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# A Fully Implicit, Moment Accelerated, Electromagnetic Particle-in-Cell Algorithm

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# Outline

- Plasma kinetic simulations: Particle-in-cell (PIC) methods
  - explicit, implicit time integrations
- Our approach: fully implicit **electromagnetic** PIC
  - Vlasov-Darwin model, space-time-centered discretization
  - Based on a JFNK solver with nonlinear elimination
- Preconditioning: Moment acceleration
  - physics based, fluid set of equations (electrons only)
  - targeting stiffest electrostatic waves (e.g. Langmuir wave)
  - targeting some fundamental electromagnetic effects (e.g. skin current)
  - some test case examples

# Introduction



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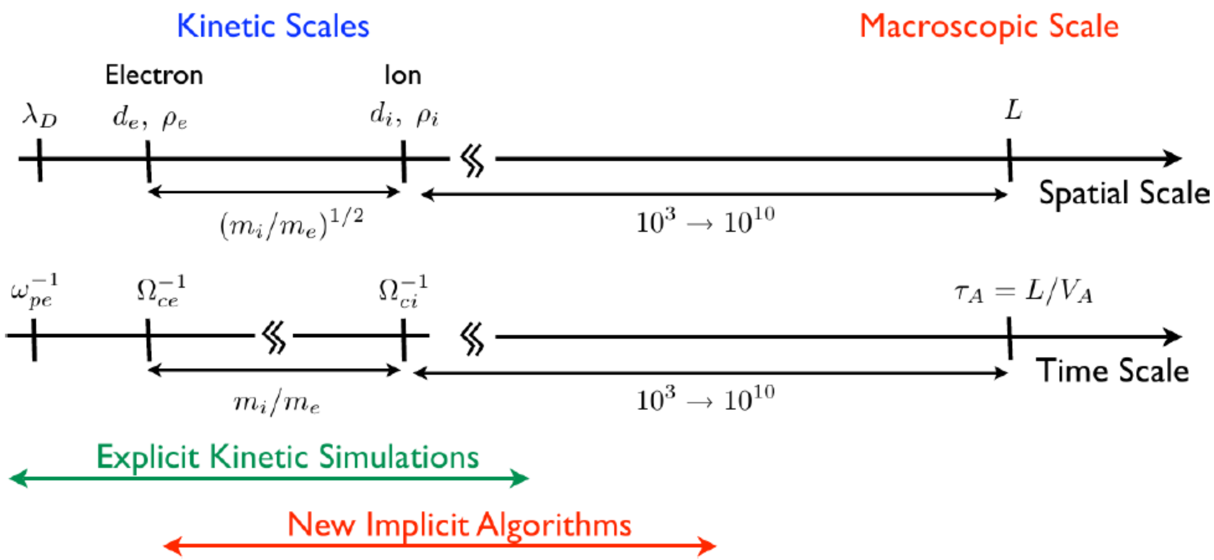
# Kinetic Plasma Simulation

- A fully ionized collisionless plasma: ions, electrons, and electromagnetic fields
- **Challenge**: integrate ion-electron kinetic system (plus Maxwell's equations) on an ion time-scale and a system length scale while retaining electron kinetic effects accurately.




(We are developing a New implicit algorithm for long-term, system-scale simulations. )

- Problem features a **hierarchical description**:
  - Kinetic scales require transport models (3D-3V): high-order problem (PIC, direct Vlasov)
  - Macroscopic scale well described by fluid models (3D): low-order problem (MHD)

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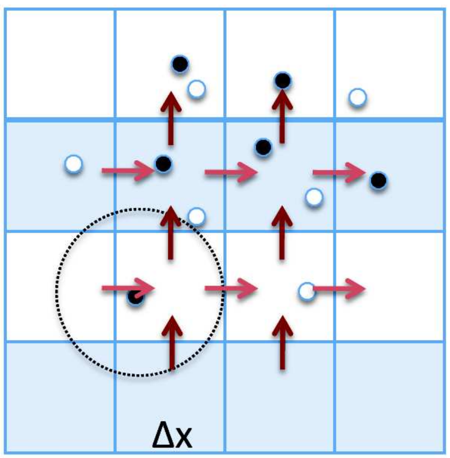
# Particle-in-cell (PIC) methods for kinetic plasma simulation

$$\partial_t f + \mathbf{v}\cdot\nabla f + \frac{\mathbf{F}}{m}\cdot\nabla_v f = \left(\frac{\partial f}{\partial t}\right)_{col}$$

