Implicit multiscale PIC and related topics

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1. Direct-implicit PIC
2. Tunable damping in time advance of particles, EM field
3. Implicit multiscale PIC (IMSPIC)
4. Some current related work

Disclaimers

- This is a retrospective
  - I have not worked actively on this topic for some time
  - I suspect that this work is not widely known
  - I suspect the method has some general applicability
- It is a personal view, describing things I've been associated with
  - It is NOT a balanced history of implicit PIC
- Implicit multiscale PIC works, but unanswered questions remain; among them:
  - How to achieve efficiency on problems that are not "embarassingly multiscale" (large "macro" regions, small "micro" regions)
  - Relationship of implicit multiscale PIC to other methods

Thanks to my collaborators on direct-implicit and multiscale work: Bruce Langdon, Bruce Cohen, Scott Parker, Ned Birdsall, Scott Ray

1. Direct Implicit PIC

Implicit PIC is motivated by desire for large Δt (and large Δx)

- Kinetic effects are important to many plasma phenomena, even those associated with low frequencies

  In such cases, would like to use a large Δt; but explicit movers such as leapfrog are unstable for large steps, *e.g.*, $\omega_p \Delta t > 2$-ish

- Routes to large Δt
  - Eliminate high frequency modes from governing equations, *e.g.*, fluid models, quasineutral models
  - Capitalize on separation of scales - projection methods, etc.
  - Use implicit advance for stability with respect to under-resolved physics that is "unimportant," *e.g.*, in localized regions of high density

    Usually want "low-pass filter" to damp away the under-resolved degrees of freedom

    Damping is possible in explicit schemes, too, but does not increase allowable Δt

Direct-implicit algorithm is conceptually very simple*

A general difference scheme can be written as:

$$x_{n+1} = \tilde{x}_{n+1} + \beta \frac{q}{m} E_{n+1} \Delta t^2 \equiv \tilde{x}_{n+1} + \delta x$$
$$\rho_{n+1} = \tilde{\rho}_{n+1}(\{\tilde{x}_{n+1}\}) + \delta\rho(\{\delta x\})$$

where the correction δx is relative to the free-streaming “tilde” position. From the continuity equation:

$$\delta\rho(x) = -\nabla \cdot [\tilde{\rho}_{n+1}(x)\delta x(x)] = -\nabla \cdot [\chi(x) E_{n+1}(x)]$$

where

$$\chi(x) \equiv \beta \frac{q}{m} \tilde{\rho}_{n+1}(x) \Delta t^2 = \beta \omega_p^2(x) \Delta t^2$$

The field equation is thus:

$$\nabla \cdot E_{n+1}(x) = \rho_{n+1}(x) = \tilde{\rho}_{n+1}(x) - \nabla \cdot [\chi(x) E_{n+1}(x)]$$

* A. Friedman, A. B. Langdon, and B. I. Cohen, “A Direct Method for Implicit Particle-in-Cell Simulation,” *Comments on Plasma Physics and Controlled Fusion* **6**, 225 (1981).

This implementation of implicit "d1" advance uses a "final push" to x_n followed by a "pre-push" to an approximate x_{n+1}

It uses integer time levels, allowing changes of Δt "between steps"

"Final push":

(1) $\tilde{x} = x_{n-1} + \Delta t \; v_{n-1}$

(2) $a = (q/m) E_n(\tilde{x})$ (interpolation of field from mesh)

(3) $\bar{a}_{n-1} = \frac{1}{2}(a + \bar{a}_{n-2})$

(4) $v_n = v_{n-1} + \Delta t(\bar{a}_{n-1} + a)/2$

(5) $x_n = \tilde{x} + (\Delta t^2/2)a$

"Pre-push" to next time level:

(6) $\tilde{x} = x_n + \Delta t \; v_n$

(7) Using this new $\tilde{x}$, compute ρ and χ for the field solver

Note that this new ρ and χ are at time level n+1;
they allow us to solve for E_{n+1} knowing only the $\{X_n\}$

