a nonlinearly converged, fully implicit PIC algorithm

What is the nature of the resulting fully-coupled algebraic system? Is it practical to invert?
Fully implicit PIC
A fully implicit formulation couples particles and fields non-trivially (integro-differential PDE):

\[
\frac{f^{n+1} - f^n}{\Delta t} + \mathbf{v} \cdot \nabla f^{n+1} + \frac{f^n}{2} - \frac{q}{m} \frac{\Phi^{n+1} + \Phi^n}{2} \cdot \nabla f^{n+1} + \frac{f^n}{2} = 0
\]

\[
\nabla^2 \Phi^{n+1} = \int d\mathbf{v} f^{n+1}(\mathbf{x}, \mathbf{v}, t)
\]

In PIC, \( f^{n+1} \) is sampled by a large collection of particles in phase space, \( \{\mathbf{x}, \mathbf{v}\}_{n+1}^p \).

- There are \( N_p \) particles, each particle requiring \( 2 \times d \) equations (\( d \rightarrow \)dimensions),
- Field requires \( N_g \) equations, one per grid point.

If implemented naively, an impractically large algebraic system of equations results:

\[
\mathbf{G}(\{\mathbf{x}, \mathbf{v}\}_{p}^{n+1}, \{\Phi^{n+1}\}_{g}) = 0 \quad \rightarrow \quad \dim(\mathbf{G}) = 2dN_p + N_g \gg N_g
\]

- No current computing mainframe can afford the memory requirements
- Algorithmic issues are showstoppers (e.g., how to precondition it?)

An alternative strategy exists: nonlinear elimination (particle enslavement)
Particle enslavement (nonlinear elimination)

- Full residual $G(\{x,v\}_p, \{\Phi\}_g) = 0$ is impractical to implement
- Alternative: nonlinearly eliminate particle quantities so that they are not dependent variables:
  - Formally, particle equations of motion are functionals of the electrostatic potential:
    \[
    x_{p}^{n+1} = x_p[\Phi^{n+1}] ; \quad v_{p}^{n+1} = v_p[\Phi^{n+1}]
    \]
    \[
    G(x_{p}^{n+1}, v_{p}^{n+1}, \Phi^{n+1}) = G(x[\Phi^{n+1}], v[\Phi^{n+1}], \Phi^{n+1}) = \tilde{G}(\Phi^{n+1})
    \]

Nonlinear residual can be unambiguously formulated in terms of electrostatic potential only!

- JFNK storage requirements are dramatically decreased, making it tractable:
  - Nonlinear solver storage requirements $\propto N_g$, comparable to a fluid simulation
  - Particle quantities $\Rightarrow$ auxiliary variables: only a single copy of particle population needs to be maintained in memory throughout the nonlinear iteration

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### Field equation: Vlasov-Poisson vs. Vlasov-Ampère

- **Nonlinear elimination** procedure leads to $G(\Phi) = 0$ (or $G(E) = 0$)
- Two formulations are possible:

<table>
<thead>
<tr>
<th>Vlasov-Poisson (VP)</th>
<th>Vlasov-Ampère (VA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\partial_t f + v \partial_x f + \frac{qE}{m} \partial_v f = 0$</td>
<td>$\partial_t f + v \partial_x f + \frac{qE}{m} \partial_v f = 0$</td>
</tr>
<tr>
<td>$\partial_x E = \frac{\rho}{\epsilon_0}$</td>
<td>$\epsilon_0 \partial_t E + j = \langle j \rangle$</td>
</tr>
<tr>
<td>$E = -\partial_x \Phi$</td>
<td></td>
</tr>
</tbody>
</table>

Two systems are equivalent in continuum, but not in the discrete.

- Conventionally used in explicit PIC.
- Exact *local* charge conservation.
- Exact *global* momentum conservation.
- Unstable with orbit averaging in implicit context [Cohen and Freis, 1982].

- Exact *local* charge conservation.
- Exact *global* energy conservation.
- Suitable for orbit averaging.
- Can be extended to electromagnetic system.

We will show, however, that an equivalent energy-conserving VP formulation exists.