- Ignoring collisions $\Rightarrow$ 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)




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

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

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

$$\delta(\mathbf{x}-\mathbf{x}_p) \longrightarrow S(\mathbf{x}-\mathbf{x}_p)\ ;\ E_p = \sum_i E_i S(x_i - x_p)\ ;\ j_i = \sum_p j_p S(x_i - x_p)$$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# Implicit vs. explicit particle-in-cell (PIC) methods

- Explicit PIC features:
  - 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**)
    - Challenging for heterogeneous architectures: memory bounded
  - Accuracy limitations: **lack of energy conservation**, problematic for long-time-scale simulations
- Fully converged, nonlinear implicit PIC [1-7] can overcome difficulties of explicit PIC:
  - Allowing stable and robust integrations with large $\Delta t$ and $\Delta x$ (2nd order accurate)
  - Ensuring exact global energy conservation and local charge conservation properties
  - Allowing adaptivity in both time and space without loss of the conservation properties
  - Nonlinear elimination: particle subcycling (large operational intensities!)
  - *Allows fluid preconditioning to accelerate the iterative (JFNK) kinetic solver*

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# Fluid equations

- Taking moments of Vlasov equation:

$$\begin{aligned}\partial_t n_\alpha &= -\nabla \cdot \mathbf{\Gamma}_\alpha \\ m_\alpha \partial_t \mathbf{\Gamma}_\alpha &= q_\alpha n_\alpha \left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) - \nabla \cdot \mathbf{\Pi}_\alpha \\ &\bullet \quad \bullet \quad \bullet\end{aligned}$$

  where

$$\begin{aligned}n_\alpha &= \int f_\alpha dv \\ \mathbf{\Gamma}_\alpha &= \int \mathbf{v} f_\alpha dv \\ \mathbf{\Pi}_\alpha &= \int \mathbf{v}\mathbf{v} f_\alpha dv\end{aligned}$$

- Our goal: Using simplified fluid equations, which expose the stiffest modes in the system, and is fast to invert, for algorithmic accelerations $\leftarrow$ IMPLICIT PIC time integrations.



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# Fully implicit electromagnetic Vlasov-Darwin PIC

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# Darwin model (potential form)

- A good approximation to the Maxwell's equation for low-frequency plasma phenomena, but without the light wave.
  - Light waves can be excited by noises, accumulate errors, and introduce numerical Cherenkov radiations/instabilities.
- We consider potentials $\phi$, $\mathbf{A}$ in the Coulomb gauge ($\nabla \cdot \mathbf{A} = 0$) such that:

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

- In 1D:

$$
\begin{aligned}
\epsilon_0 \partial_t E_x + j_x &= \langle j_x \rangle , \\
\frac{1}{\mu_0} \partial_x^2 A_y + j_y &= \langle j_y \rangle , \\
\frac{1}{\mu_0} \partial_x^2 A_z + j_z &= \langle j_z \rangle .
\end{aligned}
$$

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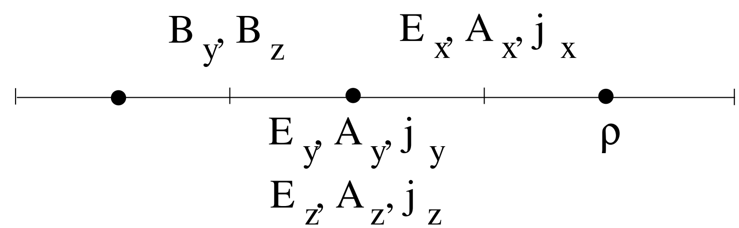
# Time-space-centered discrete 1D Darwin model

