# Speed-limited Particle-in-Cell (SLPIC): speeding up simulations while slowing down particles on the March to exascale


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- Particle-in-cell methods: powerful for kinetics, but limiting, esp. ion-scale simulations with kinetic electrons
- Avoiding limits through implicit methods painful
- SLPIC ansatz captures the required processes while ignoring the unimportant
- SLPIC can be solved by particle methods
- SLPIC shown to work on sheath problems

# Particle-in-Cell methods are indispensable for plasma simulations

- PIC provides a representation of velocity space with minimal degrees of freedom
- Provides a way of giving velocity space representation that over multiple cells provides thousands of velocity space points
- Many advances to deal with noise ($\delta f$), numerical restrictions (implicit)

But at some point, maybe 100 ppc in 2d, 1000 in 3d, one can go to a continuum rep and eliminate noise.

# Particle-in-Cell methods imply limits on time stepping, grid resolution

- $v_p \Delta t \leq \Delta x$: Particles must not move over many grid cells in a time step to get an accurate force and to provide an accurate current
- $\omega_e \Delta t \leq 1$: otherwise get strong instability, i.e., plasma CFL,
- $\Delta x \leq \lambda_e$: Debye length resolution needed to prevent grid instability
- All very related
- For electromagnetics, also EM CFL, again related for relativistic particles

# These numerical limits are not related to resolution requirements

- Cold plasma oscillations: wavelength determines the physics, not Debye length
- MHD: electrons mostly just cancel electric field
- Ion-acoustic modes (electrons basically Boltzmann response)
- Plasma sheaths (one-sided chopped electron Maxwellians)

# Current approach to avoiding limits is to apply implicit methods

- S. Markidis, G. Lapenta, The energy conserving particle-in-cell method, J. Comput. Phys. 230 (1) (2011) 7037.
- L. Chacon, G. Chen, D. Barnes, A charge-and energy-conserving implicit, electrostatic particle-in-cell algorithm on mapped computational meshes, J. Comput. Phys. 233 (2013) 1.
- G.Chen, L.Chacon, “A multi-dimensional, energy-and charge-conserving, nonlinearly implicit, electromagnetic Vlasov–Darwin particle-in-cell algorithm”, Computer Physics Communications 197 (2015): 73-87.
- Many much older
- Requires large matrix inversion at each step.
- Worse: matrix creation at each step (moment method)

# Basic PIC methods – solve for distribution function by method of characteristics

- Conservation form

$$\partial_t f(\mathbf{x},\mathbf{v},t) + \nabla_x[\mathbf{v} f(\mathbf{x},\mathbf{v},t)] + \nabla_v[\mathbf{a}(\mathbf{x},\mathbf{v},t) f(\mathbf{x},\mathbf{v},t)] = 0$$

- Advection form

$$\partial_t f(\mathbf{x},\mathbf{v},t) + \mathbf{v}\cdot\nabla_x[f(\mathbf{x},\mathbf{v},t)] + \mathbf{a}(\mathbf{x},\mathbf{v},t)\cdot\nabla_v[f(\mathbf{x},\mathbf{v},t)] = 0$$