---

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Energy-conserving (EC) Vlasov-Ampère discretization

- Fully implicit Crank-Nicolson time discretization:

\[
\frac{E_{i}^{n+1} - E_{i}^{n}}{\Delta t} + \sum_{p} q_{p} \sqrt{\frac{m_{p}}{2}} S(x_{i} - x_{p}^{n+1/2}) = 0
\]

\[
\frac{x_{p}^{n+1} - x_{p}^{n}}{\Delta t} = \frac{v_{p}^{n+1} + v_{p}^{n}}{2}
\]

\[
\frac{v_{p}^{n+1} - v_{p}^{n}}{\Delta t} = \frac{q_{p}}{m_{p}} \sum_{i} \frac{E_{i}^{n} + E_{i}^{n+1}}{2} S(x_{i} - x_{p}^{n+1/2})
\]

- C-N enforces energy conservation to numerical round-off:

\[
\sum_{p} \frac{m_{p}}{2} (v_{p}^{n+1} + v_{p}^{n})(v_{p}^{n+1} - v_{p}^{n}) = - \sum_{i} \varepsilon_{0} \frac{E_{i}^{n+1} - E_{i}^{n} E_{i}^{n+1} + E_{i}^{n}}{\Delta t} \Rightarrow \sum_{p} \frac{m_{p}}{2} v_{p}^{2} + \sum_{i} \frac{1}{2} \varepsilon_{0} E_{i}^{2} = \text{const}
\]

- As a result, the formulation does not suffer from finite-grid instabilities (normal mode analysis)

\(\Delta x \ll \lambda_D\)

- Requires a tight nonlinear tolerance

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Jacobian-Free Newton-Krylov Methods

- After spatial and temporal discretization \( \Rightarrow \) a large set of nonlinear equations: \( \vec{G}(\vec{x}^{m+1}) = \vec{0} \)

- Converging nonlinear couplings requires iteration: Newton-Raphson method:

  \[
  \left. \frac{\partial \vec{G}}{\partial \vec{x}} \right|_k \delta \vec{x}_k = -\vec{G}(\vec{x}_k)
  \]

- Jacobian linear systems result, which require a linear solver \( \Rightarrow \) Krylov subspace methods (GMRES)
  
  Only require matrix-vector products to proceed.

  Jacobian-vector product can be computed Jacobian-free (CRITICAL: no need to form Jacobian matrix):

  \[
  \left( \frac{\partial \vec{G}}{\partial \vec{x}} \right)_k \vec{y} = J_k \vec{y} = \lim_{\epsilon \to 0} \frac{\vec{G}(\vec{x}_k + \epsilon \vec{y}) - \vec{G}(\vec{x}_k)}{\epsilon}
  \]

  Krylov methods can be easily preconditioned: \( P_k^{-1} \sim J_k^{-1} \)

  \[
  J_k P_k^{-1} P_k \delta \vec{x} = -\vec{G}_k
  \]

We will explore suitable preconditioning strategies later in this talk.
Algorithmic implementation details

The nonlinear residual formulation $G(E^{n+1})$ based on Vlasov-Ampere formulation is as follows:

1. Input $E$ (given by JFNK iterative method)
2. Move particles (i.e., find $x_p[E], v_p[E]$ by solving equations of motion)
   (a) Requires inner (local) nonlinear iteration: Picard (not stiff)
   (b) Can be as complicated as we desire (substepping, adaptivity, etc)
3. Compute moments (current)
4. Form Vlasov-Ampere equation residual
5. return

Because particle move is performed within function evaluation, we have much freedom.

Rest of the talk will describe improvements in particle mover to ensure long-term accuracy

- Particle substepping and orbit averaging (ensures orbit accuracy and preserves exact energy conservation)
- Exact charge conservation strategy (a new charge-conserving particle mover)
- Orbit adaptivity (to improve momentum conservation)
Particle orbit substepping

In applications of interest, field time-scale ($\Delta t$) and orbit time-scale ($\Delta \tau$) can be well separated. FIELDS evolve slowly (dynamical time scale, $\Delta t$)

- Particle orbits may still undergo rapid change ($\Delta \tau \ll \Delta t$)

- Particle orbits need to be resolved to avoid large orbit integration errors

Accurate orbit integration requires particle substepping!

