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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)

Introduction

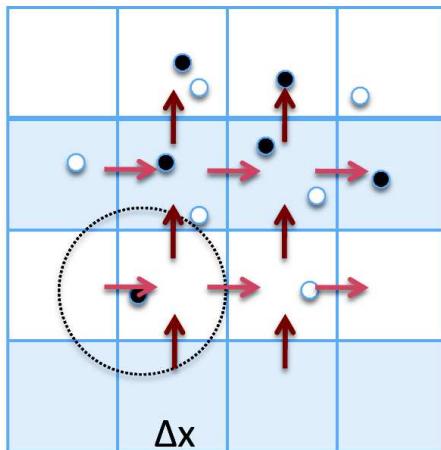
Particle-in-cell (PIC) methods for kinetic plasma simulation

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

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

$$f(\mathbf{x}, \mathbf{v}, t) = f_0 \left(\mathbf{x} - \int_0^t dt \mathbf{v}, \mathbf{v} - \frac{1}{m} \int_0^t dt \mathbf{F} \right) ; \quad \mathbf{x}(t=0) = \mathbf{x}_0 ; \quad \mathbf{v}(t=0) = \mathbf{v}_0$$

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



$$f(\mathbf{x}, \mathbf{v}, t) = \sum_p \delta(\mathbf{x} - \mathbf{x}_p) \delta(\mathbf{v} - \mathbf{v}_p)$$

$$\dot{\mathbf{x}}_p = \mathbf{v}_p$$

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

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0$$

$$-\mu_0 \epsilon_0 \partial_t \mathbf{E} + \nabla \times \mathbf{B} = \mu_0 \mathbf{j}$$

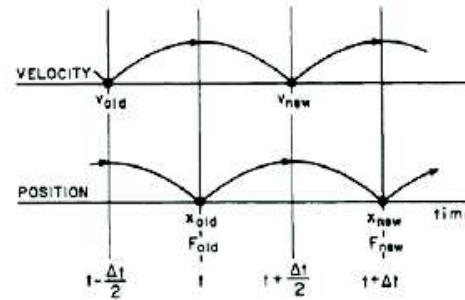
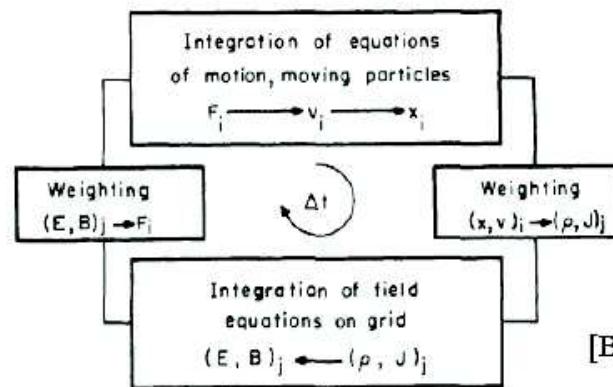
$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{e(n_i - n_e)}{\epsilon_0}$$

$$\delta(\mathbf{x} - \mathbf{x}_p) \longrightarrow S(\mathbf{x} - \mathbf{x}_p) ; \quad E_p = \sum_i E_i S(x_i - x_p) ; \quad j_i = \sum_p j_p S(x_i - x_p)$$

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:



[Birdsall and Langdon, Plasma physics via computer simulation]

- 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

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

Fully implicit PIC formulation

- A **fully implicit formulation** couples particles and fields non-trivially (integro-differential PDE):

$$\frac{f^{n+1} - f^n}{\Delta t} + \mathbf{v} \cdot \nabla \frac{f^{n+1} + f^n}{2} - \frac{q}{m} \nabla \frac{\Phi^{n+1} + \Phi^n}{2} \cdot \nabla_{\mathbf{v}} \frac{f^{n+1} + f^n}{2} = 0$$
$$\nabla^2 \Phi^{n+1} = \int d\mathbf{v} f^{n+1}(\mathbf{x}, \mathbf{v}, t)$$

- In PIC, f^{n+1} is sampled by a large collection of particles in phase space, $\{\mathbf{x}, \mathbf{v}\}_p^{n+1}$.
 - ⇒ 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:

$$\mathbf{G}(\{\mathbf{x}, \mathbf{v}\}_p^{n+1}, \{\Phi^{n+1}\}_g) = 0 \rightarrow \dim(\mathbf{G}) = 2dN_p + N_g \gg N_g$$

- ⇒ 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 $\mathbf{G}(\{x, v\}_p, \{\Phi\}_g) = 0$ 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:

$$x_p^{n+1} = x_p[\Phi^{n+1}] ; v_p^{n+1} = v_p[\Phi^{n+1}]$$

$$\mathbf{G}(\mathbf{x}_p^{n+1}, \mathbf{v}_p^{n+1}, \Phi^{n+1}) = \mathbf{G}(\mathbf{x}[\Phi^{n+1}], \mathbf{v}[\Phi^{n+1}], \Phi^{n+1}) = \tilde{\mathbf{G}}(\Phi^{n+1})$$

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

Field equation: Vlasov-Poisson vs. Vlasov-Ampere

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

Vlasov-Poisson (VP)	Vlasov-Ampère (VA)
$\partial_t f + v \partial_x f + \frac{qE}{m} \partial_v f = 0$ $\partial_x E = \frac{\rho}{\epsilon_0}$ $E = -\partial_x \Phi$	$\partial_t f + v \partial_x f + \frac{qE}{m} \partial_v f = 0$ $\epsilon_0 \partial_t E + j = \langle j \rangle$
Two systems are equivalent in continuum, but not in the discrete.	
<ul style="list-style-type: none"> ► Conventionally used in explicit PIC. ► Exact <i>local</i> charge conservation. ► Exact <i>global</i> momentum conservation. ► Unstable with orbit averaging in implicit context [Cohen and Freis, 1982]. 	<ul style="list-style-type: none"> ► Exact <i>local</i> charge conservation. ► Exact <i>global</i> energy conservation. ► Suitable for orbit averaging. ► Can be extended to electromagnetic system.

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

Energy-conserving (EC) Vlasov-Ampère discretization

- Fully implicit Crank-Nicolson time discretization:

$$\varepsilon_0 \frac{E_i^{n+1} - E_i^n}{\Delta t} + \sum_p q_p v_p^{n+1/2} S(x_i - x_p^{n+1/2}) = 0$$

$$\frac{x_p^{n+1} - x_p^n}{\Delta t} = \frac{v_p^{n+1} + v_p^n}{2}$$

$$\frac{v_p^{n+1} - v_p^n}{\Delta t} = \frac{q_p}{m_p} \sum_i \frac{E_i^n + E_i^{n+1}}{2} S(x_i - x_p^{n+1/2})$$

In time:

centered, 2nd order;
implicit;
unconditionally stable;
non-dissipative.

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

$$\sum_p \frac{m_p}{2} (v_p^{n+1} + v_p^n) (v_p^{n+1} - v_p^n) = - \sum_i \varepsilon_0 \frac{E_i^{n+1} - E_i^n}{\Delta t} \frac{E_i^{n+1} + E_i^n}{2} \Rightarrow \sum_p \frac{1}{2} m_p v_p^2 + \sum_i \frac{1}{2} \varepsilon_0 E_i^2 = \text{const}$$

- As a result, the formulation does not suffer from finite-grid instabilities (normal mode analysis)
 - ⇒ Unconstrained spatial resolution: $\Delta x \not\propto \lambda_D$!!
- Energy conservation is only realized when particles and fields are nonlinearly converged:
 - ⇒ Requires a tight nonlinear tolerance

Jacobian-Free Newton-Krylov Methods

- After spatial and temporal discretization \Rightarrow a large set of nonlinear equations:
- 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):

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

- ☞ 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

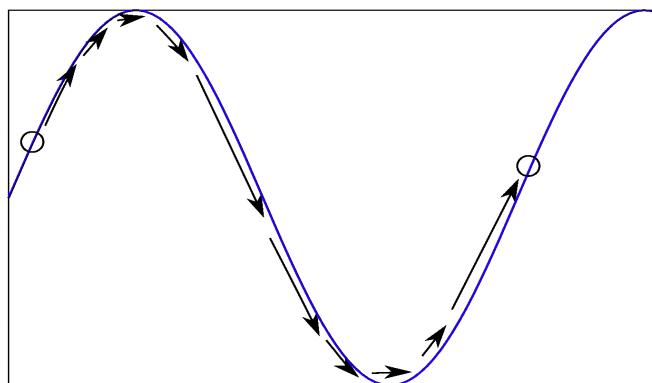
- The **nonlinear residual formulation** $\mathbf{G}(E^{n+1})$ based on Vlasov-Ampere formulation is as follows:
 1. Input E (given by JFNK iterative method)
 2. **Move particles** (i.e., find $x_p[E]$, $v_p[E]$ by solving equations of motion)
 - (a) Requires inner (local) nonlinear iteration: Picard (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 (Δt)** and **orbit time-scale ($\Delta\tau$)** can be well separated
 - ➡ Fields evolve *slowly* (dynamical time scale, Δt)
 - ➡ 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



$$\frac{x_p^{\nu+1} - x_p^\nu}{\Delta\tau} = v_p^{\nu+1/2}$$
$$\frac{v_p^{\nu+1} - v_p^\nu}{\Delta\tau} = \sum_i \underbrace{\frac{E_i^{n+1} + E_i^n}{2}}_{\text{slow}} S(x_i - x_p^{\nu+1/2})$$

