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# Implicit particle-in-cell methods


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# Outline

- Particle methods for plasma simulation (PIC)
  - explicit time differencing
  - implicit time differencing
- Our approach: energy and charge-conserving implicit **electrostatic** PIC
  - "Direct" implicit Vlasov-Ampere formulation
  - Exact energy-conserving formulation
  - Exact charge-conserving particle mover
  - Momentum conservation error control: orbit adaptivity
- Preconditioning: "Moment"-based acceleration
- Generalization to **electromagnetic** PIC: Darwin model

# Introduction



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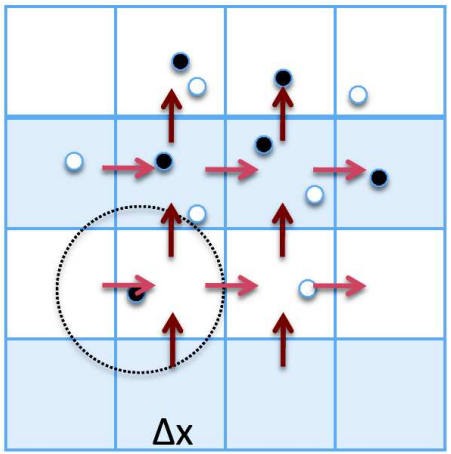
# Particle-in-cell (PIC) methods for kinetic plasma simulation

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

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

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

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




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

$$\begin{aligned}\dot{\mathbf{x}}_p &= \mathbf{v}_p\\ \dot{\mathbf{v}}_p &= \frac{q_p}{m_p}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\end{aligned}$$

$$\begin{aligned}\partial_t\mathbf{B} + \nabla\times\mathbf{E} &= 0\\ -\mu_0\epsilon_0\partial_t\mathbf{E} + \nabla\times\mathbf{B} &= \mu_0\mathbf{j}\\ \nabla\cdot\mathbf{B} &= 0\\ \nabla\cdot\mathbf{E} &= \frac{e(n_i-n_e)}{\epsilon_0}\end{aligned}$$

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

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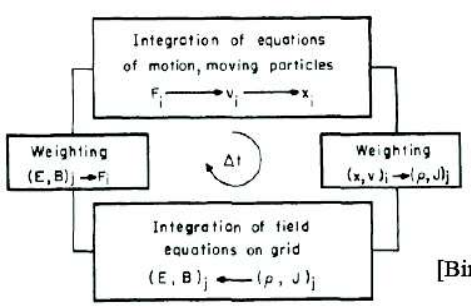
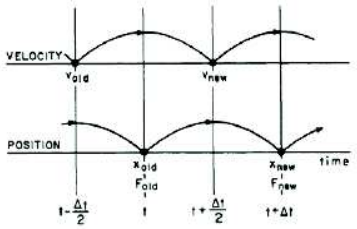
# State-of-the-art *classical* PIC algorithm is explicit[1] [2]

- Classical explicit PIC approach "leap-frog"s particle positions and velocities:

$$\frac{x_p^{n+1}-x_p^n}{\Delta t} = v_p^{n+1/2} \rightarrow \triangle\phi^{n+1} = -\sum_p q_p S(x_p^{n+1}-x)/\Delta x \rightarrow \frac{v_p^{n+3/2}-v_p^{n+1/2}}{\Delta t} = a_p^{n+1}$$




[Birdsall and Langdon, Plasma physics via computer simulation]

- Limitations:
  - $\Delta x < \lambda_{Debye}$ (finite-grid instability), $\omega_{pe}\Delta t < 1$ or $c\Delta t < \Delta x$ (CFL-type instability).
  - Cannot be used in Darwin model (which eliminates light waves).
  - No discrete energy conservation.
  - Discrete momentum conservation can only be realized in electrostatic case on a uniform grid.
- As a result, explicit schemes are not well suited for long-term system-scale simulations, even with super-computers.

---

[1] C.K. Birdsall, A.B. Langdon, Plasma Physics via Computer Simulation, McGraw-Hill, New York, 2005.

[2] R.W. Hockney, J.W. Eastwood, Computer Simulation Using Particles, Taylor & Francis Inc., Bristol, UK, 1988.

# What about implicit PIC?

- Implicit PIC holds the promise of overcoming the difficulties and inefficiencies of explicit methods for long-term system-scale simulations
- Exploration of implicit PIC started in the 1980s
  - Moment implicit method [3] [4]
  - Direct implicit method [5]
- Early approaches used linearized, semi-implicit formulations:
  - Lack of nonlinear convergence
  - Inconsistencies between particles and moments
  - Inaccuracies! $\rightarrow$Plasma self-heating/cooling [6]

[3] Mason, R. J. (1981)
[4] Brackbill, J. U., and Forslund, D. W. (1982)
[5] Friedman, A., Langdon, A. B. and Cohen, B. I.(1981)
[6] Cohen, B. I., Langdon, A. B., Hewett, D. W., and Procassini, R. J. (1989)

# Our approach to implicit PIC

Electrostatic example:

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

$$\frac{v_p^{n+1} - v_p^n}{\Delta t} = a_p\left(\frac{x_p^{n+1} + x_p^n}{2}\right)$$

$$\triangle \phi^{n+1} = -\sum_p q_p S(x_p^{n+1} - x)/\Delta x$$

Nonlinearly converged, fully implicit PIC algorithm

- Implicit PIC can eliminate CFL-type instability and the finite-grid instability.
- Can conserve total energy and local charge exactly in a discrete setting (crucial for long term accuracy).
- Can be easily extended to electromagnetic model ( Darwin, or Maxwell).

What is the nature of the resulting fully-coupled algebraic system?
Is it practical to invert?

# Jacobian-Free Newton-Krylov Methods[7]

- A large set of nonlinear equations (in the residual form, Newton-Raphson method):

$$A\vec{x}^{n+1} = \vec{b} \Rightarrow \boxed{\vec{G}(\vec{x}^{n+1}) = \vec{0}} \Rightarrow \left.\frac{\partial \vec{G}}{\partial \vec{x}}\right|_k \delta\vec{x}_k = -\vec{G}(\vec{x}_k)$$

- Jacobian $\left(J = \frac{\partial \vec{G}}{\partial \vec{x}}\right)$ linear systems are solved by a *Krylov subspace method (GMRES)*:
  - Only requires matrix-vector products to proceed. Jacobian-vector product can be computed Jacobian-free (CRITICAL):

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

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

$$\left(\frac{\partial \vec{G}}{\partial \vec{x}}\right)_k P_k^{-1}(P_k \delta\vec{x}) = -\vec{G}_k$$

[7] Knoll, D. A., and Keyes, D. E. (2004)

# Particle enslavement (nonlinear elimination)

- Full residual $\mathbf{G}(\{x,v\}_p,\{\Phi\}_g)=0$ is impractical by GMRES method (too much memory requirement for $\vec{x}=K\vec{a}$ where $K=span\{\vec{b},A\vec{b},A^2\vec{b}...\}$ and $\vec{a}$ is some appropriate vector).
- Alternative: nonlinearly eliminate particle quantities **(from dependent variables)**:
  - Formally, particle equations of motion are functionals of the electrostatic potential:

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

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

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

- JFNK storage requirements are dramatically decreased, making it tractable:
  - 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
- Moment preconditioning becomes suitable.