Field does not change appreciably: time-averaged value over long time scale is sufficient

\[
\frac{x_p^{v+1} - x_p^v}{\Delta \tau} = v_p^{v+1/2}
\]

\[
\frac{v_p^{v+1} - v_p^v}{\Delta \tau} = \sum_i \frac{E_i^{n+1} + E_i^n}{2} S(x_i - x_p^{v+1/2})
\]
Energy conservation and orbit averaging

- Particle substepping breaks energy conservation.
- Energy conservation theorem can be recovered by orbit averaging Ampère’s law:

\[
\epsilon_0 \partial_t E + J = \langle j \rangle, \quad \frac{1}{\Delta t} \int_t^{t+\Delta t} d\tau [\cdots] \Rightarrow \epsilon_0 \frac{E^{n+1} - E^n}{\Delta t} + \bar{j} = \langle \bar{j} \rangle
\]

- Orbit-averaged current is found as:

\[
\bar{j} = \frac{1}{\Delta t} \int_t^{t+\Delta t} d\tau j \approx \frac{1}{\Delta t} \sum_p \sum_{\nu=1}^{N_p} q_p \nu_p S(x - x_p) \Delta \tau^\nu
\]

- With these definitions, exact energy conservation is recovered:

\[
\sum_p \sum_{\nu} \frac{m_p}{2} \left( v_{p,\nu}^{v+1} + v_{p,\nu}^v \right) \left( v_{p,\nu}^{v+1} - v_{p,\nu}^v \right) = -\sum_i \epsilon_0 \frac{E_{i,n+1} - E_{i,n} E_{i,n+1}^2 + E_{i,n}^2}{\Delta t} \\
\Rightarrow \sum_p \frac{1}{2} m_p v_p^2 + \sum_i \frac{1}{2} \epsilon_0 E_i^2 = \text{const.}
\]
Exact charge conservation: charge-conserving particle mover

- Local charge conservation (enforced in the continuum by Gauss' law) is violated in discrete Vlasov-Ampère formulation.
- Local charge conservation is essential to ensure long-term accuracy of numerical algorithm.
- Exact charge conservation requires a particle mover that satisfies a discrete charge continuity equation, \( \partial_t \rho + \nabla \cdot j = 0 \) [Buneman 1968, Morse and Nielson, 1971]

- **Standard strategy** based on current redistribution when particle crosses boundary.
- In our context, current redistribution breaks energy conservation. **Need new strategy.**

Here, charge conservation is enforced by stopping particles at cell boundaries.

\[
\rho_{i+\frac{1}{2}} = \sum_p q_p \frac{S_m(x-x_i+\frac{1}{2})}{\Delta x}
\]

\[
\begin{align*}
\rho_{i+\frac{1}{2}} & = \sum_p q_p \frac{S_m(x-x_i+\frac{1}{2})}{\Delta x} \\
\partial_t \rho + \nabla \cdot j & = 0 \\
S'_{m}(x) & = \frac{S_{m-1}(x+\Delta x/2)-S_{m-1}(x-\Delta x/2)}{\Delta x}
\end{align*}
\]

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Momentum conservation: adaptive orbit integrator

- EC/CC PIC algorithm does not enforce momentum conservation exactly.
  - Controlling error in momentum conservation is crucial for long-term accuracy.
- Orbit integration errors can significantly affect momentum conservation: particle tunneling.

- Adaptive orbit integration can be effective in suppressing particle tunneling and thus improve momentum conservation.
- Approach: find $\Delta \tau$ to control local truncation error. Second order estimator gives:

$$\Delta \tau \leq \sqrt{12\varepsilon_r \frac{m_p}{q_p} \left| \frac{dE}{dx} \right|_p^{-1}}$$

- Electric field gradient is estimated from cell-based gradient:
  $$\frac{\partial E}{\partial x} \bigg|_p \approx \frac{E_{i+1} - E_i}{\Delta x}.$$ Provides potential barrier!