Energy conservation and orbit averaging

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

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

- Orbit-averaged current is found as:

$$\bar{j} = \frac{1}{\Delta t} \int_t^{t+\Delta t} d\tau j \approx \frac{1}{\Delta t} \sum_p \sum_{\nu=1}^{N_\nu} q_p v_p S(x - x_p) \Delta \tau^\nu$$

- With these definitions, exact energy conservation is recovered:

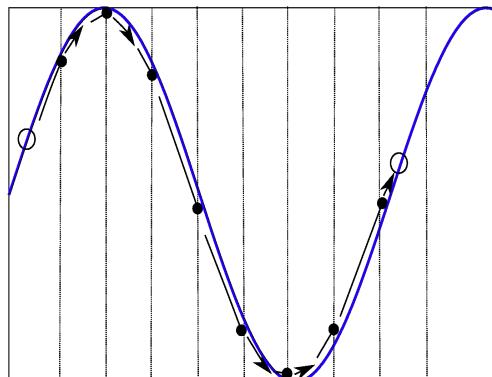
$$\sum_p \sum_{\nu} \frac{m_p}{2} (v_p^{\nu+1} + v_p^{\nu}) (v_p^{\nu+1} - v_p^{\nu}) = - \sum_i \epsilon_0 \frac{E^{n+1} - E^n}{\Delta t} \frac{E_i^{n+1} + E_i^n}{2}$$

$$\Rightarrow \sum_p \frac{1}{2} m_p v_p^2 + \sum_i \frac{1}{2} \epsilon_0 E_i^2 = \text{const.}$$

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, $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$ [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.

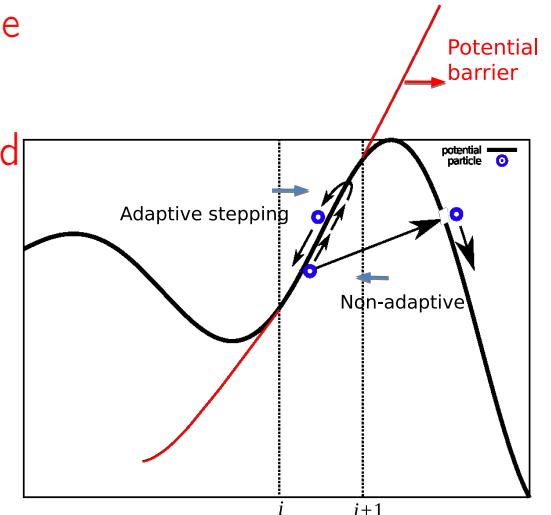


$$\left. \begin{aligned} \rho_{i+\frac{1}{2}} &= \sum_p q_p \frac{S_m(x - x_{i+\frac{1}{2}})}{\Delta x} \\ j_i &= \sum_p q_p v_p \frac{S_{m-1}(x - x_i)}{\Delta x} \\ S'_m(x) &= \frac{S_{m-1}(x + \frac{\Delta x}{2}) - S_{m-1}(x - \frac{\Delta x}{2})}{\Delta x} \end{aligned} \right\} \stackrel{(m=1,2)}{\implies} [\partial_t \rho + \nabla \cdot \mathbf{j} = 0]_{i+\frac{1}{2}}^{n+\frac{1}{2}} = 0$$

Momentum conservation: adaptive orbit integrator

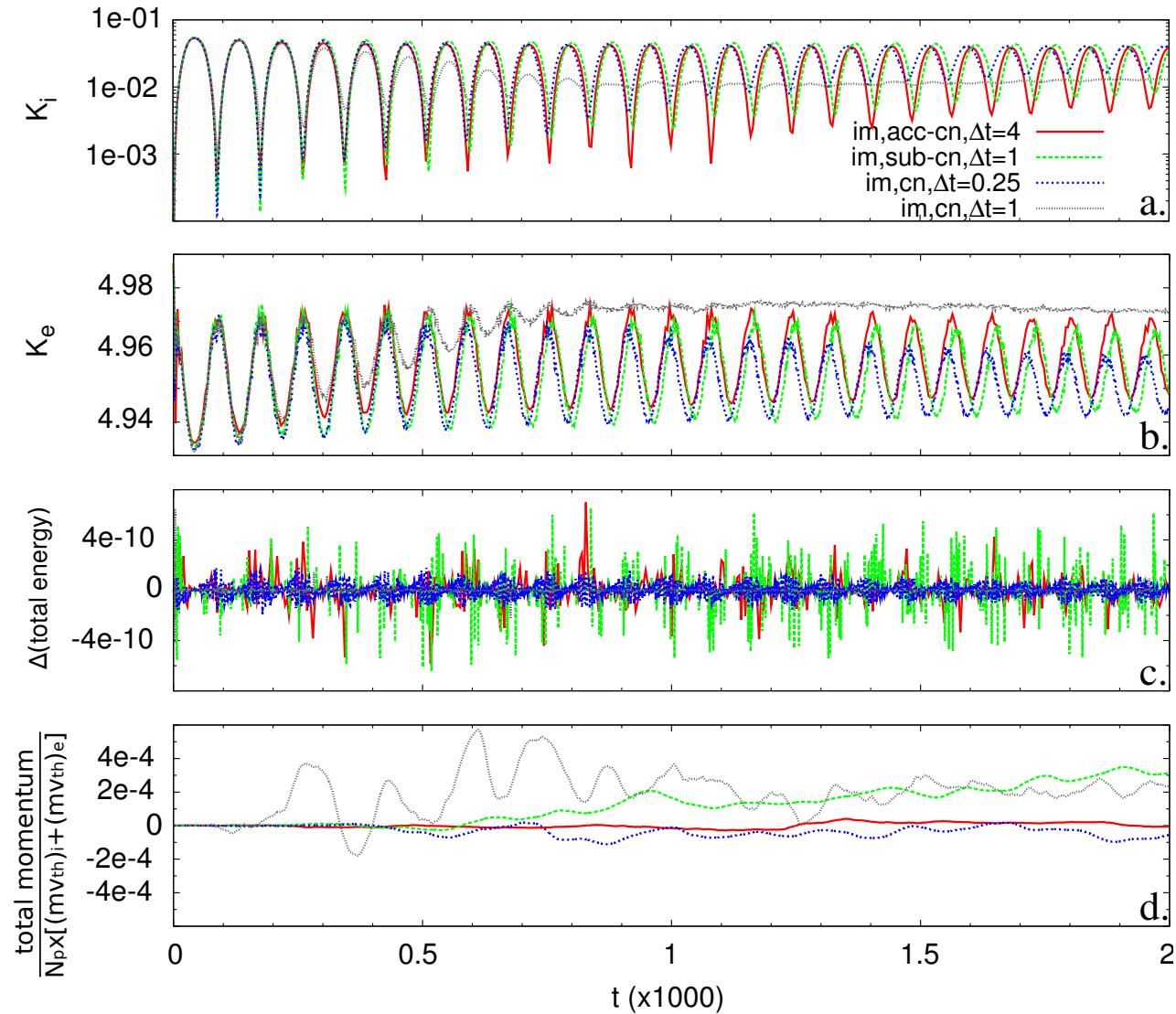
- EC/CC PIC algorithm does not enforce momentum conservation exactly.
 - ➥ **Controlling error** in momentum conservation is **crucial** for long-term accuracy
- Orbit integration errors can significantly affect momentum conservation: **particle tunneling**
- Adaptive orbit integration can be **effective** in suppressing particle tunneling and thus improve momentum conservation
- **Approach:** find $\Delta\tau$ to control local truncation error. Second order estimator gives:

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

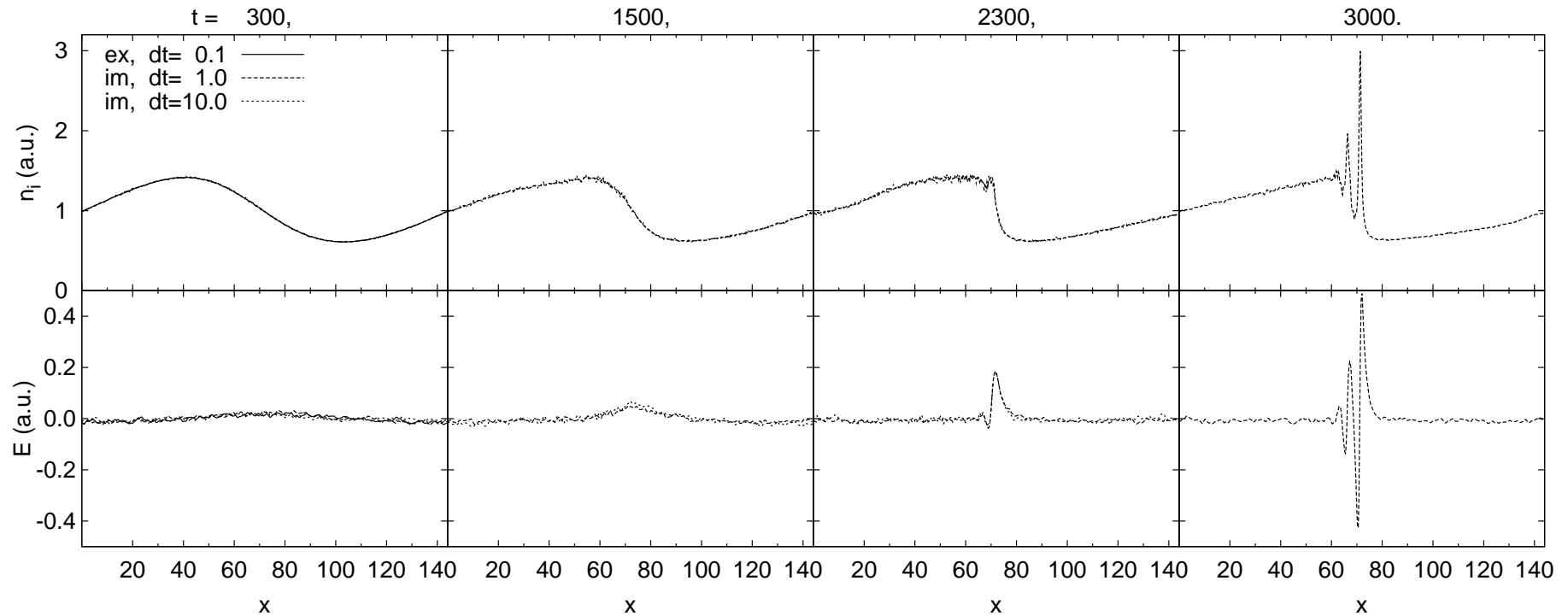


- Electric field gradient is estimated from **cell-based gradient**: $\frac{\partial E}{\partial x} \Big|_p \approx \frac{E_{i+1} - E_i}{\Delta x}$. **Provides potential barrier!**
- Particle is stopped at **cell boundaries** to ensure charge conservation.

Ion acoustic wave (IAW): accuracy impact of different EC movers



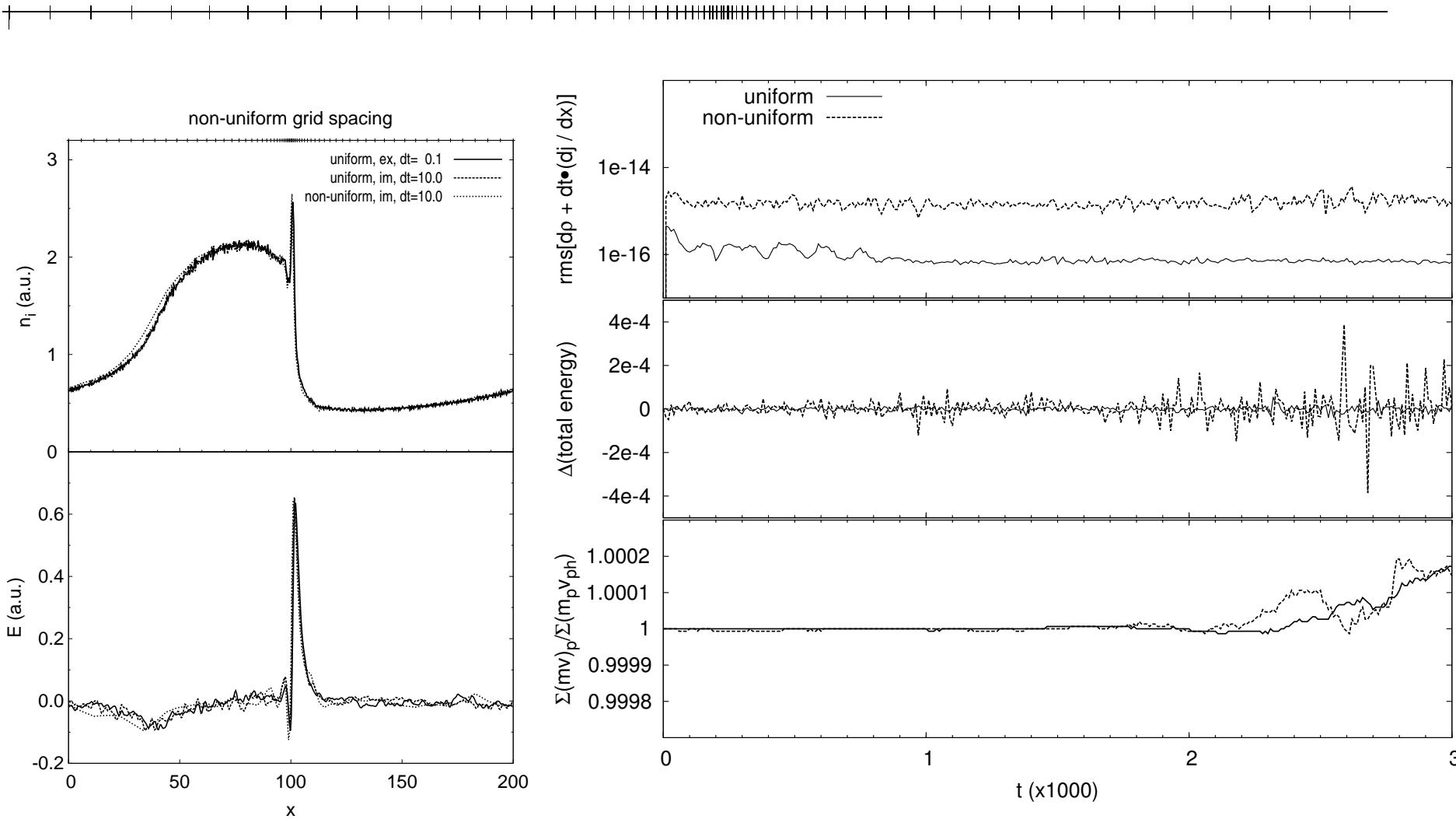
Ion acoustic shock wave



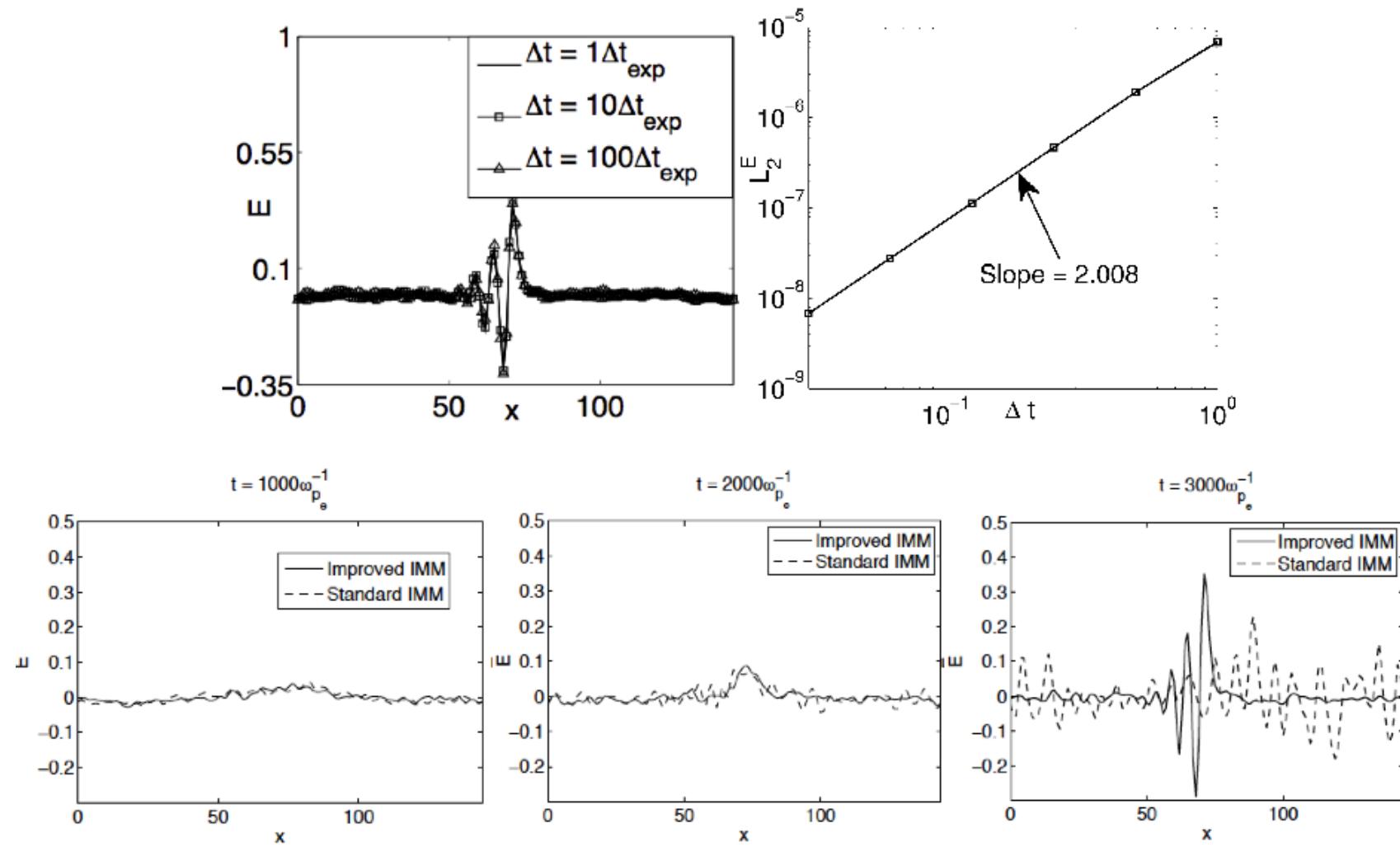
- Propagating IAW with perturbation level $\epsilon = 0.4$, with 4000 particles/cell.
- Realistic mass ratio ($m_i/m_e = 2000$).
- Shock wave length scale \sim Debye length.