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# Fully implicit electrostatic PIC

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# Energy-conserving *Vlasov-Ampère* (1D) formulation

- A time-centered, fully implicit discretization:

$$\varepsilon_0 \frac{E_i^{n+1} - E_i^n}{\Delta t} + j_i^{n+1/2} - \langle j \rangle = 0;$$

$$\frac{x_p^{n+1} - x_p^n}{\Delta t} - v_p^{n+1/2} = 0;$$

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

$$j_i^{n+1/2} = \sum_p q_p v_p^{n+1/2} S(x_p^{n+1/2} - x_i).$$

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

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

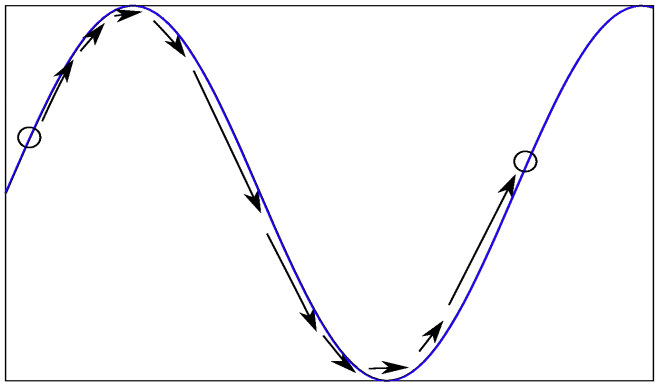
  - Does not suffer from finite-grid instabilities: $\Delta x \not< \lambda_D$ !!
  - Requires that particles and fields are nonlinearly converged.

# Particle orbit integration: a multi-scale problem

- 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, $\Delta t = t^{n+1} - t^n$)
  - Particle orbits may still undergo *rapid change* (Lagrangian time scale $\Delta\tau = t^{\nu+1} - t^{\nu} \leq \Delta t$)
- Particle orbits need to be resolved to **avoid large orbit integration errors**[8]

> Particle sub-stepping is necessary for orbit integration, and can be easily implemented in implicit PIC.

- Field does not change appreciably in $\Delta t$: time-averaged value over long time scale is sufficient



$$\frac{x_p^{\nu+1} - x_p^{\nu}}{\Delta\tau^{\nu}} = \frac{v_p^{\nu+1} + v_p^{\nu}}{2}$$

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

$$\Delta t = \sum \Delta\tau^{\nu}$$

[8] Parker, S. E., Friedman, A., Ray, S. L., and Birdsall, C. K. (1993)

# Energy conservation with orbit averaging

- Orbit averaging Ampère's law[9]:

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

- Orbit-averaged current is found as:

$$\bar{j} = \frac{1}{\Delta t}\int_t^{t+\Delta t} d\tau\, j \approx \frac{1}{\Delta t}\sum_p \sum_{\nu=1}^{N_\nu} q_p v_p^{\nu+1/2} S(x - x_p)\Delta\tau^\nu$$

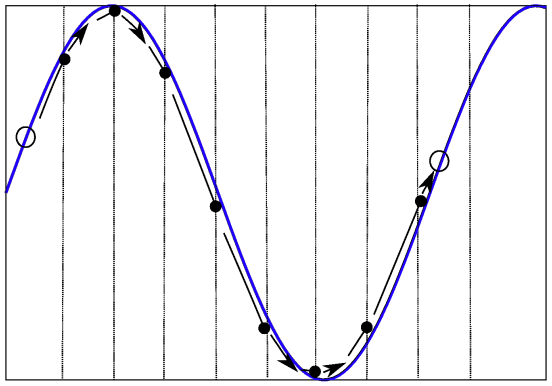
- With these definitions, exact energy conservation is retained:

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

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

[9] Cohen, B. I., Freis, R. P. and Thomas, V. (1982)

# Exact charge conservation: charge-conserving particle mover



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

- Exact charge conservation [10]
  - Strictly satisfied per particle when it is moving within a cell.
  - When a particle crosses boundary, **standard strategy** based on current redistribution.
  - In our context, **charge conservation is enforced by stopping particles at cell boundaries**, without breaking energy conservation.
- Local charge conservation is essential to ensure long-term accuracy of numerical algorithm:

$$\left.\begin{aligned} \epsilon_0 \frac{E_i^{n+1} - E_i^n}{\Delta t} + \bar{j}_i^{n+1/2} &= \left\langle \bar{j} \right\rangle^{n+1/2} \\ \frac{\rho_{i+1/2}^{n+1} - \rho_{i+1/2}^n}{\Delta t} + \frac{\bar{j}_{i+1}^{n+1/2} - \bar{j}_i^{n+1/2}}{\Delta x} &= 0 \end{aligned}\right\} \Rightarrow \left(\frac{E_{i+1} - E_i}{\Delta x} - \rho_{i+1/2}\right)^{n+1} = \left(\frac{E_{i+1} - E_i}{\Delta x} - \rho_{i+1/2}\right)^{n}$$

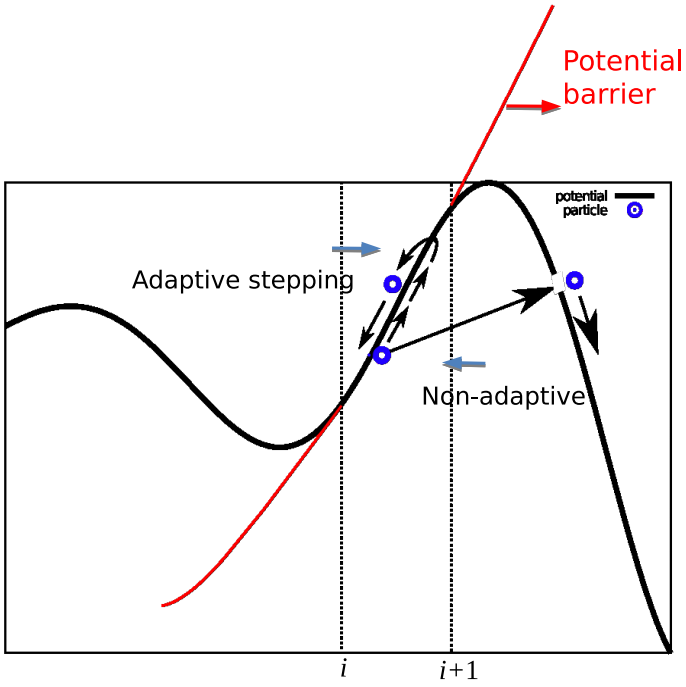
[10] BUNEMAN, O. (1968)

# 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**

- **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!**
  - No sub-step crosses a cell boundary.