- Particle is stopped at cell boundaries to ensure charge conservation.
Ion acoustic wave (IAW): accuracy impact of different EC movers

![Graphs showing compared results](image)

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Ion acoustic shock wave

- Propagating IAW with perturbation level $\epsilon = 0.4$, with 4000 particles/cell.
- Realistic mass ratio ($m_i/m_e = 2000$).
- Shock wave length scale $\sim$ Debye length.

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Ion acoustic shock wave test

non-uniform grid spacing

non-uniform grid spacing

uniform, ex, dt= 0.1
uniform, im, dt=10.0
non-uniform, im, dt=10.0

rms $[\rho + dt \cdot (dj / dx)]$

uniform
non-uniform

-4e-4
-2e-4
0
2e-4
4e-4

Δ (total energy)

0.9998
0.9999
1
1.0001
1.0002

Σ (mv)$_p$/Σ (mpv)ph

t (x1000)

0 1 2 3

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Comparison against Implicit Moment Method

1 Taitano et al., *SISC*, accepted (2013)

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Moment-based acceleration for fully implicit PIC
CPU gain potential of implicit PIC vs. explicit PIC

➤ Back-of-the-envelope estimate of CPU gain:

\[ CPU \sim \left( \frac{T}{\Delta t} \right) \left( \frac{L}{\Delta x} \right)^d n_p C_{\text{solver}} \]

\[ \frac{C_{\text{imp}}}{C_{\text{ex}}} \sim N_{FE} \frac{\Delta t_{\text{imp}}}{\Delta \tau_{\text{imp}}} \]

\[ \frac{CPU_{\text{ex}}}{CPU_{\text{imp}}} \sim \left( \frac{\Delta x_{\text{imp}}}{\Delta x_{\text{ex}}} \right)^d \frac{\Delta \tau_{\text{imp}}}{\Delta t_{\text{ex}}} \frac{1}{N_{FE}} \]

➤ Using reasonable estimates:

\[ \Delta \tau_{\text{imp}} \sim \min \left[ 0.1 \frac{\Delta x_{\text{imp}}}{v_{th}}, \Delta t_{\text{imp}} \right] \]

\[ \Delta t_{\text{imp}} \sim 0.1 \omega_{pi}^{-1} \]

\[ \Delta t_{\text{exp}} \sim 0.1 \omega_{pe}^{-1} \]

\[ k \Delta x_{\text{imp}} \sim 0.2 \]

\[ \Delta x_{\text{ex}} \sim \lambda_D \]

➤ CPU speedup is:

✔ Independent of time step!

✔ Better for realistic mass ratios!

✔ Limited by solver performance \( N_{FE} \) (preconditioning!)

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Moment-based acceleration of fully kinetic simulations

- Particle elimination ⇒ nonlinear residual is formulated in terms of fields/moments ONLY: \( G(E) \)
- Within JFNK, preconditioner ONLY needs to provide field/moment update:

\[
\delta E \approx -P^{-1}G
\]

Premise of acceleration: obtain \( \delta E \) from a fluid model using current particle distribution for closure.

We begin with corresponding fluid nonlinear model:

\[
\begin{align*}
\partial_t n_\alpha &= -\nabla \cdot \Gamma_\alpha \\
m_\alpha \left[ \partial_t \Gamma_\alpha + \nabla \cdot \left( \frac{1}{n_\alpha} \Gamma_\alpha \Gamma_\alpha \right) \right] &= q_\alpha n_\alpha E + \nabla \cdot \left( n_\alpha \left( \frac{\Pi_\alpha}{n_\alpha} \right)_p \right) \\
\varepsilon_0 \partial_t E &= \sum_\alpha q_\alpha \Gamma_\alpha
\end{align*}
\]

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We formulate approximate linearized fluid equations (neglect linear temperature response):

\[
\frac{\delta n_\alpha}{\Delta t} = -\nabla \cdot \delta \Gamma_\alpha
\]

\[
m_\alpha \frac{\delta \Gamma_\alpha}{\Delta t} \approx q_\alpha (\delta n_\alpha E + n_{\alpha,p} \delta E) + \nabla \cdot \left( \left( \frac{\Pi_\alpha}{n_\alpha} \right)_p \delta n_\alpha \right)
\]

\[
\epsilon_0 \delta E = \Delta t \left[ \sum_\alpha q_\alpha \delta \Gamma_\alpha - G(E) \right]
\]

\(\delta E\) can be obtained from Newton state \(E\), Newton residual \(G(E)\),

and particle closures \(\Pi_{\alpha,p}\) and \(n_{\alpha,p}\)

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Preconditioner performance with $\Delta t$

- Number of FE remains constant with $\Delta t$ (preconditioning)
- Overall CPU time of algorithm is independent of $\Delta t$ (as predicted!)