Ion acoustic shock wave test

non-uniform grid spacing



Comparison against Implicit Moment Method¹



¹Taitano et al., *S/SC*, accepted (2013)

Moment-based acceleration for fully implicit PIC

CPU gain potential of implicit PIC vs. explicit PIC

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

$$CPU \sim \left(\frac{T}{\Delta t} \right) \left(\frac{L}{\Delta x} \right)^d n_p C^{solver} ; \quad \frac{C^{imp}}{C^{ex}} \sim N_{FE} \frac{\Delta t_{imp}}{\Delta \tau_{imp}} ; \quad \frac{CPU_{ex}}{CPU_{imp}} \sim \left(\frac{\Delta x_{imp}}{\Delta x_{ex}} \right)^d \frac{\Delta \tau_{imp}}{\Delta t_{ex}} \frac{1}{N_{FE}}$$

- Using reasonable estimates:

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

$$\Delta t_{imp} \sim 0.1 \omega_{pi}^{-1}$$

$$\Delta t_{exp} \sim 0.1 \omega_{pe}^{-1}$$

$$k \Delta x_{imp} \sim 0.2$$

$$\Delta x_{ex} \sim \lambda_D$$

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

- CPU speedup is:

- ☞ Independent of time step!
- ☞ Better for realistic mass ratios!
- ☞ Limited by solver performance N_{FE} (preconditioning!)

Moment-based acceleration of fully kinetic simulations

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

$$\delta E \approx -P^{-1}\mathbf{G}$$

Premise of acceleration: obtain δE from a fluid model using current particle distribution for closure.

- We begin with corresponding fluid nonlinear model:

$$\begin{aligned}\partial_t n_\alpha &= -\nabla \cdot \boldsymbol{\Gamma}_\alpha \\ m_\alpha \left[\partial_t \boldsymbol{\Gamma}_\alpha + \nabla \cdot \left(\frac{1}{n_\alpha} \boldsymbol{\Gamma}_\alpha \boldsymbol{\Gamma}_\alpha \right) \right] &= q_\alpha n_\alpha \mathbf{E} + \nabla \cdot \left(n_\alpha \left(\frac{\boldsymbol{\Pi}_\alpha}{n_\alpha} \right)_p \right) \\ \epsilon_0 \partial_t \mathbf{E} &= \sum_\alpha q_\alpha \boldsymbol{\Gamma}_\alpha\end{aligned}$$

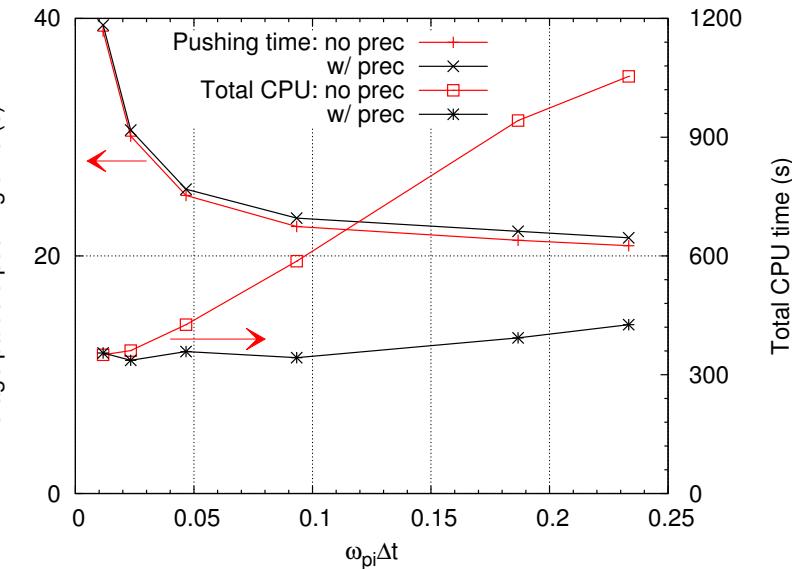
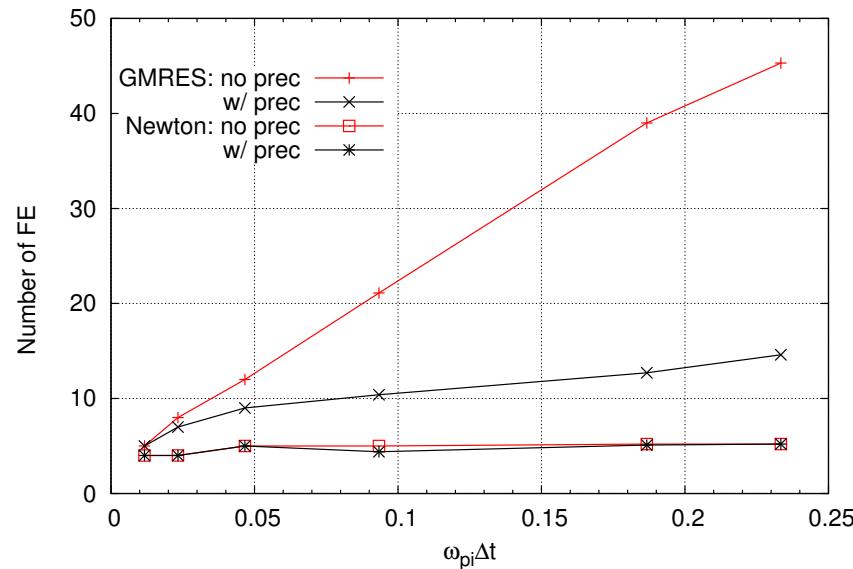
Moment-based acceleration of fully kinetic simulations (cont.)

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

$$\begin{aligned}\frac{\delta n_\alpha}{\Delta t} &= -\nabla \cdot \delta \Gamma_\alpha \\ m_\alpha \frac{\delta \Gamma_\alpha}{\Delta t} &\approx q_\alpha (\delta n_\alpha \mathbf{E} + n_{\alpha,p} \delta \mathbf{E}) + \nabla \cdot \left(\left(\frac{\mathbf{\Pi}_\alpha}{n_\alpha} \right)_p \delta n_\alpha \right) \\ \epsilon_0 \delta \mathbf{E} &= \Delta t \left[\sum_\alpha q_\alpha \delta \Gamma_\alpha - \mathbf{G}(\mathbf{E}) \right]\end{aligned}$$

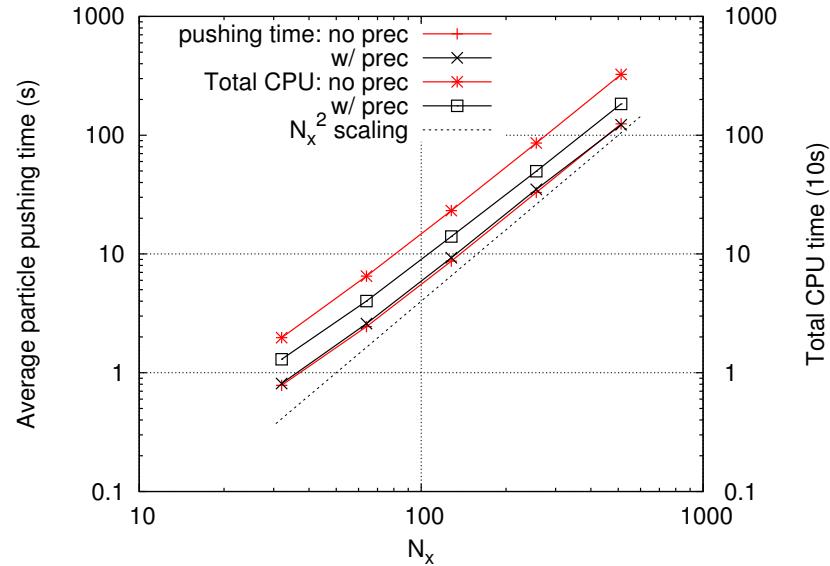
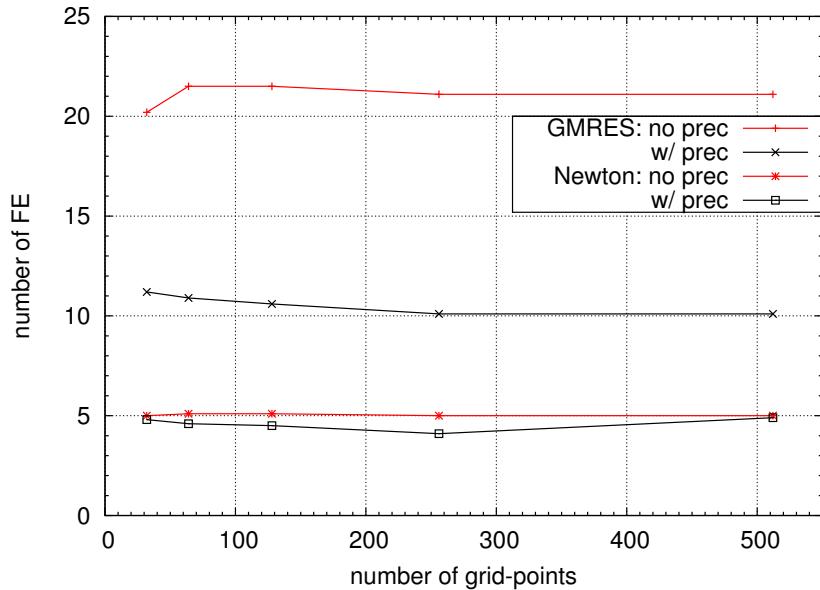
$\delta \mathbf{E}$ can be obtained from Newton state \mathbf{E} , Newton residual $\mathbf{G}(\mathbf{E})$, and particle closures $\mathbf{\Pi}_{\alpha,p}$ and $n_{\alpha,p}$