"Conventional" implicit PIC must obey a Δt constraint if a short scale length anywhere is to be resolved

- The need to resolve field variations (scale length λ) couples Δt and Δx:

Along orbit: $v\,\Delta t / \lambda < \varepsilon_1$ (1)

On grid: $\Delta x / \lambda < \varepsilon_2$ (2)

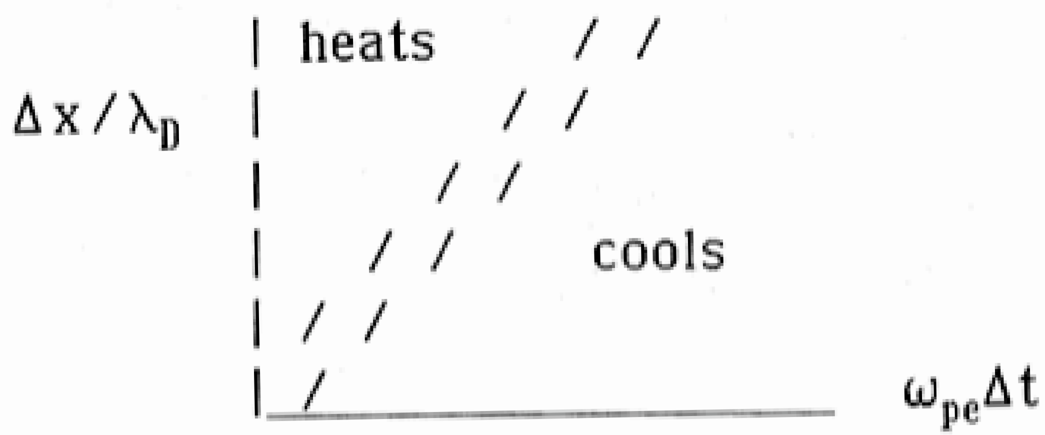
- In a sheath region, the relevant λ is the electron Debye length, λ_{De}

  Using (1) with the characteristic velocity $v = v_{Thermal,e}$, and noting that $\lambda_{De} = v_{Thermal,e} / \omega_{pe}$, the global constraint is $\omega_{pe}\Delta t < \varepsilon_1$

- In such cases, implicit PIC offers no timestep advantage over conventional explicit PIC

Limitations of “conventional” implicit PIC simulation

- There is a narrow “valley of goodness” (with small absolute energy error) in parameter space that well-behaved implicit PIC simulations should occupy*



The optimum lies along $v_{th}\Delta t/\Delta x \sim 0.3$ +- 0.1

- However, at large Δt the “valley” results from a balance between spurious heating and imposed damping; coherent structures may be replaced by random motions
- This motivates schemes with “tunable” damping - discussed next
- It also motivates use of independent particle timesteps - discussed later

*B. I. Cohen, A. B. Langdon, and A. Friedman, *J. Comp. Phys.* **46**, 15 (1982)

2. “Tunably” damped methods

Adjustable implicit particle advance is tunable between undamped and “d1” limits*

The algorithm is written here in a form that displays the time-centering:

$$v_{n+1} = v_n + \Delta t\ [a_{n+1} + \bar{A}_n]/2$$
$$x_{n+1} = x_n + \Delta t\ [v_n + (\Delta t/2)a_{n+1}]$$

where:

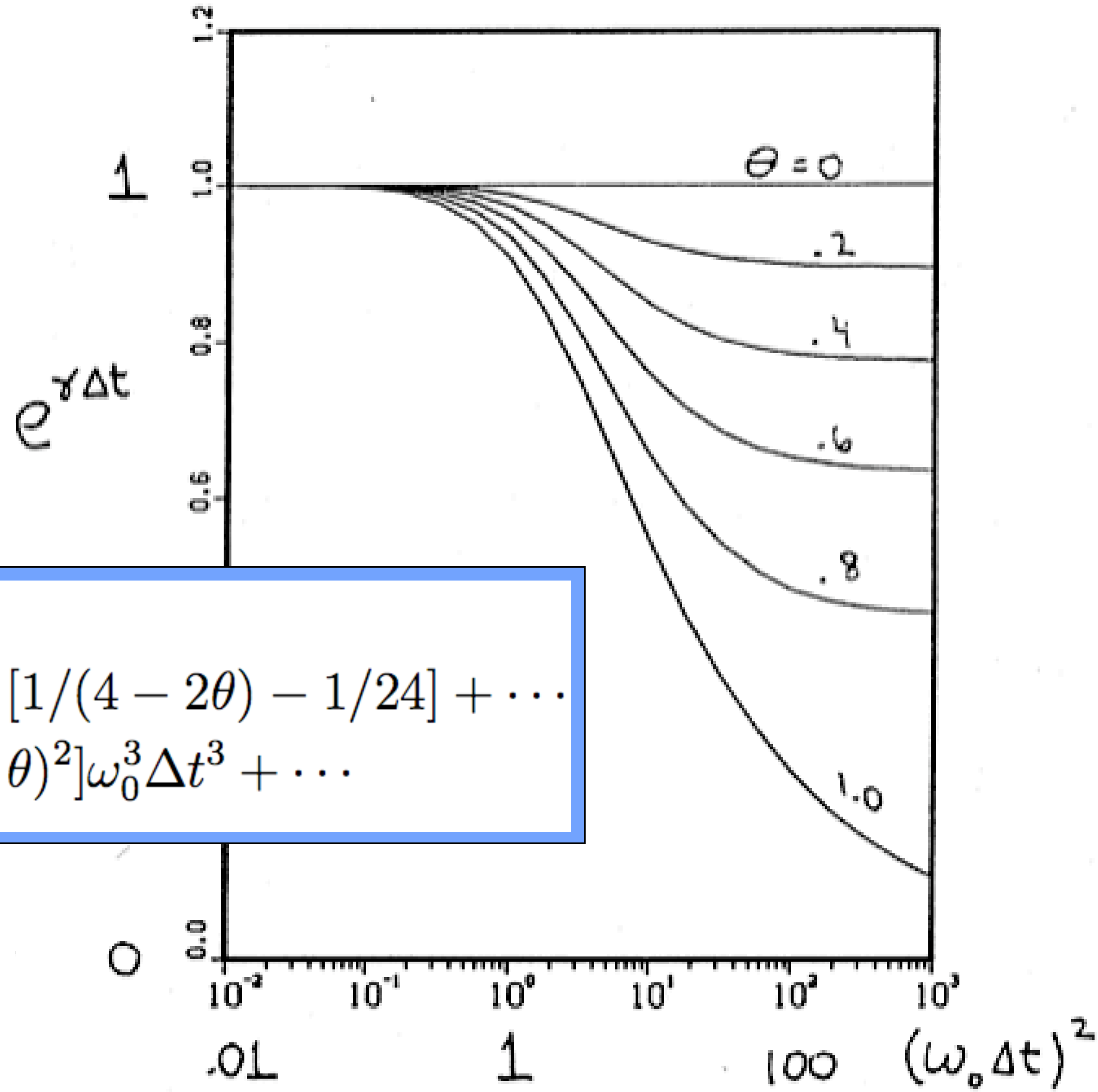
$$\bar{A}_n = (\theta/2)a_{n+1} + (1-\theta/2)\bar{a}_{n-1} \qquad \text{(temporary qty's)}$$
$$\bar{a}_{n-1} = (1-\theta/2)a_n + (\theta/2)\bar{a}_{n-2} \qquad \text{(running sums)}$$

The “blend” is adjustable between “d1” ($\theta = 1$)

and undamped “c0” ($\theta = 0$) limits

*A. Friedman, *J. Comp. Phys.* **90**, 292 (1990).