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Preconditioner performance with $N_x$

- Number of FE independent of $N_x$ (as expected from plasma freq.)
- CPU cost grows as $N_x^2$
  - $\times N_x$ due to particles, and $\times N_x$ due to crossings
  - In multi-D: $CPU \propto N \times N^{1/d}$

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Preconditioner performance: CPU scaling

\[
\frac{CPU_{ex}}{CPU_{imp}} \sim \frac{1}{(k\lambda_D)^d} \frac{1}{N_{FE}} \min \left[ \frac{1}{k\lambda_D}, \sqrt{\frac{m_i}{m_e}} \right]
\]

Transition occurs at \( k\lambda_D \sim \sqrt{\frac{m_e}{m_i}} \sim 0.025 \), as predicted.
Electromagnetic PIC: non-radiative Darwin formulation
Darwin approximation to Maxwell equations: motivation

- To avoid enhanced radiative aliasing noise due to electromagnetic waves in an exactly energy-conserving algorithm:

![Figure 1: Fourier phase space for exactly energy conserving PIC (left) and energy dissipative PIC (right) [Markidis and Lapenta, JCP 2011].](image)

- Darwin approximation analytically removes light-wave in non-relativistic plasma simulations while preserving charge separation effects

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Darwin model (potential form)

We consider potentials $\phi$, $A$ in the Coulomb gauge ($\nabla \cdot A = 0$) such that:

\[
B = \nabla \times A, \\
E = -\nabla \phi - \partial_t A.
\]

Darwin model projects out the speed of light without enforcing quasineutrality (i.e., allowing for charge separation effects).

\[
\nabla^2 \chi = \nabla \cdot j, \\
-\nabla^2 A = \mu_0 [j - \nabla \chi], \\
\chi = \epsilon_0 \partial_t \phi.
\]

Problem becomes elliptic (not hyperbolic): no issue for implicit algorithm

\[
\begin{align*}
\epsilon_0 \partial_t E_x + j_x &= \langle j_x \rangle, \\
\frac{1}{\mu_0} \partial_x^2 A_y + j_y &= \langle j_y \rangle, \\
\frac{1}{\mu_0} \partial_y^2 A_z + j_z &= \langle j_z \rangle.
\end{align*}
\]

In 1D:

\[
\begin{align*}
E_{y,i}^{n+1/2} &= -\frac{A_{y,i}^{n+1} - A_{y,i}^n}{\Delta t}, \\
E_{z,i}^{n+1/2} &= -\frac{A_{z,i}^{n+1} - A_{z,i}^n}{\Delta t}.
\end{align*}
\]
Implicit EM particle mover

Subcycled particle equations of motion:

\[
\begin{align*}
\frac{x_{p}^{v+1} - x_{p}^{v}}{\Delta \tau^{v}} &= v_{x}^{v+1/2}, \\
\frac{v_{p}^{v+1} - v_{p}^{v}}{\Delta \tau^{v}} &= \frac{q_{p}}{m_{p}} \left( E_{p}^{v+1/2}(x_{p}^{v+1/2}) + v_{p}^{v+1/2} \times B_{p}^{v+1/2}(x_{p}^{v+1/2}) \right). 
\end{align*}
\]

Implicit Boris update (analytical inversion):

\[
\begin{align*}
\hat{v}_{p} &= v_{p}^{v} + \alpha E_{p}^{v+1/2}, \quad \alpha = \frac{q_{p}\Delta \tau^{v}}{m_{p}2} \\
v_{p}^{v+1/2} &= \frac{\hat{v}_{p} + \alpha [\hat{v}_{p} \times B_{p}^{v+1/2} + \alpha (\hat{v}_{p} \cdot B_{p}^{v+1/2}) B_{p}^{v+1/2}]}{1 + (\alpha B_{p})^{2}}. 
\end{align*}
\]