Preconditioner performance with Δt



- Number of FE remains constant with Δt (preconditioning)
- Overall CPU time of algorithm is independent of Δt (as predicted!)

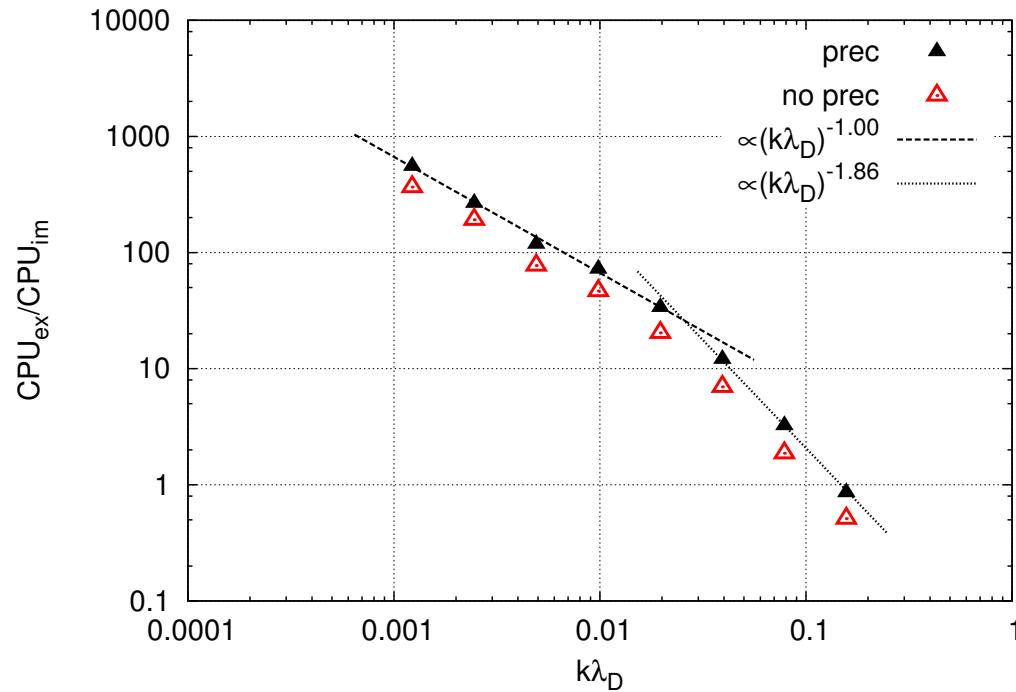
Preconditioner performance with N_x



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

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 analytically remove light-wave in non-relativistic plasma simulations *while preserving charge separation effects*
- If one keeps light wave with exact energy conservation in non-relativistic setting, one gets enhanced **numerical noise due to numerical Cherenkov radiation**

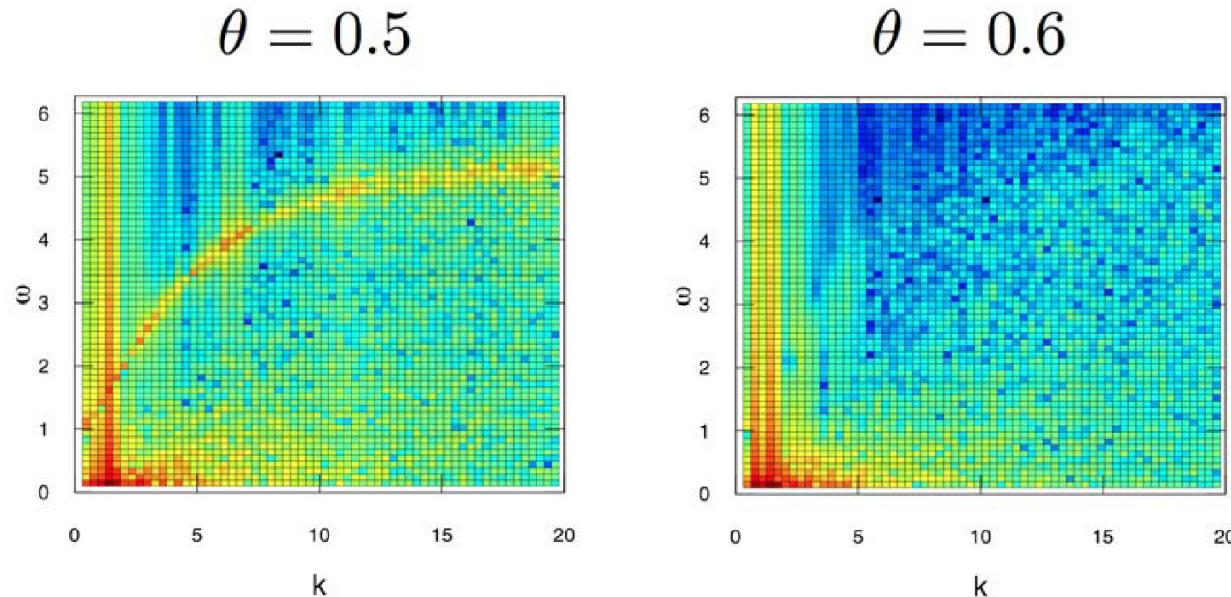


Figure 1: Fourier phase space for exactly energy conserving PIC (left) and dissipative PIC (right) [Markidis and Lapenta, JCP 2011].

Darwin model (potential form)

- We consider potentials ϕ, \mathbf{A} in the Coulomb gauge ($\nabla \cdot \mathbf{A} = 0$) such that:

$$\begin{aligned}\mathbf{B} &= \nabla \times \mathbf{A}, \\ \mathbf{E} &= -\nabla\phi - \partial_t \mathbf{A}.\end{aligned}$$

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

$$\begin{aligned}\nabla^2\chi &= \nabla \cdot \mathbf{j}, \\ -\nabla^2\mathbf{A} &= \mu_0 [\mathbf{j} - \nabla\chi], \\ \chi &= \epsilon_0\partial_t\phi.\end{aligned}$$

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

► In 1D:

$$\begin{aligned}\epsilon_0\partial_t E_x + \mathbf{j}_x &= \langle j_x \rangle, & E_{y,i}^{n+1/2} &= -\frac{A_{y,i}^{n+1} - A_{y,i}^n}{\Delta t}, \\ \frac{1}{\mu_0}\partial_x^2 A_y + \mathbf{j}_y &= \langle j_y \rangle, & E_{z,i}^{n+1/2} &= -\frac{A_{z,i}^{n+1} - A_{z,i}^n}{\Delta t}. \\ \frac{1}{\mu_0}\partial_x^2 A_z + \mathbf{j}_z &= \langle j_z \rangle.\end{aligned}$$

Implicit EM particle mover

- Subcycled particle equations of motion:

$$\begin{aligned}\frac{x_p^{\nu+1} - x_p^{\nu}}{\Delta\tau^{\nu}} &= v_x^{\nu+1/2}, \\ \frac{\mathbf{v}_p^{\nu+1} - \mathbf{v}_p^{\nu}}{\Delta\tau^{\nu}} &= \frac{q_p}{m_p} \left(\mathbf{E}_p^{\nu+1/2}(x_p^{\nu+1/2}) + \mathbf{v}_p^{\nu+1/2} \times \mathbf{B}_p^{\nu+1/2}(x_p^{\nu+1/2}) \right).\end{aligned}$$