“Dispersion” of tunably-damped implicit mover is attractive



At small timestep:

$$\omega_r/\omega_0 = 1 - \omega_0^2 \Delta t^2 \left[1/(4-2\theta) - 1/24\right] + \cdots$$

$$\gamma/\omega_0 = -\theta/[2(2-\theta)^2]\omega_0^3 \Delta t^3 + \cdots$$

Tunably-damped mover offers flexibility

- By adjusting θ we can move the "valley of goodness" around in parameter space; this in itself has utility
- We'd like to actually widen the valley, perhaps by:
  - Using a different θ for each particle, depending upon its location in phase space
  - Using a different θ for each component of the motion, e.g., $\perp$, $||$
- To do this in a long simulation, must vary θ with time, for each particle. This can be done while preserving second-order accuracy.

- Explicit tunably-damped particle advances also exist
  - Derive by extrapolating E forward along the trajectory by one timestep: $E_{n+1} \Rightarrow 2E_n - E_{n-1}$
  - Simpler than implicit, may have utility, but I don't know of any examples

Damped implicit EM field advances have been developed

- As suggested in [A. Friedman, *J. Comp. Phys.* **90**, 292 (1990)], damping can be applied to time-domain electromagnetics by folding a tuning parameter into the method of [Hewett & Langdon, *JCP* **72**, 121 (1987)]:

$$E_{n+1} - E_n = c\Delta t \nabla \times B_{n+1/2} - 4\pi \Delta t J_{n+1/2}$$

$$B_{n+1/2} - B_{n-1/2} = -\frac{c\Delta t}{2} \nabla \times [E_{n+1} + \bar{A}_{n-1}]$$

where:

$$\bar{A}_{n-1} = (\theta/2)E_n + (1-\theta/2)\bar{E}_{n-2} \quad \text{(temporary qty's)}$$

$$\bar{E}_{n-1} = (1-\theta/2)E_n + (\theta/2)\bar{E}_{n-2} \quad \text{(running sums)}$$

- This method is used in the LSP code.

- Another proposed method [Langdon and Barnes, in *Multiple Time Scales* J. U. Brackbill and B. I. Cohen, Eds., Academic,1985, p. 335] blends d1 and leapfrog

  They suggest setting the d1 fraction nonzero only where cells are small, to enable violating the light-wave Courant condition locally
- I do not know if this method has been tested.

An explicit EM method has proven useful for noise reduction

- From [A. Friedman, *J. Comp. Phys.* **90**, 292 (1990)] :

$$\mathbf{E}_{n+1} = \mathbf{E}_n + c\,\Delta t\,\nabla\times\mathbf{B}_{n+1/2} - 4\pi\,\Delta t\,\mathbf{J}_{n+1/2}; \qquad (34a)$$

$$\mathbf{B}_{n+3/2} = \mathbf{B}_{n+1/2} - c\,\Delta t\,\nabla\times\left[\left(1+\frac{\theta}{4}\right)\mathbf{E}_{n+1} - \frac{1}{2}\mathbf{E}_n + \left(\frac{1}{2}-\frac{\theta}{4}\right)\bar{\mathbf{E}}_{n-1}\right], \qquad (34b)$$

where

$$\bar{\mathbf{E}}_{n-1} = \left(1-\frac{\theta}{2}\right)\mathbf{E}_n + \frac{\theta}{2}\bar{\mathbf{E}}_{n-2}. \qquad (35)$$