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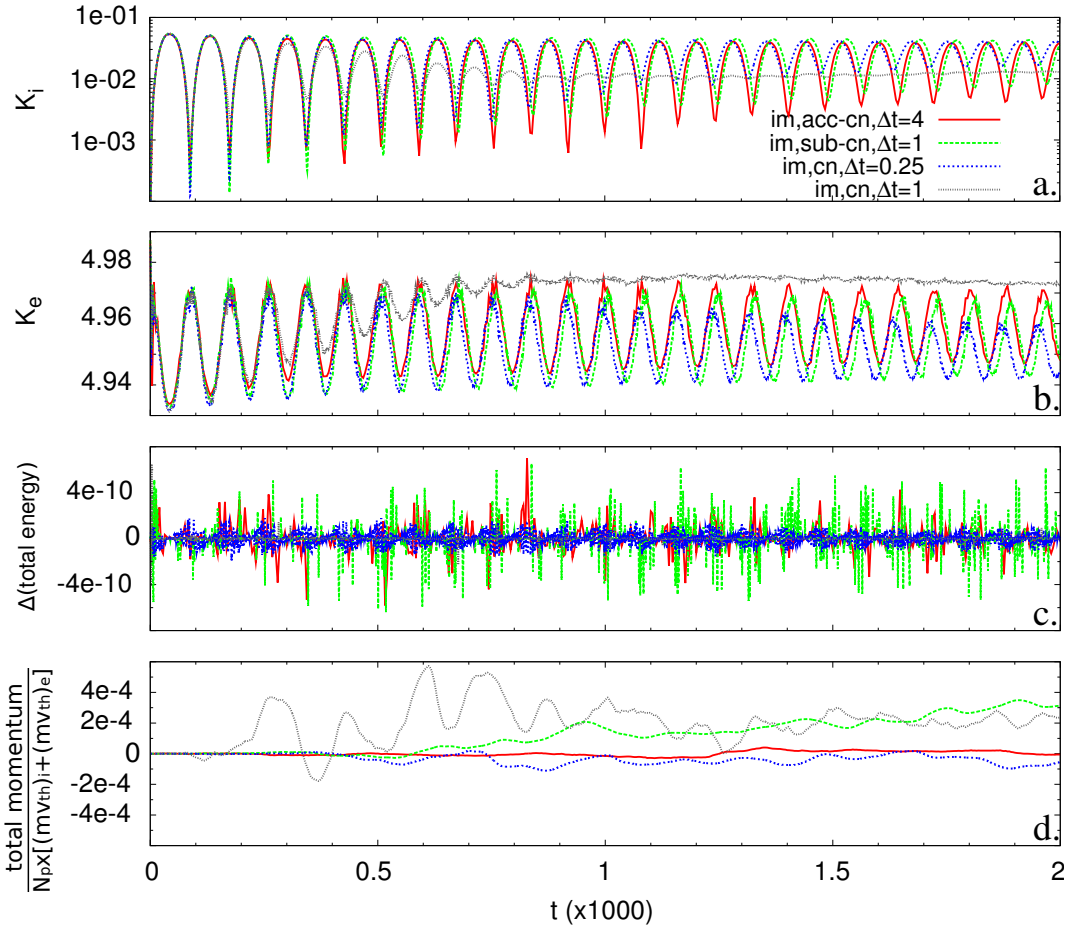
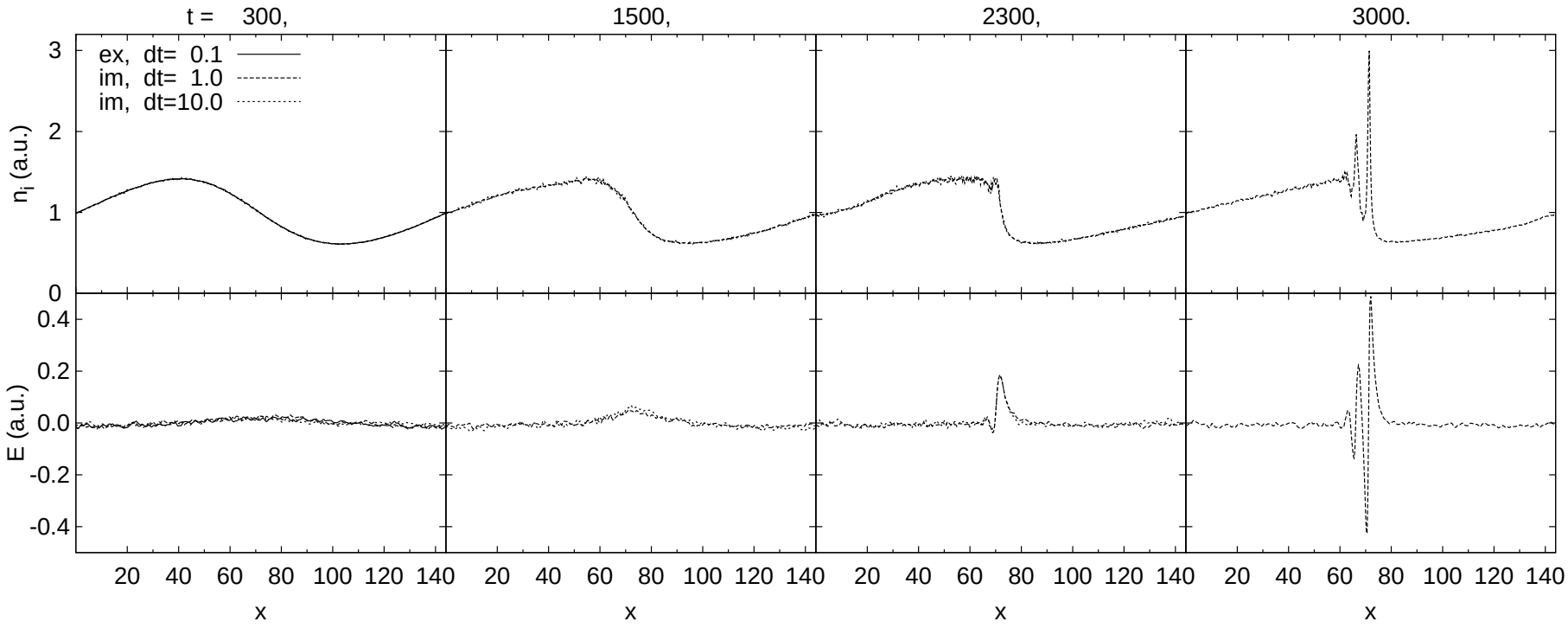
# Ion acoustic oscillation (1D1V): accuracy impact of different energy-conserving movers[11]