- Field equations on a Yee grid:

$$
\begin{aligned}
\epsilon_0 \frac{E_{x,i+1/2}^{n+1} - E_{x,i+1/2}^{n}}{\Delta t} + \bar{j}_{x,i+1/2}^{n+1/2} &= \langle j_x \rangle \,, \\
\frac{1}{\mu_0}\, \partial_x^2 \frac{A_y^{n+1} + A_y^{n}}{2}\bigg|_i + \bar{j}_{y,i}^{n+1/2} &= \langle j_y \rangle \,, \\
\frac{1}{\mu_0}\, \partial_x^2 \frac{A_z^{n+1} + A_z^{n}}{2}\bigg|_i + \bar{j}_{z,i}^{n+1/2} &= \langle j_z \rangle
\end{aligned}
$$




- Current gather (with orbit averaging):

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

# Implicit particle mover

- Subcycled particle equations of motion:

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

- This in an implicit nonlinear system. We invert it locally using Picard iterations.
- We use an implicit Boris push:

$$\hat{\mathbf{v}}_p = \mathbf{v}_p^{\nu} + \alpha\mathbf{E}_p^{\nu+1/2}\,,\ \alpha = \frac{q_p\Delta\tau^{\nu}}{m_p 2}$$

$$\mathbf{v}_p^{\nu+1/2} = \frac{\hat{\mathbf{v}}_p + \alpha\left[\hat{\mathbf{v}}_p \times \mathbf{B}_p^{\nu+1/2} + \alpha(\hat{\mathbf{v}}_p \cdot \mathbf{B}_p^{\nu+1/2})\mathbf{B}_p^{\nu+1/2}\right]}{1 + \left(\alpha B_p\right)^2}.$$

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# Jacobian-Free Newton-Krylov Methods

- A large set of nonlinear equations (in the residual form): $A\vec{x}^{n+1} = \vec{b} \Rightarrow \boxed{\vec{G}(\vec{x}^{n+1}) = \vec{0}}$
- 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 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):

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

  - 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 explore physics-based preconditioning strategies.

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# Nonlinear elimination by Particle enslavement

- Full residual $\mathbf{G}(\{x,v\}_p,\{\Phi\}_g) = 0$ is impractical by GMRES method (too much memory requirement for $\vec{x} = \mathcal{K}\vec{c}$ where $\mathcal{K} = span\{\vec{b}, A\vec{b}, A^2\vec{b}...\}$ and $\vec{c}$ is some appropriate vector).
- Alternative: nonlinearly eliminate particle quantities **so that they are not dependent variables**:
  - Formally, particle equations of motion are functionals of the electrostatic potential:

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

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

Nonlinear residual can be *unambiguously* formulated in terms of fields only!

- 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 possible!**



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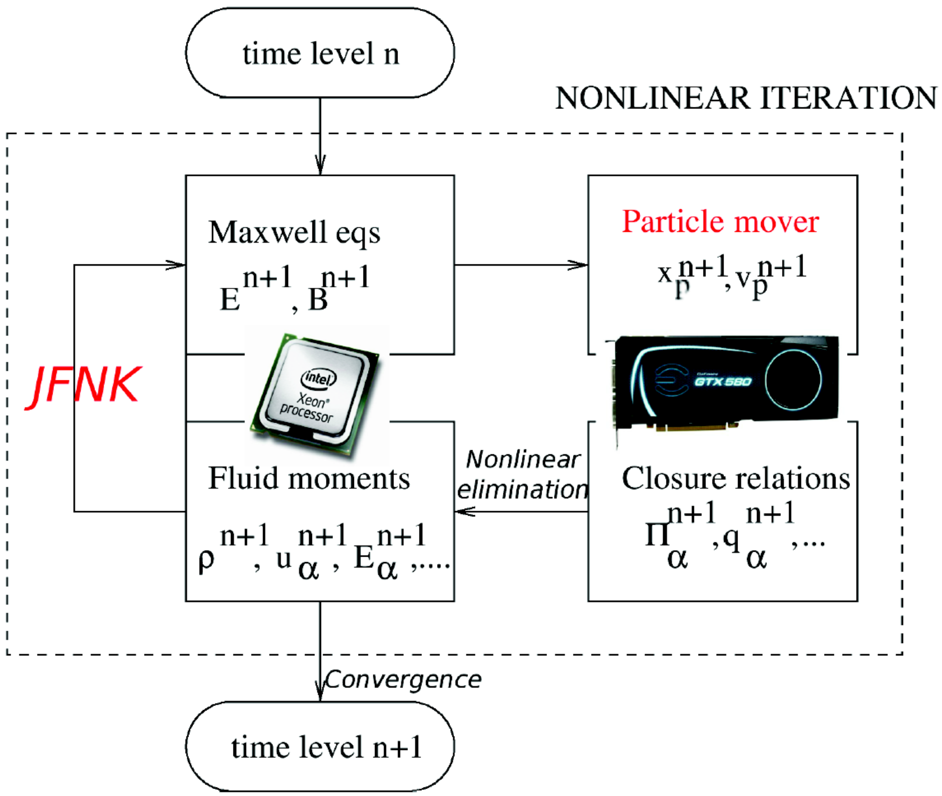
# Algorithmic implementation details