- Implicit Boris update (analytical inversion):

$$\begin{aligned}\hat{\mathbf{v}}_p &= \mathbf{v}_p^{\nu} + \alpha \mathbf{E}_p^{\nu+1/2}, \quad \alpha = \frac{q_p \Delta\tau^{\nu}}{m_p 2} \\ \mathbf{v}_p^{\nu+1/2} &= \frac{\hat{\mathbf{v}}_p + \alpha \left[\hat{\mathbf{v}}_p \times \mathbf{B}_p^{\nu+1/2} + \alpha (\hat{\mathbf{v}}_p \cdot \mathbf{B}_p^{\nu+1/2}) \mathbf{B}_p^{\nu+1/2} \right]}{1 + (\alpha B_p)^2}.\end{aligned}$$

- Final particle position and velocity are found from:

$$\begin{aligned}x_p^{\nu+1} &= x_p^{\nu} + \Delta\tau^{\nu} \mathbf{v}_{x,p}^{\nu+1/2}, \\ \mathbf{v}_p^{\nu+1} &= 2\mathbf{v}_p^{\nu+1/2} - \mathbf{v}_p^{\nu}.\end{aligned}$$

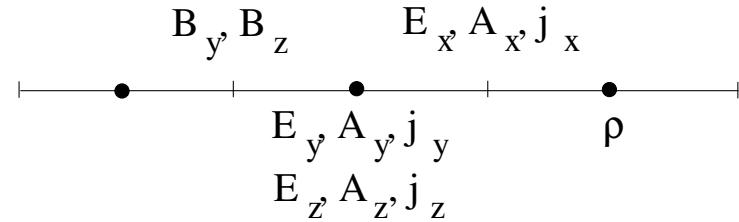
Energy conserving discrete 1D Darwin model

► Field equations:

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

$$\frac{1}{\mu_0} \partial_x^2 \frac{A_y^{n+1} + A_y^n}{2} \bigg|_i + \bar{j}_{y,i}^{n+1/2} = \langle j_y \rangle,$$

$$\frac{1}{\mu_0} \partial_x^2 \frac{A_z^{n+1} + A_z^n}{2} \bigg|_i + \bar{j}_{z,i}^{n+1/2} = \langle j_z \rangle$$



► Current gather (with orbit averaging):

$$\bar{j}_{x,i+1/2}^{n+1/2} = \frac{1}{\Delta t \Delta x} \sum_p \sum_\nu q_p v_{p,x}^{\nu+1/2} S_m(x_p^{\nu+1/2} - x_{i+1/2}) \Delta \tau^\nu,$$

$$\bar{j}_{y,i}^{n+1/2} = \frac{1}{\Delta t \Delta x} \sum_p \sum_\nu q_p v_{p,y}^{\nu+1/2} S_l(x_p^{\nu+1/2} - x_i) \Delta \tau^\nu,$$

$$\bar{j}_{z,i}^{n+1/2} = \frac{1}{\Delta t \Delta x} \sum_p \sum_\nu q_p v_{p,z}^{\nu+1/2} S_l(x_p^{\nu+1/2} - x_i) \Delta \tau^\nu,$$

Field scatter to particles (with orbit averaging)

► Electric field scatter:

$$E_{x,p}^{\nu+1/2} = \sum_i \frac{E_{x,i+1/2}^{n+1} + E_{x,i+1/2}^n}{2} S_m(x_p^{\nu+1/2} - x_{i+1/2}),$$

$$E_{y,p}^{\nu+1/2} = - \sum_i \frac{A_{y,i}^{n+1} - A_{y,i}^n}{\Delta t} S_l(x_p^{\nu+1/2} - x_i),$$

$$E_{z,p}^{\nu+1/2} = - \sum_i \frac{A_{z,i}^{n+1} - A_{z,i}^n}{\Delta t} S_l(x_p^{\nu+1/2} - x_i).$$

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

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

$$B_{y,p}^{\nu+1/2} = - \sum_i \frac{A_{z,i+1}^{\nu+1/2} - A_{z,i}^{\nu+1/2}}{\Delta x} S_{l-1}(x_{i+1/2} - x_p^{\nu+1/2}) - \boxed{\sum_i \frac{\Delta A_{z,i-1}^\nu - 2\Delta A_{z,i}^\nu + \Delta A_{z,i+1}^\nu}{8} (x_p^{\nu+1} - x_p^\nu)},$$

$$B_{z,p}^{\nu+1/2} = \sum_i \frac{A_{y,i+1}^{\nu+1/2} - A_{y,i}^{\nu+1/2}}{\Delta x} S_{l-1}(x_{i+1/2} - x_p^{\nu+1/2}) + \boxed{\sum_i \frac{\Delta A_{y,i-1}^\nu - 2\Delta A_{y,i}^\nu + \Delta A_{y,i+1}^\nu}{8} (x_p^{\nu+1} - x_p^\nu)}.$$

$\mathcal{O}(\Delta \tau^\nu \Delta x)^2$

Energy conservation in Darwin

$$\begin{aligned}\frac{K_p^{n+1} - K_p^n}{\Delta t} &= \frac{1}{\Delta t} \sum_p m_p \sum_{\nu} \Delta \tau^{\nu} \frac{\mathbf{v}_p^{\nu+1} + \mathbf{v}_p^{\nu}}{2} \cdot \frac{\mathbf{v}_p^{\nu+1} - \mathbf{v}_p^{\nu}}{\Delta \tau^{\nu}} = \frac{1}{\Delta t} \sum_{p,\nu} q_p \Delta \tau^{\nu} \mathbf{E}_p^{\nu+1/2} \cdot \mathbf{v}_p^{\nu+1/2} \\ &= \sum_i \Delta x \left(\frac{E_{x,i+1/2}^{n+1} + E_{x,i+1/2}^n}{2} j_{x,i+1/2}^{n+1/2} + E_{y,i}^{n+1/2} j_{y,i}^{n+1/2} + E_{z,i}^{n+1/2} j_{z,i}^{n+1/2} \right)\end{aligned}$$

$$\begin{aligned}\sum_i \Delta x \frac{E_{x,i+1/2}^{n+1} + E_{x,i+1/2}^n}{2} j_{x,i+1/2}^{n+1/2} &= -\frac{\epsilon_0}{2\Delta t} \sum_i \Delta x \left(\left(E_{x,i+1/2}^{n+1} \right)^2 - \left(E_{x,i+1/2}^n \right)^2 \right) = -\frac{W_{\phi x}^{n+1} - W_{\phi x}^n}{\Delta t} \\ \sum_i \Delta x E_{y,i}^{n+1/2} j_{y,i}^{n+1/2} &= -\frac{1}{2\mu_0 \Delta t} \sum_i \Delta x \left[\left(\partial_x A_y^{n+1} \right)_{i+1/2}^2 - \left(\partial_x A_y^n \right)_{i+1/2}^2 \right] = -\frac{W_{Bz}^{n+1} - W_{Bz}^n}{\Delta t} \\ \sum_i \Delta x E_{z,i}^{n+1/2} j_{z,i}^{n+1/2} &= -\frac{1}{2\mu_0 \Delta t} \sum_i \Delta x \left[\left(\partial_x A_z^{n+1} \right)_{i+1/2}^2 - \left(\partial_x A_z^n \right)_{i+1/2}^2 \right] = -\frac{W_{By}^{n+1} - W_{By}^n}{\Delta t}\end{aligned}$$

$$(K_p + W_{\phi x} + W_{By} + W_{Bz})^{n+1} = (K_p + W_{\phi x} + W_{By} + W_{Bz})^n$$