Final particle position and velocity are found from:

\[
\begin{align*}
x_{p}^{v+1} &= x_{p}^{v} + \Delta \tau^{v} v_{x,p}^{v+1/2}, \\
v_{p}^{v+1} &= 2v_{p}^{v+1/2} - v_{p}^{v}. 
\end{align*}
\]
Energy conserving discrete 1D Darwin model

Field equations:

\[ \epsilon_0 \frac{E_{x,i+1/2}^{n+1} - E_{x,i+1/2}^n}{\Delta t} + \tilde{j}_{x,i+1/2}^{n+1/2} = \langle j_x \rangle, \]

\[ \frac{1}{\mu_0} \frac{\partial^2 A_y^n + A_y^n}{2} \bigg|_{i}^{n+1/2} + \tilde{j}_{y,i}^{n+1/2} = \langle j_y \rangle, \]

\[ \frac{1}{\mu_0} \frac{\partial^2 A_z^n + A_z^n}{2} \bigg|_{i}^{n+1/2} + \tilde{j}_{z,i}^{n+1/2} = \langle j_z \rangle. \]

Current gather (with orbit averaging):

\[ \tilde{j}_{x,i+1/2}^{n+1/2} = \frac{1}{\Delta t \Delta x} \sum_p \sum_v q_p \sigma_{p,x}^{v+1/2} S_m (x_p^{v+1/2} - x_{i+1/2}) \Delta \tau^v, \]

\[ \tilde{j}_{y,i}^{n+1/2} = \frac{1}{\Delta t \Delta x} \sum_p \sum_v q_p \sigma_{p,y}^{v+1/2} S_l (x_p^{v+1/2} - x_i) \Delta \tau^v, \]

\[ \tilde{j}_{z,i}^{n+1/2} = \frac{1}{\Delta t \Delta x} \sum_p \sum_v q_p \sigma_{p,z}^{v+1/2} S_l (x_p^{v+1/2} - x_i) \Delta \tau^v, \]

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Field scatter to particles (with orbit averaging)

- **Electric field scatter:**

  \[
  E_{x,p}^{v+1/2} = \frac{1}{2} \sum_i \left( E_{x,i+1/2}^{n+1} + E_{x,i+1/2}^n \right) S_m \left( x_p^{v+1/2} - x_i^{v+1/2} \right),
  \]

  \[
  E_{y,p}^{v+1/2} = -\sum_i \frac{A_{y,i}^{n+1} - A_{y,i}^n}{\Delta t} S_l \left( x_p^{v+1/2} - x_i \right),
  \]

  \[
  E_{z,p}^{v+1/2} = -\sum_i \frac{A_{z,i}^{n+1} - A_{z,i}^n}{\Delta t} S_l \left( x_p^{v+1/2} - x_i \right).
  \]

- **Magnetic field scatter:** conservation of canonical momenta in ignorable directions

  \[
  \dot{p}_y = m_p \ddot{v}_{p,y} + q_p \dot{A}_{p,y} = 0, \quad \dot{p}_z = m_p \ddot{v}_{p,z} + q_p \dot{A}_{p,z} = 0
  \]

  \[
  B_{y,p}^{v+1/2} = -\sum_i \left[ \frac{A_{z,i}^{v+1/2} - A_{z,i}^{v+1/2}}{\Delta x} \right] S_{l-1} \left( x_{i+1/2}^{v+1/2} - x_p^{v+1/2} \right) - \frac{(\Delta \tau^v)^2}{8\Delta x^2} \frac{\dot{A}_{z,ip-1}^v - 2 \dot{A}_{z,ip}^v + \dot{A}_{z,ip+1}^v}{8} v_p^{v+1/2},
  \]