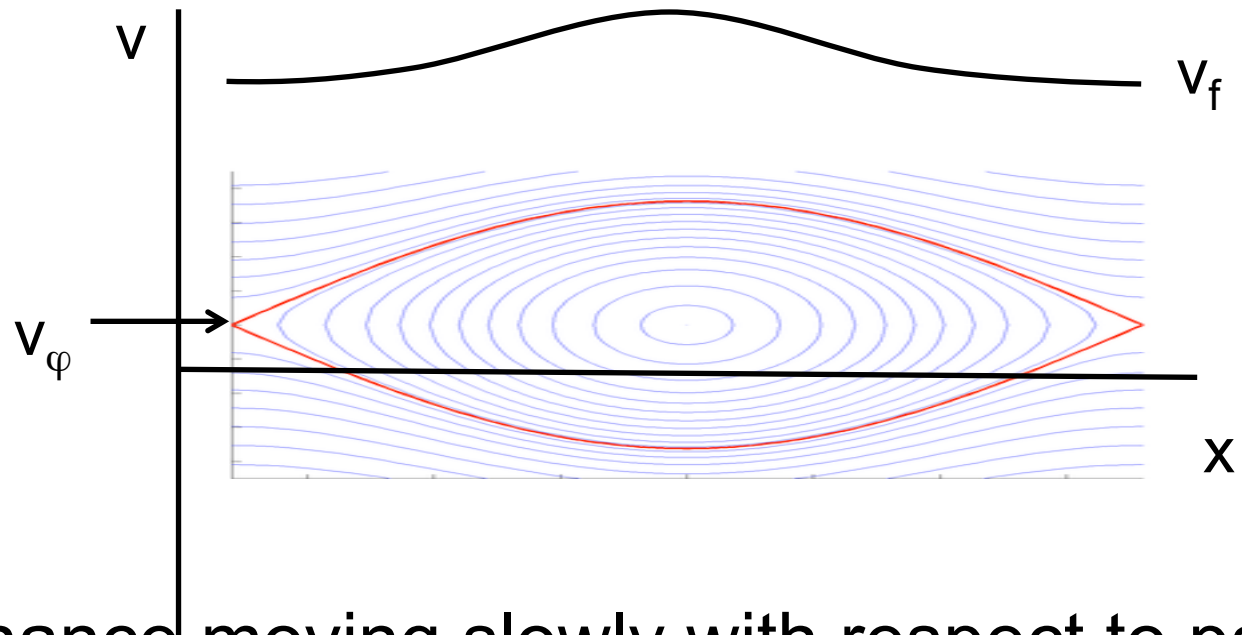
- Solution:

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

- $w_p$= particle weight
- $x_p$, $v_p$ = particle trajectory, satisfying

$$\dot{\mathbf{x}}_p = \mathbf{v}_p \qquad \dot{\mathbf{v}}_p = \mathbf{a}(\mathbf{x}_p,\mathbf{v}_p,t)$$

# Fast electrons are in equilibrium with slow (ion-scale) dynamics




- Resonance moving slowly with respect to particles at some velocity
- Particles at that velocity essentially in equilibrium with the perturbation
- Time derivative can be ignored

# SLPIC is based on a simple ansatz

$$f(\mathbf{x},\mathbf{v},t) = \beta(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)$$

$$\partial_t\left[\beta g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta\mathbf{v}g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta\mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = 0$$

$$\partial_t\left[g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta\mathbf{v}g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta\mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = \partial_t\left[(1-\beta)g(\mathbf{x},\mathbf{v},t)\right]$$

- Choose $\beta$ such that
  - For slow particles, $\beta = 1$ (RHS vanishes)
  - For fast particles, $\beta \rightarrow 0$, RHS unimportant compared with phase space derivatives
  - In both cases, RHS can be neglected

$$\partial_t\left[g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta\mathbf{v}g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta\mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = 0$$

- Distribution evolves as if velocity *and* acceleration reduced for fast particles

# Significant freedom in the prefactor

- Choose β such that
  - For slow particles, β = 1 (RHS vanishes)
  - For fast particles, β ➔0, RHS unimportant compared with phase space derivatives

$$\beta(\mathbf{x},\mathbf{v},t) = \frac{v_0}{\sqrt{v_0^2 + v^2}} \qquad \beta\mathbf{v} = \frac{\mathbf{v}}{\sqrt{1+\left(v/v_0\right)^2}}$$

- Freedom to pick β to be a function of position
  - Variable grid: refine in plasma sheath, choose smaller β there
  - Increase β in time when faster phenomena appear

# SLPIC equations can be solved identically to original

$$g(\mathbf{x},\mathbf{v},t) = \sum_p w_p \delta\left(\mathbf{x} - \mathbf{x}_p(t)\right)\delta\left(\mathbf{v} - \mathbf{v}_p(t)\right)$$

$$\dot{\mathbf{x}}_p = \beta(\mathbf{x}_p,\mathbf{v}_p,t)\mathbf{v}_p \qquad \dot{\mathbf{v}}_p = \beta(\mathbf{x}_p,\mathbf{v}_p,t)a(\mathbf{x}_p,\mathbf{v}_p,t)$$

- Particle accelerate, move more slowly
- Follow same trajectories
- Transform back to get actual distribution function

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

- Slowing down the particles makes them more dense. The prefactor counteracts that.