im=implicit, cn=Crank-Nicolson, acc=adaptive charge conserving, sub=fixed-substepping




[11] Chen, G., Chacón, L. and Barnes, D. C. (2011)

# 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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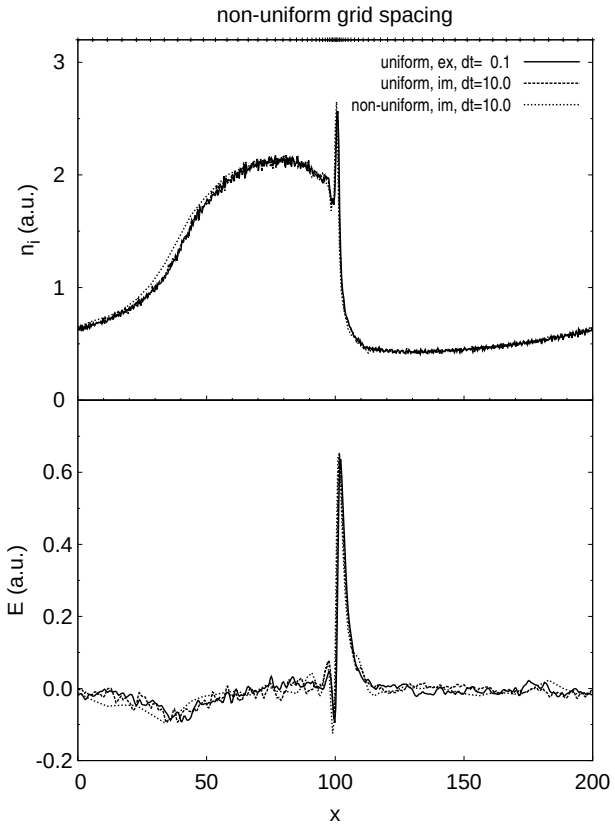
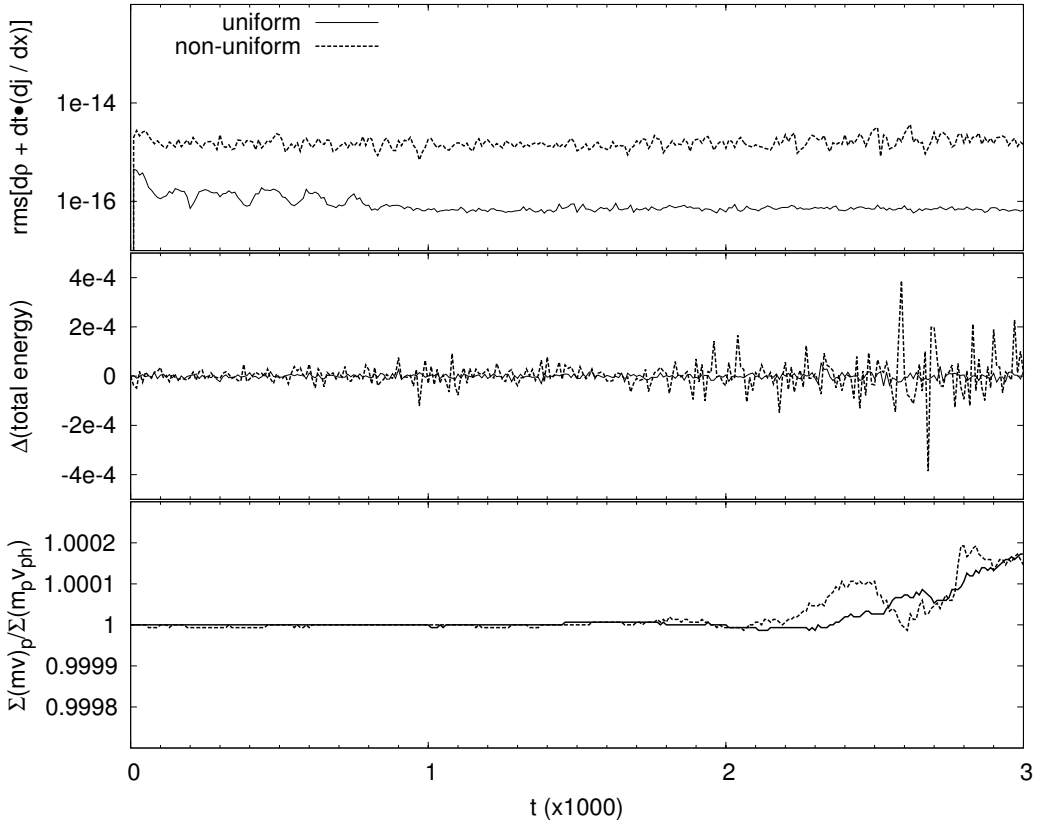
# Ion acoustic shock wave (cont.)[12]

## non-uniform grid spacing




[12] Chacón, L., Chen, G. and Barnes, D. C. (2013)

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# Moment preconditioning for fully implicit PIC

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# CPU gain potential of implicit PIC vs. explicit PIC

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

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

- Using reasonable estimates:

$$\begin{aligned}
\Delta \tau_{imp} &\sim \min\left[0.1\frac{\Delta x_{imp}}{v_{th}}, \Delta t_{imp}\right] \\
\Delta t_{imp} &\sim 0.1/\omega_{pi} \\
\Delta t_{exp} &\sim 0.1/\omega_{pe} \\
k\Delta x_{imp} &\sim 0.2 \\
\Delta x_{ex} &\sim \lambda_D
\end{aligned}$$

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

- 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 $\delta E$ from a fluid model using current particle distribution for closure.