CPU speedup potential of EM implicit PIC vs. explicit PIC

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

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

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

$$\Delta t_{exp} \sim \frac{\Delta x_{exp}}{c}$$

$$k\Delta x_{imp} \sim 0.2$$

$$\Delta x_{ex} \sim \lambda_D$$

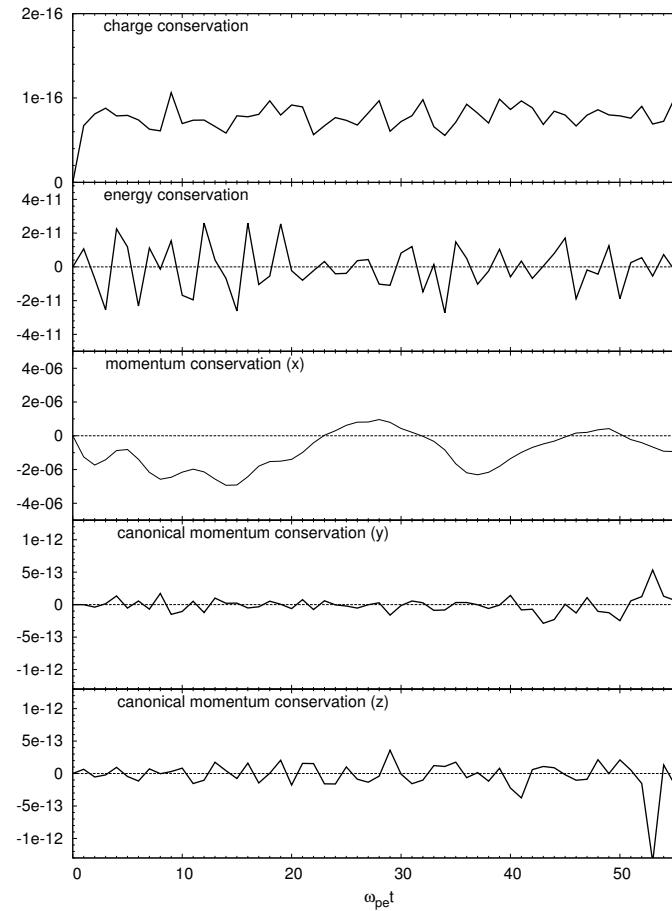
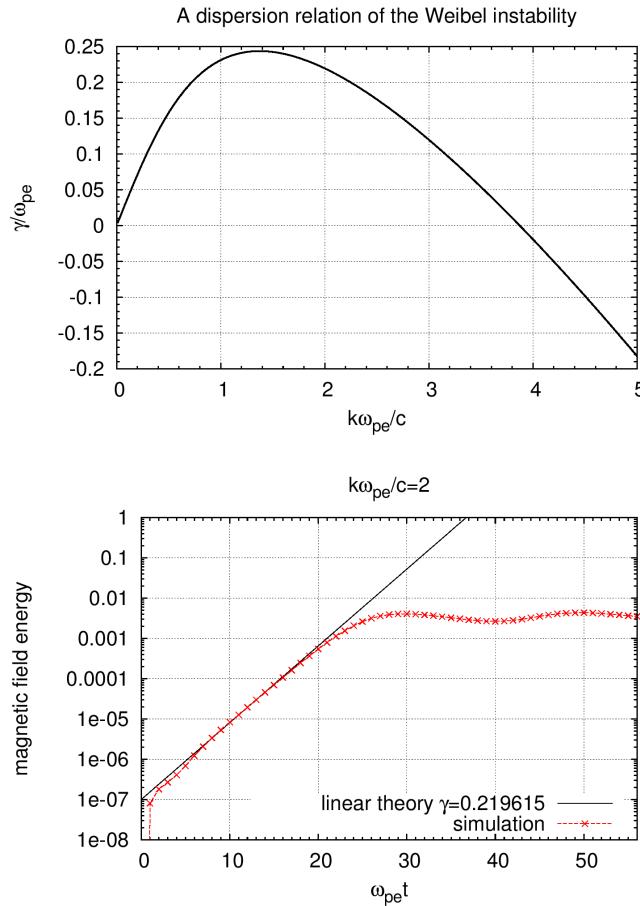
$$\frac{CPU_{ex}}{CPU_{imp}} \sim \frac{\min [1, kd_e]}{(k\lambda_D)^{d+1}} \frac{1}{N_{FE}}$$

- CPU speedup is:
 - ☛ Independent of time step
 - ☛ Impacted by electron scales
- Again, **key is to minimize N_{FE}** .
 - ☛ We are in the process of developing a moment-based preconditioner.

Verification: Electron Weibel instability

- Isotropic ions, bi-Maxwellian electrons

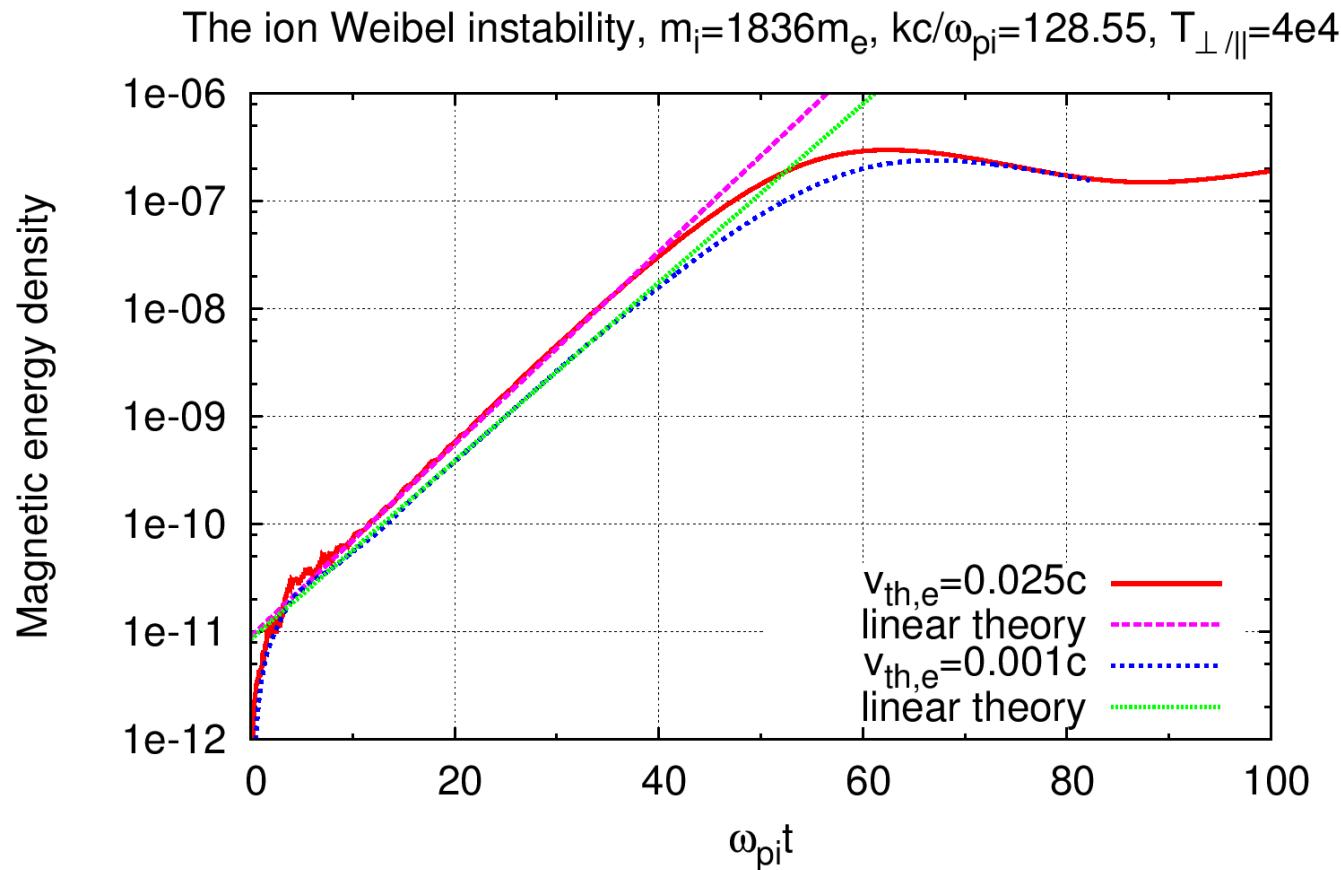
$$m_i/m_e = 1836, T_{e\perp}/T_{e\parallel} = 16, N_{e,i}=128,000, L = 2\pi c/\omega_{pe}, N_g=32.$$



Verification: Ion Weibel instability (large T anisotropy)

- Isotropic electrons, bi-Maxwellian ions

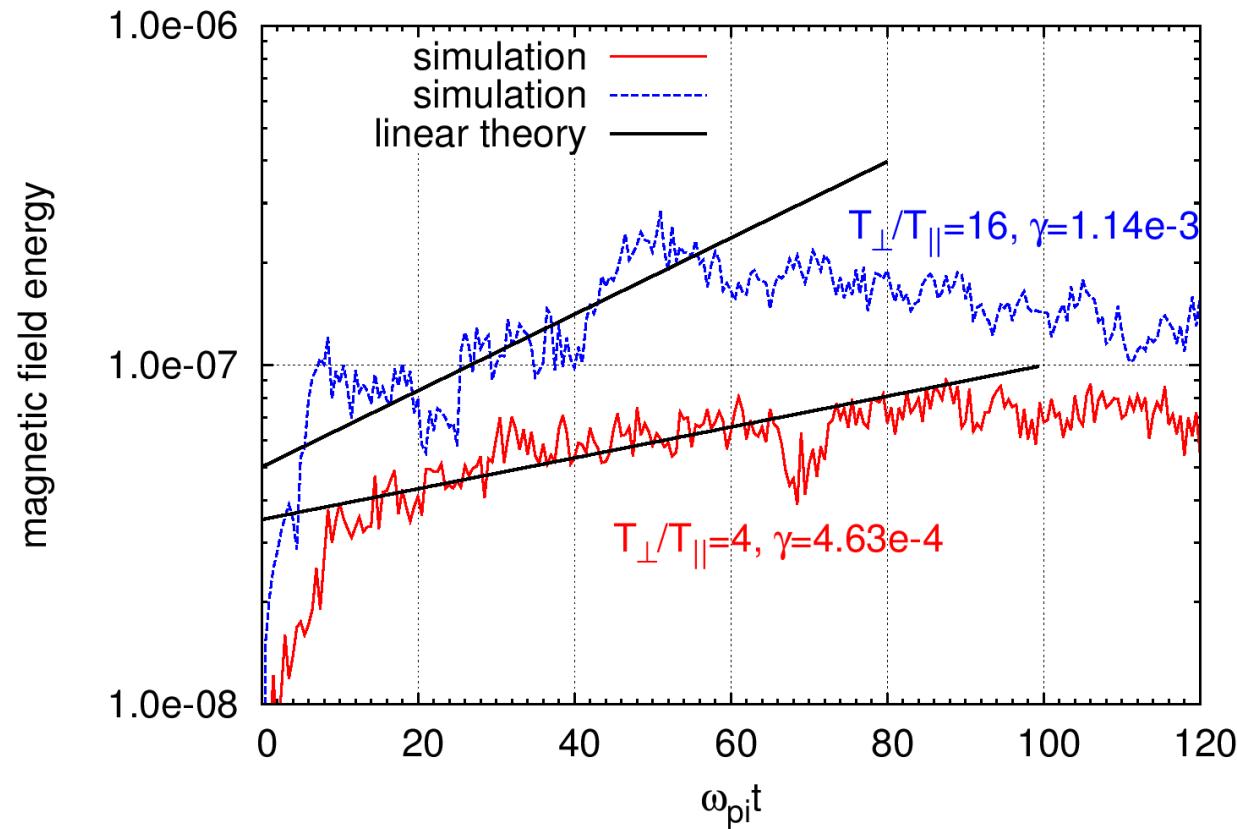
$$m_i/m_e = 1836, T_{i\perp}/T_{i\parallel} = 4 \times 10^4, N_{e,i}=128,000, L = \frac{2}{3}\pi c/\omega_{pe}, N_g=64, \gamma \approx 0.1\omega_{pi}.$$