But solving with particles not a requirement. Could use continuum methods on the speed limited equation

# SLPIC is NOT

- A coordinate transformation (would not change the way particles move through space)
- A delta-f approach (the weight does not vary in time; not separation into two distributions)
- Even necessarily a PIC approach. One could use continuum methods.

SLPIC is simply an ansatz that allows one to treat fast particles as if in equilibrium while treating slow particles exactly

# SLPIC fits easily into the PIC cycle

- Field solve (unchanged)
- Particles
  - Interpolate: same
  - Accelerate: modified acceleration, point-wise implicit algorithms solved by quartic for unmagnetized
  - Move: Just move less by $\beta$ (could be implicit when $\beta$ depends on x)
  - Deposit: only change from standard pic is the variation of $\beta$ from one end to other. Treatment known from $\delta f$.

# To determine the plasma oscillation stability need to know plasma frequency

- Standard analysis, 1D

$$-i(\omega - k\beta v)\tilde{g}_1 = -\tilde{a}_1 \partial_v [\beta g_0(v)] \qquad g_1 = \tilde{g}_1 \exp(ikx - i\omega t)$$

$$\tilde{n}_1 = \int dv \tilde{f}_1 = \int dv \beta \tilde{g}_1 = -ia_1 \int dv \frac{\beta}{\omega - k\beta v} \partial_v \left[\beta g_0\right]$$

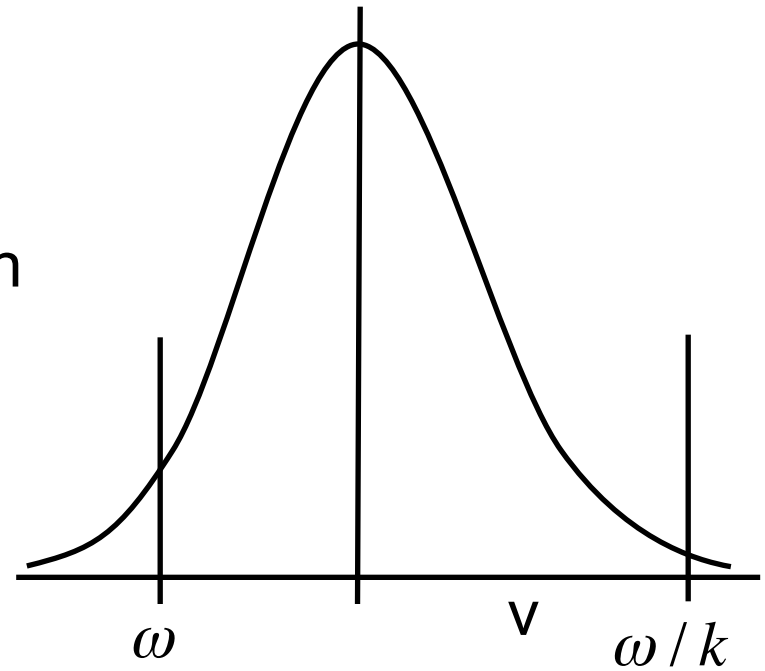
$$\tilde{n}_1 = ia_1 \left\langle \partial_v \frac{\beta}{\omega - k\beta v} \right\rangle \qquad 1 - \frac{\omega_p^2}{\omega^2} \left\langle \frac{\beta^2 + \beta' \omega / k}{\left(1 - k\beta v / \omega\right)^2} \right\rangle = 0$$

$$\omega_s^2 \approx \omega_p^2 \frac{v_0^2}{v_e^2}$$

- Plasma frequency reduced by $v_0/v_e$
- Both $\Delta t$ limits relaxed by same factor

# Expect grid instability to be much reduced

- Grid instability occurs for k near Brillouin zone limit
  - Damping of mode small due to being at tail of distribution
  - Growth due to interaction of alias with opposite side of distribution, giving Landau growth
- Grid instability growth rate scales with $\omega_e$, which is now much reduced
- SLPIC velocity distribution much changed, can it be tailored to prevent alias-induced Landau growth?
- NSF will determine whether we find out




$$\frac{\omega}{k - k_B} \qquad k_B = \frac{2\pi}{\Delta x} \qquad \omega / k$$

k larger in magnitude, phase velocity smaller, but on growth side of distribution