  \[
  B_{z,p}^{v+1/2} = \sum_i \left[ \frac{A_{y,i}^{v+1/2} - A_{y,i}^{v+1/2}}{\Delta x} \right] S_{l-1} \left( x_{i+1/2}^{v+1/2} - x_p^{v+1/2} \right) + \frac{(\Delta \tau^v)^2}{8\Delta x^2} \frac{\dot{A}_{y,ip-1}^v - 2 \dot{A}_{y,ip}^v + \dot{A}_{y,ip+1}^v}{8} v_p^{v+1/2}.
  \]
Energy conservation in Darwin

\[
\frac{K_{p}^{n+1} - K_{p}^{n}}{\Delta t} = \frac{1}{\Delta t} \sum_{p} m_{p} \sum_{v} \Delta \tau_{v} \frac{v_{p}^{v+1} + v_{p}^{v}}{2} \cdot \frac{v_{p}^{v+1} - v_{p}^{v}}{\Delta \tau_{v}} = \frac{1}{\Delta t} \sum_{p,v} q_{p} \Delta \tau_{v} E_{p}^{v+1/2} \cdot v_{p}^{v+1/2}
\]

\[
= \sum_{i} \Delta x \left( \frac{E_{x,i+1/2}^{n+1} + E_{x,i+1/2}^{n}}{2} j_{x,i+1/2}^{n+1/2} + E_{y,i}^{n+1/2} j_{y,i}^{n+1/2} + E_{z,i}^{n+1/2} j_{z,i}^{n+1/2} \right)
\]

\[
\sum_{i} \Delta x E_{x,i+1/2}^{n+1} + E_{x,i+1/2}^{n} j_{x,i+1/2}^{n+1/2} = -\frac{e_{0}}{2\Delta t} \sum_{i} \Delta x \left( \left( E_{x,i+1/2}^{n+1} \right)^{2} - \left( E_{x,i+1/2}^{n} \right)^{2} \right) = -\frac{W_{\phi x}^{n+1} - W_{\phi x}^{n}}{\Delta t}
\]

\[
\sum_{i} \Delta x E_{y,i}^{n+1/2} j_{y,i}^{n+1/2} = -\frac{1}{2\mu_{0}\Delta t} \sum_{i} \Delta x \left[ \left( \partial_{x} A_{y}^{n+1} \right)_{i+1/2}^{2} - \left( \partial_{x} A_{y}^{n} \right)_{i+1/2}^{2} \right] = -\frac{W_{Bz}^{n+1} - W_{Bz}^{n}}{\Delta t}
\]

\[
\sum_{i} \Delta x E_{z,i}^{n+1/2} j_{z,i}^{n+1/2} = -\frac{1}{2\mu_{0}\Delta t} \sum_{i} \Delta x \left[ \left( \partial_{x} A_{z}^{n+1} \right)_{i+1/2}^{2} - \left( \partial_{x} A_{z}^{n} \right)_{i+1/2}^{2} \right] = -\frac{W_{By}^{n+1} - W_{By}^{n}}{\Delta t}
\]

\[
(K_{p} + W_{\phi x} + W_{By} + W_{Bz})^{n+1} = (K_{p} + W_{\phi x} + W_{By} + W_{Bz})^{n}
\]
CPU speedup potential of EM implicit PIC vs. explicit PIC

- Back-of-the-envelope estimate of CPU gain:

\[
\frac{CPU_{ex}}{CPU_{imp}} \sim \left(\frac{\Delta x_{imp}}{\Delta x_{ex}}\right)^d \frac{\Delta t_{imp}}{\Delta t_{ex}} \frac{1}{N_{FE}}
\]

- \(\Delta t_{imp} \sim 0.1\) min \left[\frac{\Delta x_{imp}}{v_{th,e}}, \omega_{ce}^{-1}, \Delta t_{imp}\right]

- \(\Delta t_{exp} \sim \frac{\Delta x_{exp}}{c}\)

- \(k\Delta x_{imp} \sim 0.2\)

- \(\Delta x_{ex} \sim \lambda_D\)

- CPU speedup is:
  - Independent of time step
  - Impacted by electron-ion mass ratio, how close electrons are to relativistic speeds.

- Again, key is to minimize \(N_{FE}\).
  - We are in the process of developing a moment-based preconditioner.