- We begin with corresponding fluid nonlinear model:

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

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

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

$$\frac{\delta n_\alpha}{\Delta t} = -\nabla \cdot \delta \mathbf{\Gamma}_\alpha$$

$$m_\alpha \frac{\delta \mathbf{\Gamma}_\alpha}{\Delta t} \approx q_\alpha (\delta n_\alpha \mathbf{E} + n_{\alpha,p} \delta \mathbf{E}) + \nabla \cdot \left( \left( \frac{\mathbf{\Pi}_\alpha}{n_\alpha} \right)_p \delta n_\alpha \right)$$

$$\epsilon_0 \delta \mathbf{E} = \Delta t \left[ \sum_\alpha q_\alpha \delta \mathbf{\Gamma}_\alpha - \mathbf{G}(\mathbf{E}) \right]$$

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



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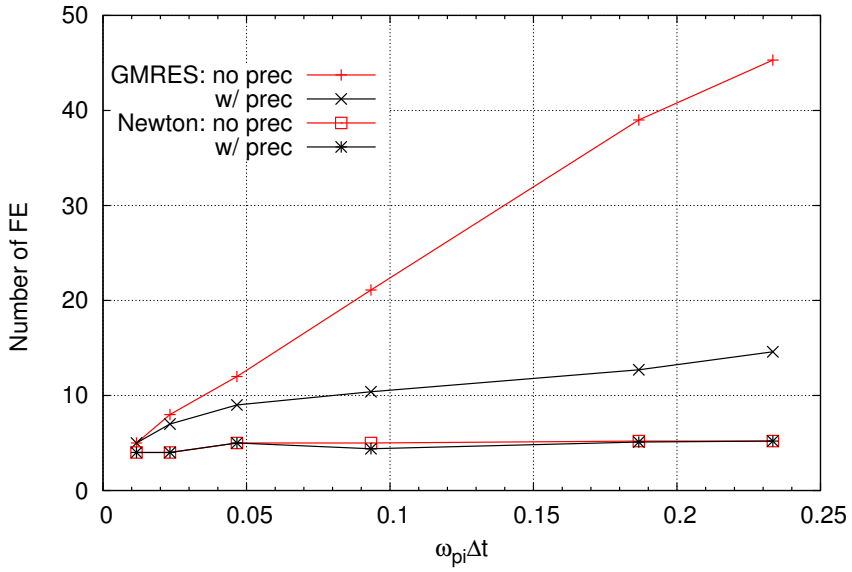
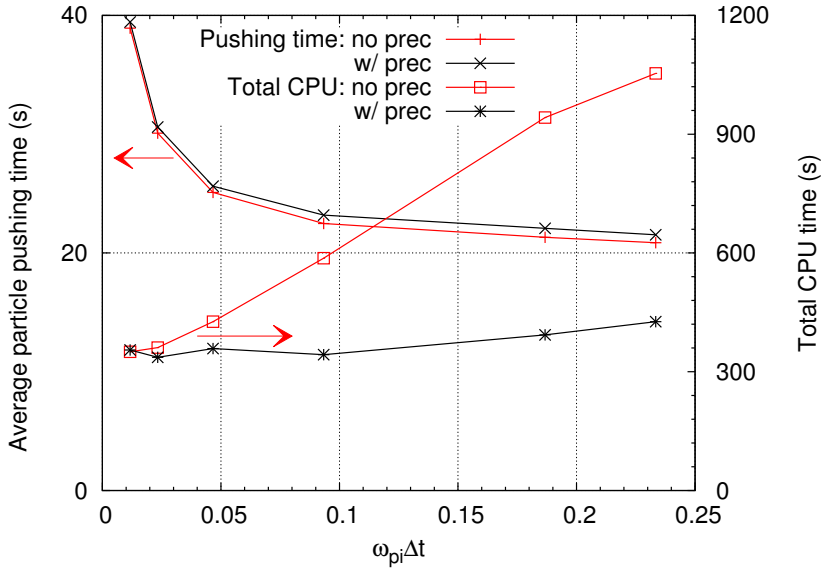
# Preconditioner performance with $\Delta t$




- 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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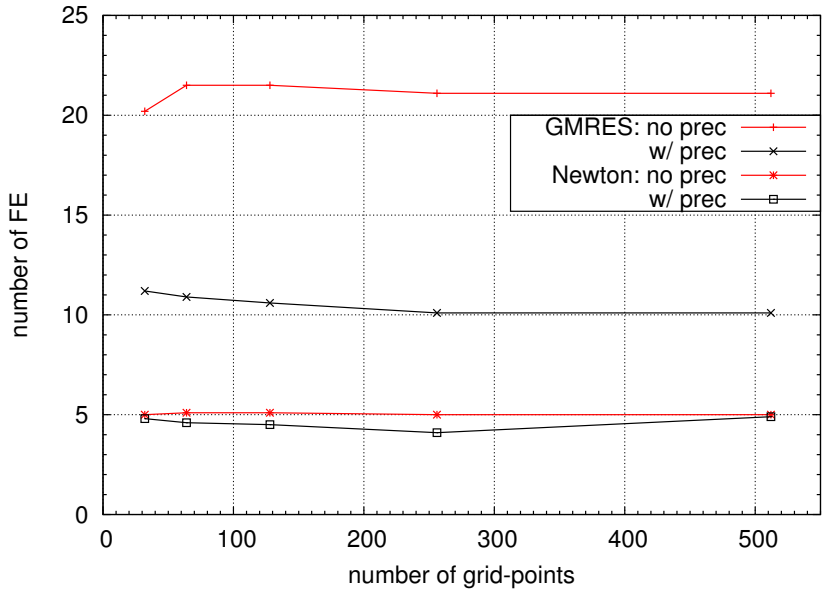
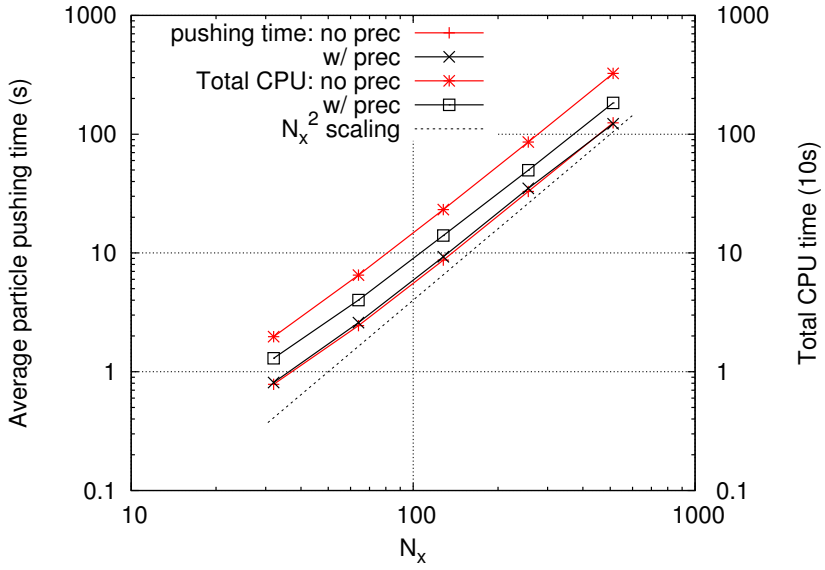
# Preconditioner performance with $N_x$