# Any changes to stability?

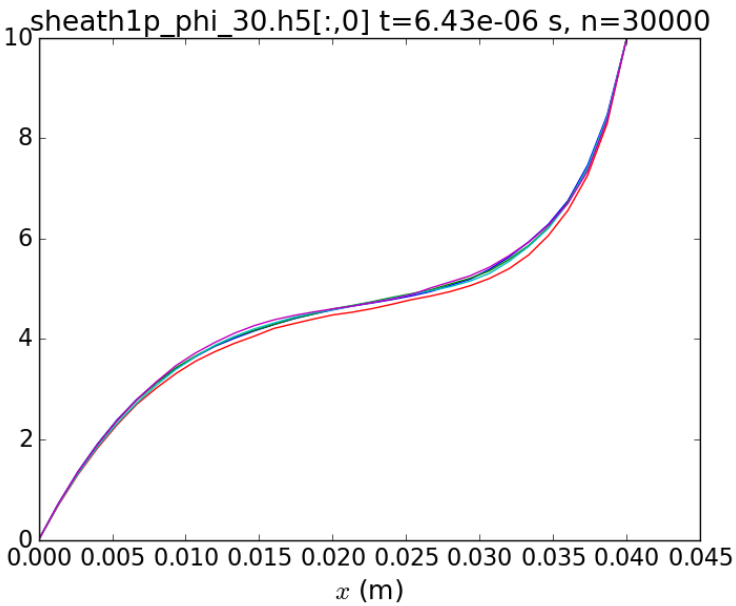
- $v_p \Delta t \leq \Delta x$: Relaxed by ratio of electron thermal velocity to perturbation velocity
- $\omega_e \Delta t \leq 1$: Relaxed by ratio of electron thermal velocity to perturbation velocity
- $\Delta x \leq \lambda_e$: Conjecture: much reduced
- EM CF (if relevant): the same

# Expect big gains in computational speeds when

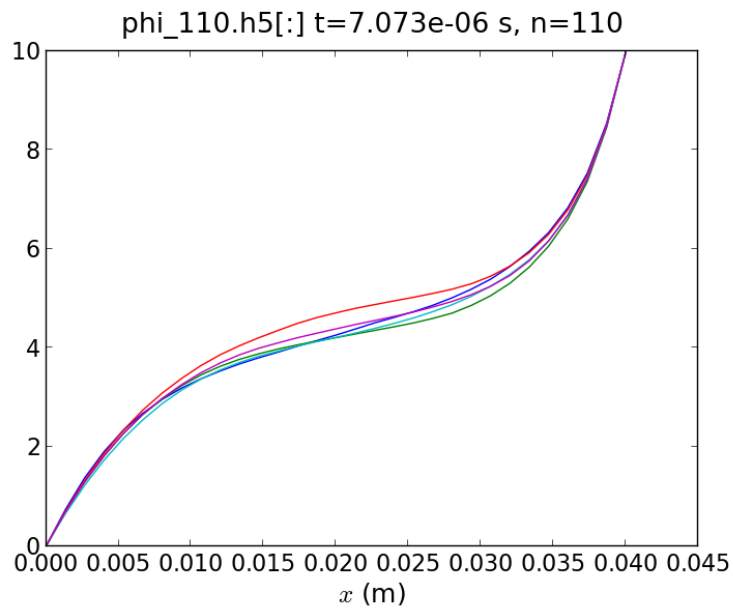
- $v_0 << v_e$
- Need not resolve electron plasma oscillations
- Especially good for $T_e > T_i$
- Example: plasma sheath

# SLPIC finds sheaths in many fewer steps

- In sheath, electron velocity distribution critical
- But Boltzmann approximation not accurate near boundary: at best a clipped Maxwellian




Standard PIC, 30000 steps for stability




SLPIC, 110 steps for stability

# Summary of SLPIC (but there's more)

- SLPIC speeds up simulations by slowing down particles
- The trajectories are the same, but they are traversed more slowly
- Gets around electron step limitations when simulating ion-scale phenomena
- Explicit, so very good for exascale
- Grid instability needs further research