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Verification: Electron Weibel instability

- Isotropic ions, bi-Maxwellian electrons

\[ \frac{m_i}{m_e} = 1836, \frac{T_{e\perp}}{T_{e\parallel}} = 16, N_{e,i} = 128,000, L = \frac{2\pi c}{\omega_{pe}}, N_g = 32. \]
Verification: Ion Weibel instability (small $T$ anisotropy)

- Isotropic electrons, bi-Maxwellian ions

$$m_i/m_e = 128, \quad N_{e,i}=128,000, \quad L = 0.88\pi c/\omega_{pi}, \quad N_g=32$$
Paradigm change: 1D Kinetic Alfven Wave

\[ m_i / m_e = 1836 ; \ k \lambda_D e = 0.003 ; \ \nu_{th,e} / c = 0.07 \]

\[ \frac{m_i}{m_e} = 1836 ; \ k\lambda_D e = 0.003 ; \ \nu_{th,e} / c = 0.07 \]

**Explicit PIC:**

- 2048 mesh points, 32,000 pcles/cell (overkill for this problem), **0.05 energy error**
- 500 CPUs x 24 hr, \(7 \times 10^6\) time steps

**Implicit PIC:**

- 32 mesh points, 2,000 pcles/cell (1000× fewer particles), **\(10^{-6}\) energy error**
- 16 CPUs x 29 hr, \(1.3 \times 10^5\) time steps, \(N_{FE} \sim 30\) \(r_{tol} = 10^{-6}\)

**CPU speedup \(\sim 26\) (\(\times 100\) in 2D, \(\times 10^4\) in 3D)**

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\(^2\)Yin et al., POP 14 (2007)

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Algorithm co-design and hierarchical multiphysics coupling
Mapping to hierarchical architectures (e.g., CPU-GPU)

- Particle orbits are independent of each other ⇒ PIC algorithms are naturally data parallel.

Key aspects:
- Performance of particle push on accelerators (algorithm co-design)
- HO-LO communication costs

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Example of algorithm co-design on GPU: roofline model

Chen, Chacon, Barnes, JCP, 2012

Luis Chacon, chacon@lanl.gov

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3 Chen, Chacon, Barnes, JCP, 2012
HO-LO hierarchical algorithms minimize communication costs

Two stream Instability on 32 nodes 16 Cores per Node

- Particle Read
- Time Step Estimator
- Cell Crossing
- Interp Accel
- Current Tally
- Picard Math
- Comm
- LO-Solve

Time per particle-subcycle (ns)

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Summary and conclusions

- We have demonstrated a fully implicit, fully nonlinear PIC formulation that features:
  - Exact charge conservation (via a novel particle mover strategy).
  - Exact energy conservation (no particle self-heating or self-cooling).
  - Adaptive particle orbit integrator to control errors in momentum conservation.
  - Canonical momenta (EM-PIC only, reduced dimensionality).

- The approach is free of numerical instabilities: \( \omega_{pe} \Delta t \gg 1 \), and \( \Delta x \gg \lambda_D \).

- Requires many fewer dofs for comparable accuracy in challenging problems.

- The method has much potential for efficiency gains vs. explicit in long-time-scale applications:
  \[
  \frac{CPU_{ex}}{CPU_{imp}} \sim \frac{1}{(k\lambda_D)^d \nu_{th,e}} \min \left[ \frac{1}{k\lambda_D', \nu_A \sqrt{m_i/m_e', \sqrt{m_i/m_e}}} \frac{1}{N_{FE}} \right].
  \]

  - CPU speedup benefits from not resolving Debye length \( (k\lambda_D \ll 1) \), dimensionality \( d \).
  - Independent of \( \Delta t \): pick largest one compatible with physics AND preconditioner.
  - Minimize the number of nonlinear function evaluations \( N_{FE} \Rightarrow \) preconditioning!

- Moment-based acceleration is effective in minimizing \( N_{FE} \), leading to an optimal algorithm.

- We have demonstrated the potential of the approach for hierarchical heterogeneous computing:
  - Optimal use of accelerators (e.g., GPUs)
  - Minimization of communication costs

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