1. Input $\mathbf{E}$, $\mathbf{B}$ (given by JFNK iterative method)
2. *Move particles (i.e., find $x_p[E]$, $v_p[E]$ by solving equations of motion)*
3. *Compute moments (current density)*
4. Form the Darwin equation residual



# JFNK preconditioning via moment equations

- We start with 1D electrostatic equations (x direction) :

$$\partial_t n_e = -\partial_x \Gamma_{ex} \quad (1)$$

$$m_e \partial_t \Gamma_{ex} = q_e n_e E_x + \partial_x \mathbf{\Pi}_e \quad (2)$$

$$\epsilon_0 \partial_t E_x = q_e \Gamma_{ex} \quad (3)$$

- Linearize and discretize:

$$\frac{\delta n_e}{\Delta t} = -\partial_x \delta \Gamma_{ex} \quad (4)$$

$$m_e \frac{\delta \Gamma_{ex}}{\Delta t} \approx q_e \left[ \delta n_e \, E_x + (n_e)_p \, \delta E_x \right] + \partial_x \left[ \left( \frac{\mathbf{\Pi}_e}{n_e} \right)_p \delta n_e \right] \quad (5)$$

$$\epsilon_0 \, \delta E_x = \Delta t \left[ q_e \delta \Gamma_{ex} - G(E_x) \right] \quad (6)$$

  - Eq.(4) (5) can be combined, and inverted by a tri-diagonal solver;
  - $\delta E$ can be obtained from Eq.(6).



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# JFNK preconditioning via moment equations (cont.)

- We then deal with electromagnetic equations (y,z directions) :

$$m_e \partial_t \Gamma_{y,z} = q_e n_e \left[ E_{y,z} + \cancel{(\mathbf{v} \times \mathbf{B})}_{y,z} \right] + \cancel{\partial_x \mathbf{\Pi}}_e \quad (7)$$

$$E_{y,z} = -\partial_t A_{y,z} \quad (8)$$

$$\frac{1}{\mu_0} \partial_{xx} A_{y,z} = -q \Gamma_{y,z} \quad (9)$$

- Linearize and discretize:

$$2 m_e \delta \Gamma_{y,z} + q_e n_e \delta A_{y,z} = 0 \quad (10)$$

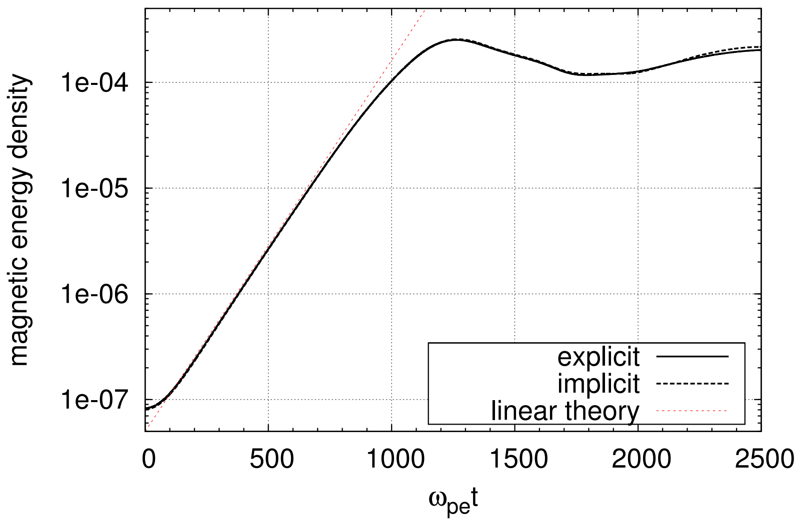
$$\frac{1}{\mu_0} \partial_{xx} \delta A_{y,z} + q_e \delta \Gamma_{y,z} = -G(A_{y,z}) \quad (11)$$