- 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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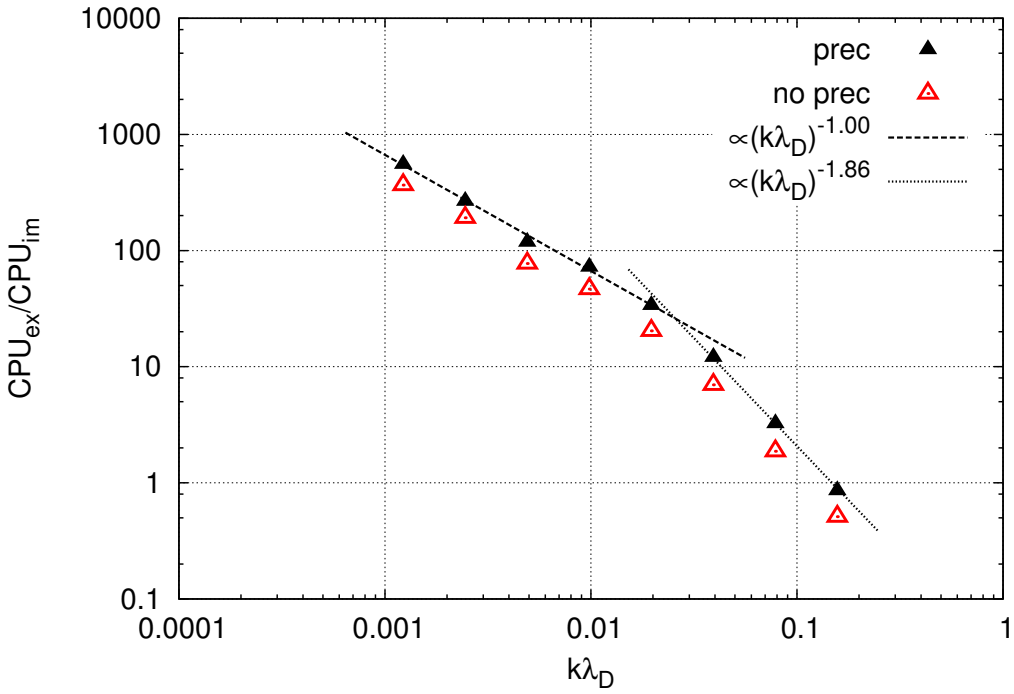
# Preconditioner performance: CPU scaling

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




Transition occurs at $k\lambda_D \sim \sqrt{\frac{m_e}{m_i}} \sim 0.025$, as predicted.

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# Generalization to electromagnetic PIC: Darwin (non-radiative) formulation

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# Darwin approximation to Maxwell equations

- Motivation: To analytically remove light-wave in non-relativistic plasma simulations.[13] [14]
  - If one keeps light wave with exact energy conservation in non-relativistic setting, one gets enhanced **numerical noise due to numerical Cherenkov radiation** [15]

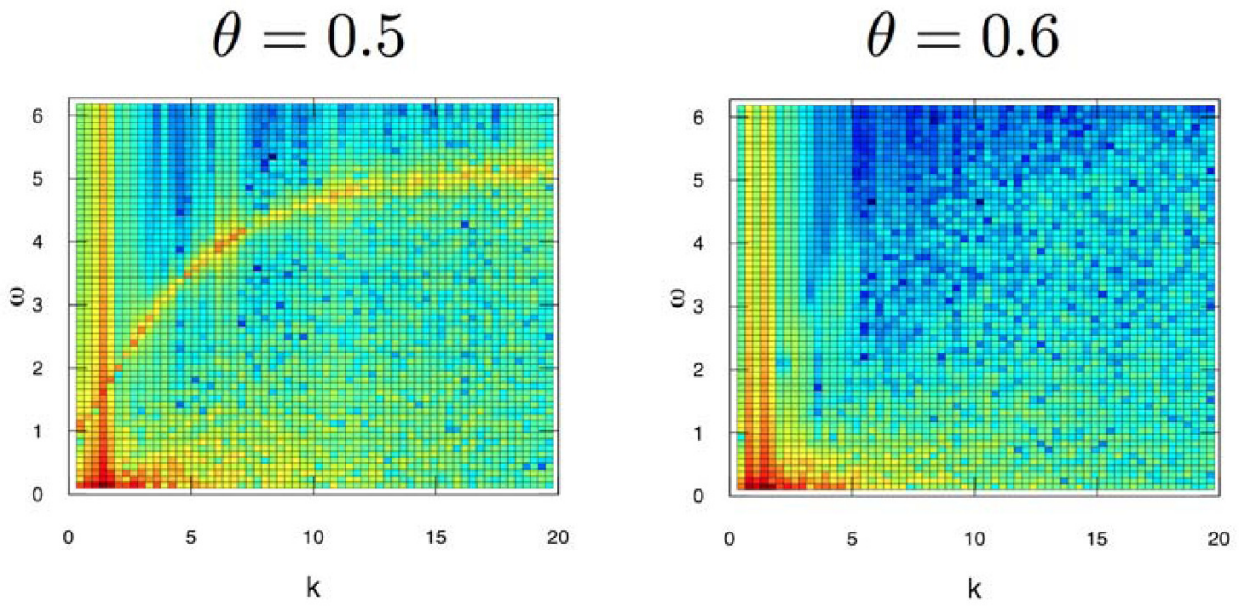


Figure 1: Fourier phase space for exactly energy conserving PIC (left) and dissipative PIC (right).