Verification: Ion Weibel instability (small T anisotropy)

- Isotropic electrons, bi-Maxwellian ions

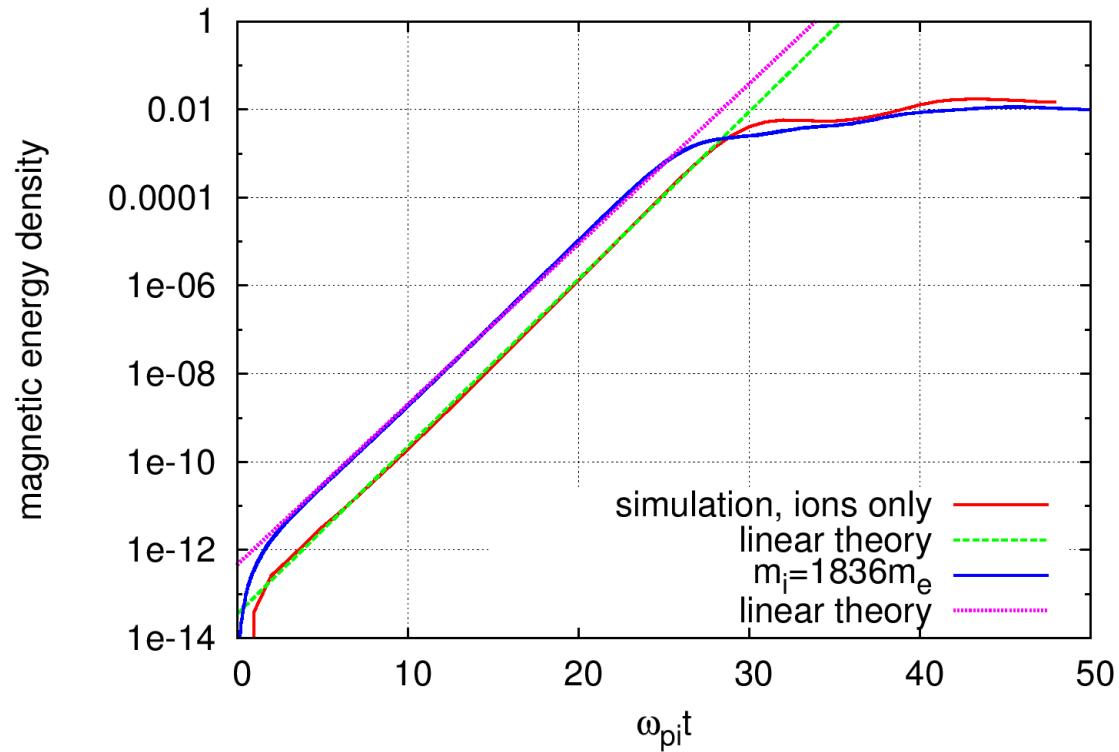
$$m_i/m_e = 128, N_{e,i}=128,000, L = 0.88\pi c/\omega_{pi}, N_g=32$$



Ion cyclotron instability (large T anisotropy)

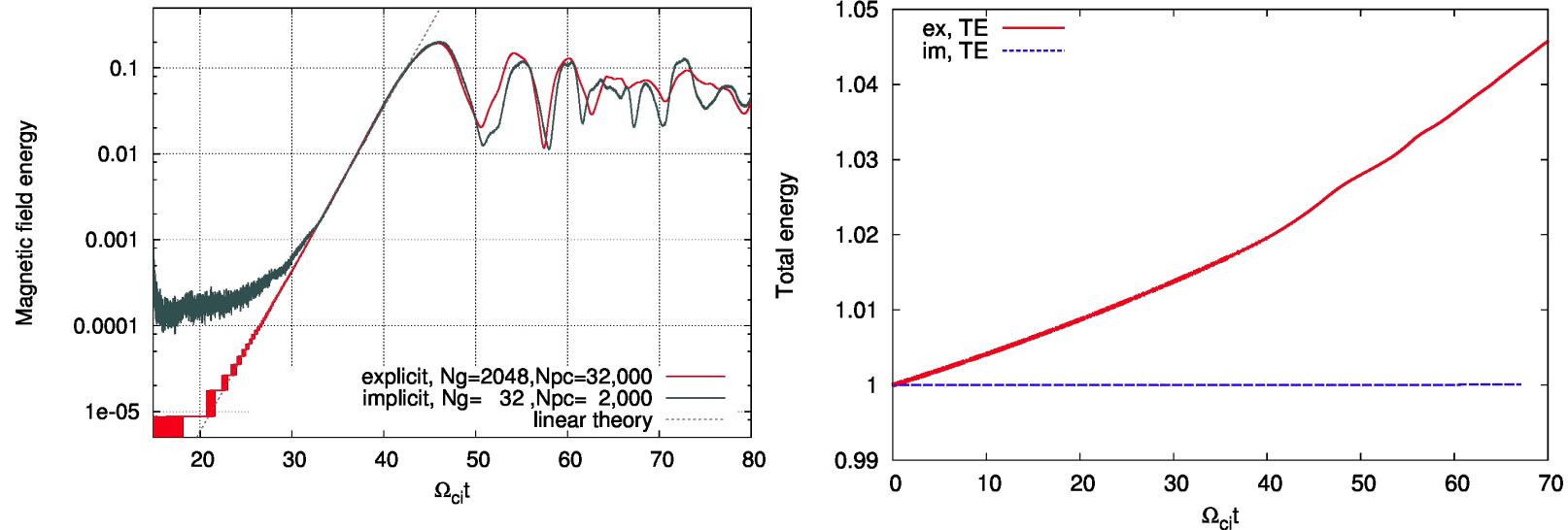
- Isotropic electrons, bi-Maxwellian ions, magnetized ion dynamics ($\beta_{i\perp} = 1$)

$$m_i/m_e = 1836, T_{i\perp}/T_{i\parallel} = 2.5 \times 10^5, N_{e,i} = 128,000, L = \pi c/\omega_{pi}, N_g = 32, \gamma \approx 0.4\omega_{pi}.$$



Paradigm change: 1D Kinetic Alfvén Wave²

$$m_i/m_e = 1836 ; k\lambda_{De} = 0.003 ; v_{th,e}/c = 0.07$$



- **Explicit PIC:**
 - ⇒ 2048 mesh points, 32,000 pcles/cell (overkill for this problem), **0.05 energy error**
 - ⇒ **500 CPUs x 24 hr**, 7×10^6 time steps
- **Implicit PIC:**
 - ⇒ 32 mesh points, 2,000 pcles/cell (1000× fewer particles), 10^{-6} **energy error**
 - ⇒ **16 CPUs x 29 hr**, 1.3×10^5 time steps, $N_{FE} \sim 30$ ($r_{tol} = 10^{-6}$)
- **CPU speedup ~ 26** ($\times 100$ in 2D, $\times 10^4$ in 3D)

²Yin et al., POP 14 (2007)

Summary and conclusions

- We have demonstrated, for the first time, a **fully implicit, fully nonlinear electrostatic 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.
- The approach has been shown to be **free of CFL and finite-grid numerical instabilities**.
- As a result, the **method is able to take time steps many times larger than explicit**, and resolutions many times coarser.
- Central to our implementation is the **concept of particle enslavement**.
- We have generalized formulation to use **spatial adaptivity via mapped coordinates**.
- The method has **much potential for efficiency gains vs. explicit** in long-time-scale applications, with the CPU speedup scaling as $(k\lambda_D)^{-(d+1)}/N_{FE}$.
 - ⇒ Minimize the number of nonlinear function evaluations N_{FE} for given Δt , $\Delta x \Rightarrow$ preconditioning!
 - ⇒ We have formulated and implemented a **very efficient moment-based preconditioner**.
- We have **ported the algorithm to GPU architectures** (not shown)
- We have **generalized the algorithm to non-radiative electromagnetic regimes** (Darwin model), where, **in addition to charge and energy, we also conserve canonical momenta**.