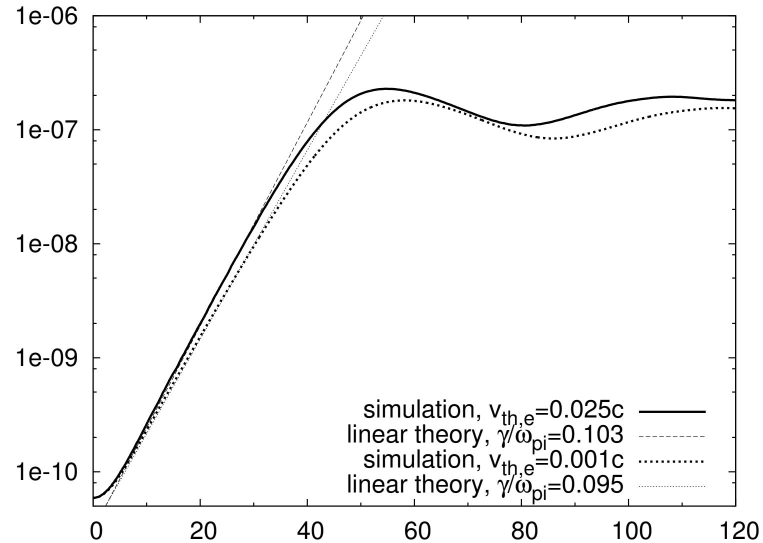
  - Eq.(10) (11) can be combined,

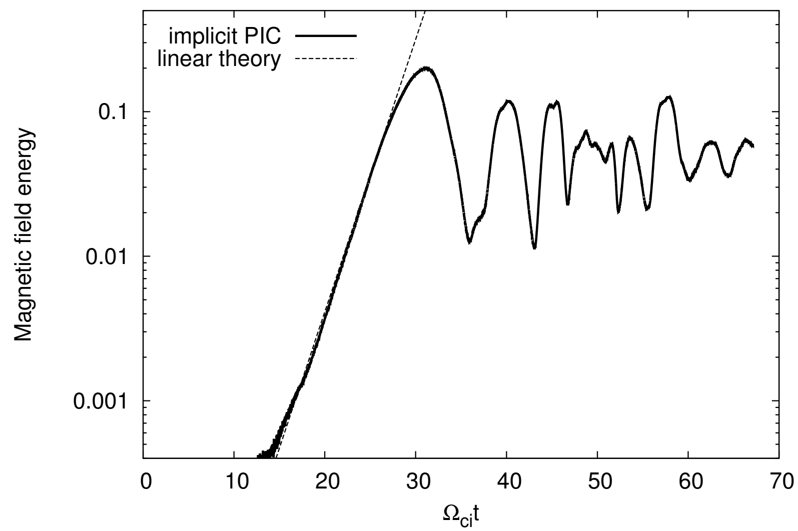
$$\frac{\partial \delta A_{y,z}}{\partial x^2} - \frac{1}{d_e^2} \delta A_{y,z} = -2\mu_0 \, G(A_{y,z}) \quad (12)$$

  where $d_e = c/\omega_{pe}$ is the skin depth.
  - Eq. 12 is inverted by a tri-diagonal solver.