[13] Kaufman, A. N., and Rostler, P. S. (1971)
[14] Nielson, C. W. and Lewis, H. R. (1976)
[15] Markidis, S., and Lapenta, G. (2011)

# Darwin model (potential form)

- We consider potentials $\phi$, $\mathbf{A}$ 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).

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

- In 1D:

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



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# Implicit particle mover

➤ Sub-stepping particle equations of motion:

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

➤ This in an implicit nonlinear system. We invert it locally using Picard.

➪ We use implicit Boris's push:

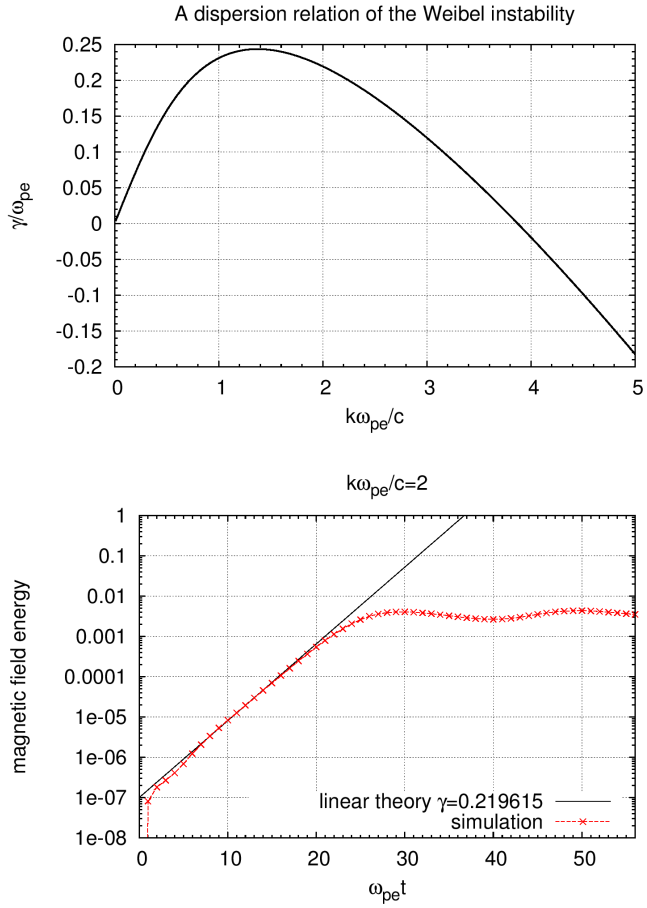
$$\begin{aligned}
\hat{\mathbf{v}}_p &= \mathbf{v}_p^{\nu} + \alpha \mathbf{E}_p^{\nu+1/2}\ ,\ \alpha = \frac{q_p \Delta\tau^{\nu}}{m_p 2} \\
\mathbf{v}_p^{\nu+1/2} &= \frac{\hat{\mathbf{v}}_p + \alpha\left[\hat{\mathbf{v}}_p \times \mathbf{B}_p^{\nu+1/2} + \alpha(\hat{\mathbf{v}}_p \cdot \mathbf{B}_p^{\nu+1/2})\mathbf{B}_p^{\nu+1/2}\right]}{1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

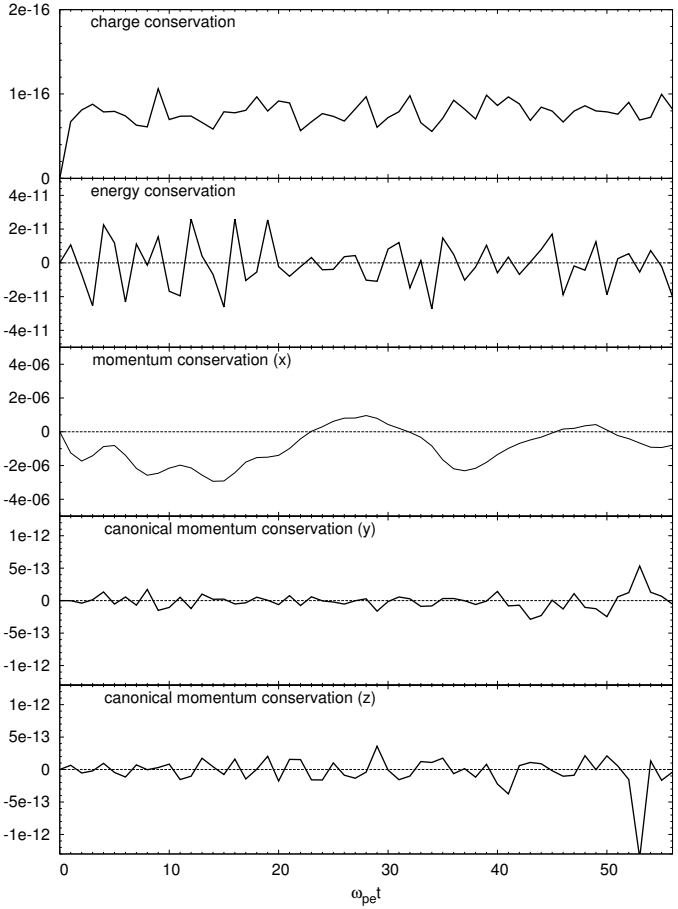
We interpolate the B field such that the $(y, z)$ canonical momentum can be exactly satisfied.