# Test cases: from unmagnetized to magnetized plasmas

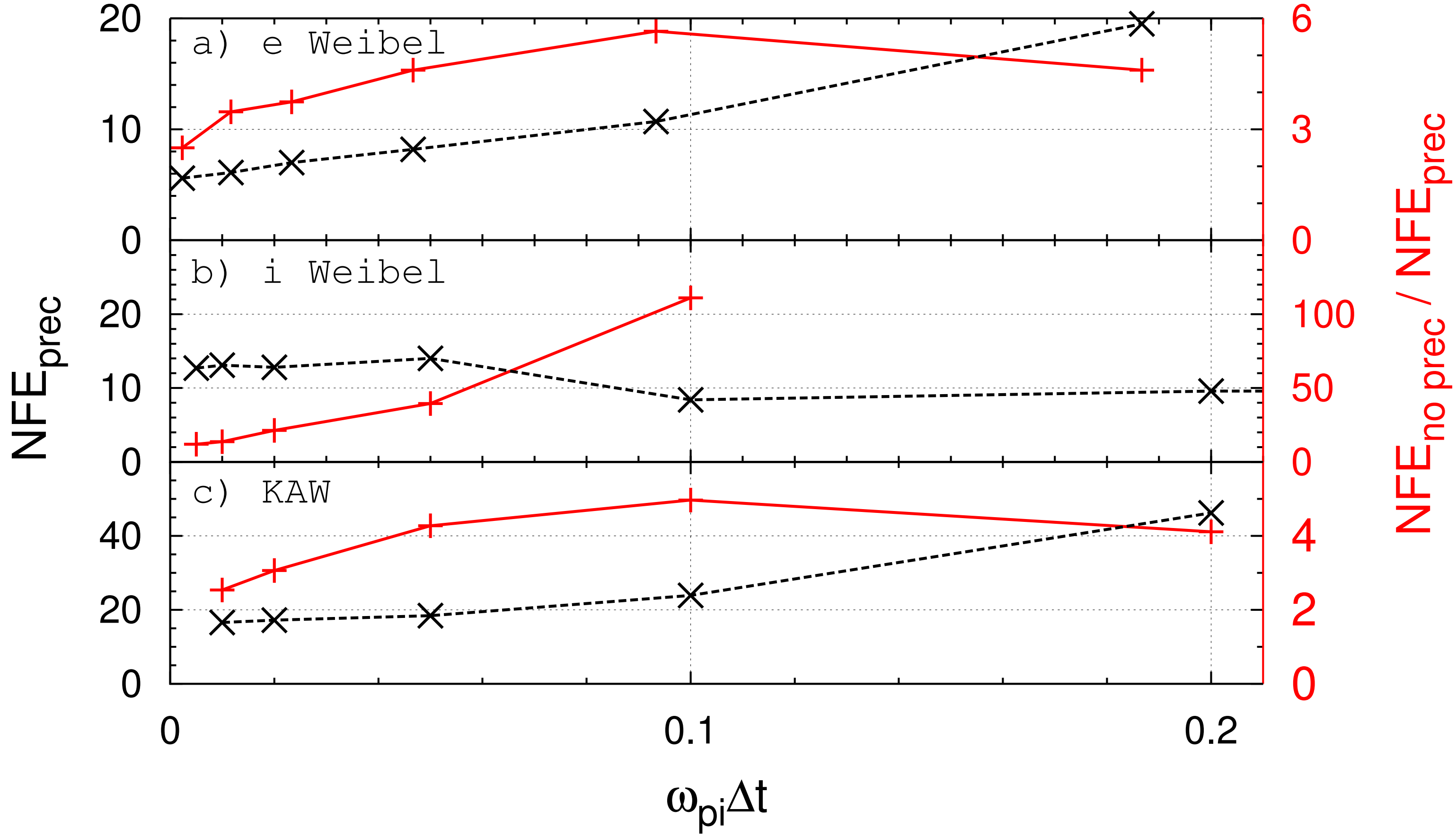



1)electron Weibel instability; 2) ion Weibel instability ; 3) Kinetic Alfven wave with ion-ion streaming instability.

# Preconditioner performance

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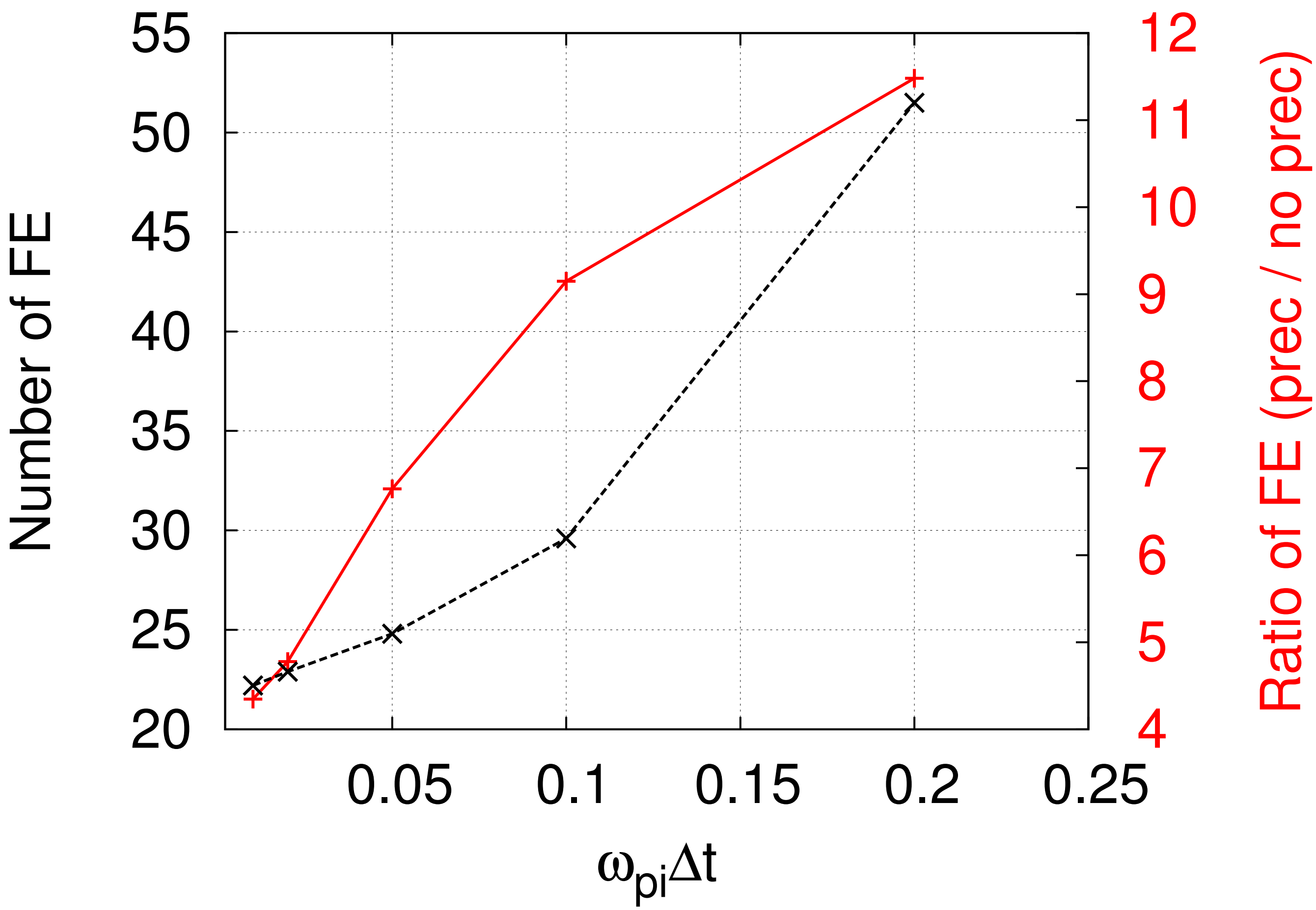
# Preconditioner performance (cont.)

We change the Ion Webel instability case from L=0.05 to a larger domain L=32 (Nx=64). Correspondingly, $k_{max} d_e \simeq 100 \rightarrow 6.4$ (see Eq. 12) :

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# Summary and conclusions

- Implicit PIC methods become practical by JFNK with nonlinear elimination.
  - JFNK solves for the field equations only; particle equations of motion can be solved separately.
- The nonlinear elimination allows us to construct an efficient moment-based preconditioner:
  - The fluid preconditioner is physics based, taking into account the electrostatic electron wave physics, and electromagnetic skin current shielding effects.
  - The fluid preconditioner (in 1D) allows good performance upto $\Delta t = 0.1\omega_{pi}^{-1}$.
  - The preconditioner is tested for unmagnetized and weakly unmagnetized problems, the ratio between un-preconditioned and preconditioned NFE is from 5 to 10 (in the case of $kd_e \gg 1$, ratio=100!)

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