# Verification: Electron Weibel instability

- Isotropic ions, bi-Maxwellian electrons

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

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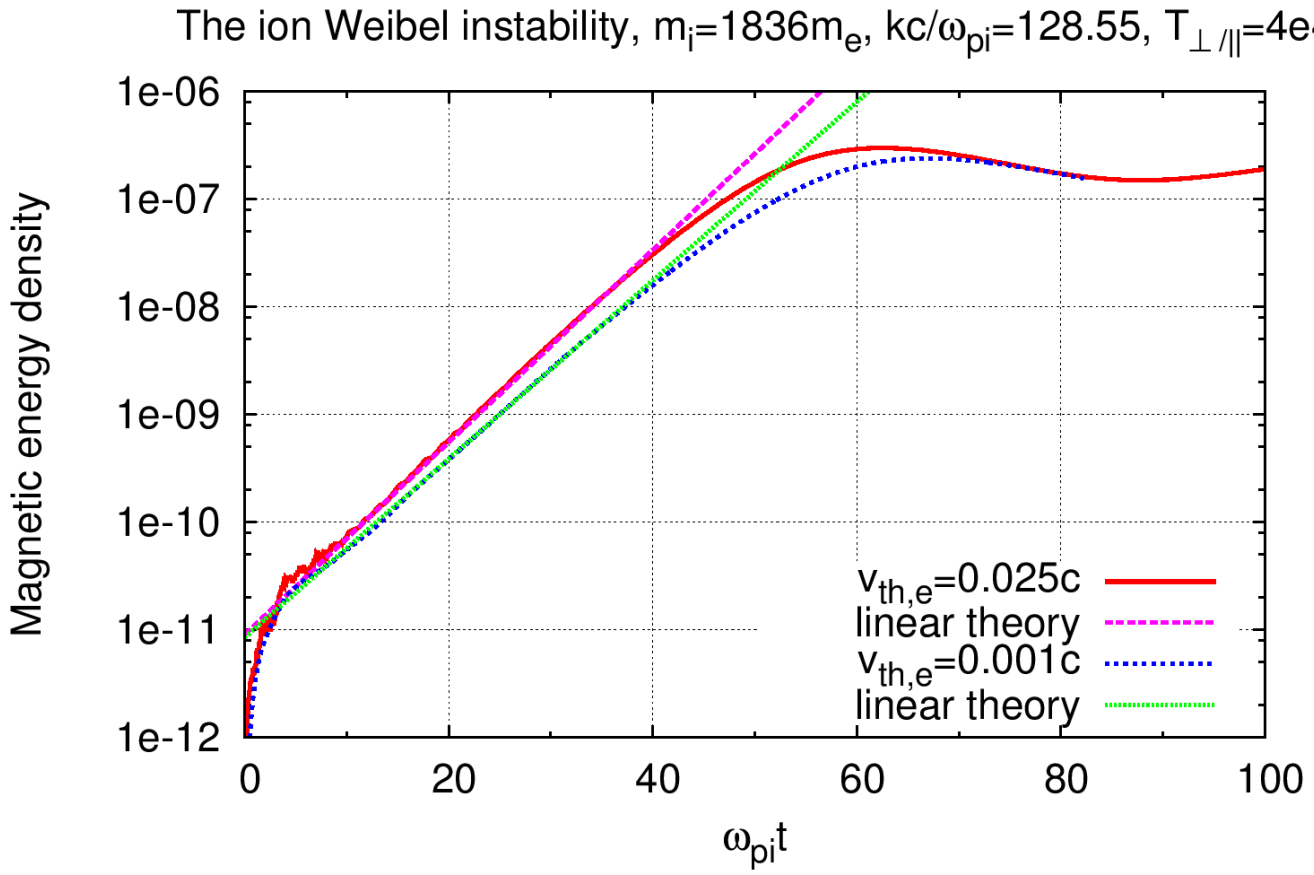
# Verification: Ion Weibel instability (large T anisotropy)

- 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, $\gamma \approxeq 0.1\omega_{pi}$.

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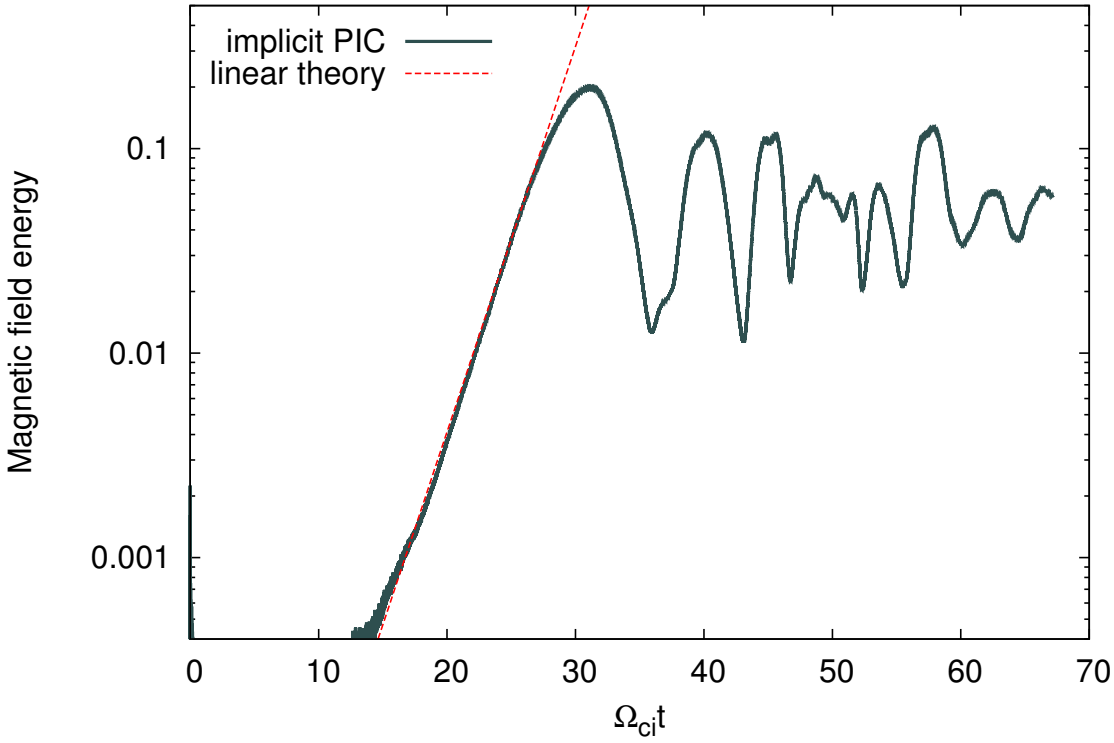
# Kinetic Alfven wave ion-ion streaming instability

- KAW generated by ion-ion streaming at relatively low (2.5 Alfvén) speed and low plasma beta ($\beta$e=0.1) with a realistic mass ratio ($m_i/m_e = 1836$).

$$N_{e,i}\text{=128,000, } L = 4\pi c/3\omega_{pi}\text{, } N_g\text{=64, } \gamma \approxeq 0.22\omega_{ci}.$$

$$\Delta x/\lambda_D \simeq 40,\ \Delta t_{im}/\Delta t_{ex} \simeq 20.$$

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# 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.
- 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 $\Delta t$, $\Delta x \Rightarrow$ preconditioning!
  - We have formulated and implemented a very efficient moment-based preconditioner.
- We have generalized the algorithm to non-radiative electromagnetic regimes (Darwin model), where, **in addition to charge and energy, we also conserve canonical momenta**.
- We have demonstrated potential of the approach via numerical experiments.