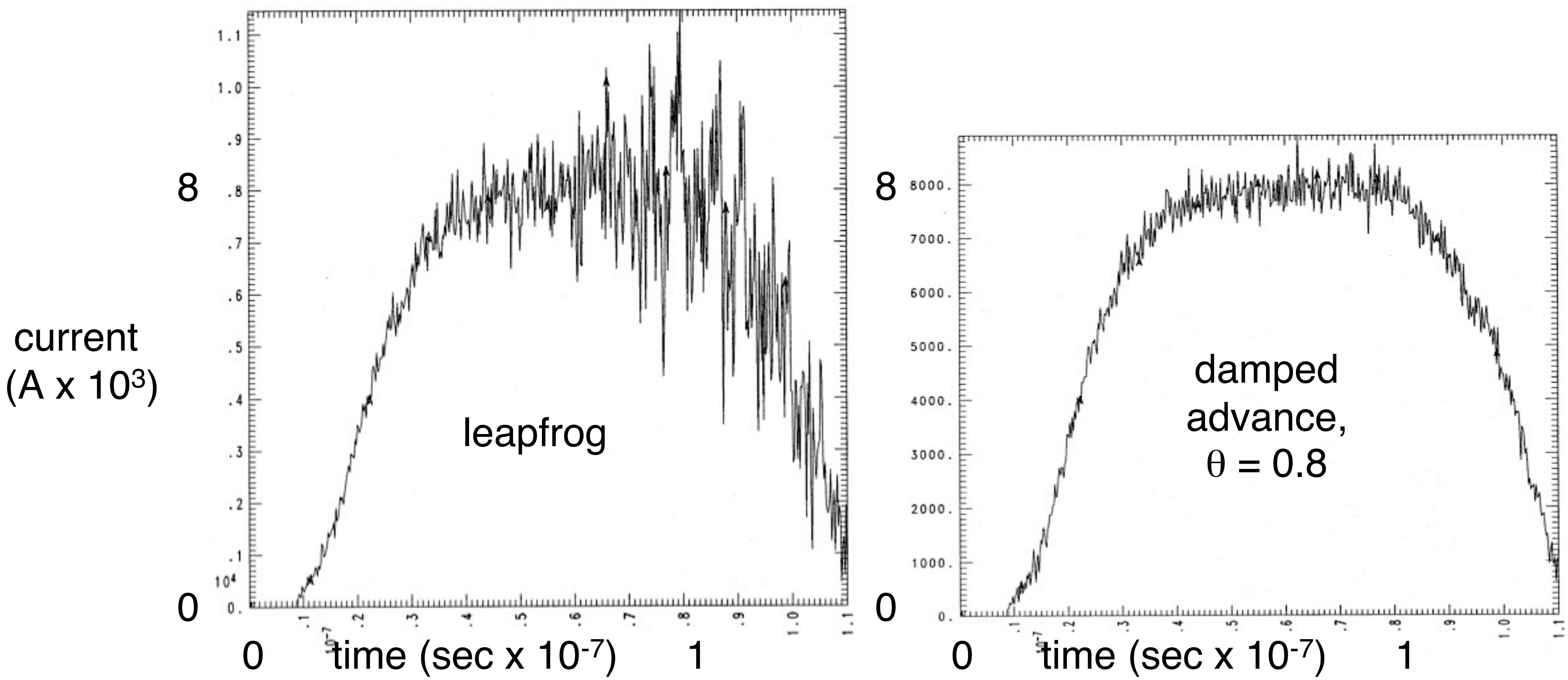
- In 1D with central differencing, a dispersion relation was obtained. Define $\Omega = (c\Delta t/\Delta x)\sin(k\Delta x/2)$. Then, for small timestep, the damping is:

$$\gamma\,\Delta t \approx -8\theta/(2-\theta)^2\,\Omega^4, \text{ and so } \gamma \propto (k\,\Delta x)^4.$$

- The method has attractive properties; see [Greenwood, *et al.*, *JCP* **201**, 665 (2004)]

Condor simulation of ATA injector (from 1990)*

- S. T. Brandon & J. K. Boyd studied how timing errors in the EM pulses that create the diode voltage affect the electron beam properties
- Here, the simulated history of the beam current vs. time at a downstream plane is corrupted by noisy fields that are generated by fluctuations in the particle injection



* A. Friedman, J. J. Ambrosiano, J. K. Boyd, S. T. Brandon, D. E. Nielson, Jr., and P. W. Rambo, “Damped Time Advance Methods for Particles and EM Fields,” *Proc. US-Japan Workshop on Advanced Computer Techniques Applied to Plasmas and Fusion*, Los Angeles, Sept. 26-8, 1990; LLNL Report UCRL-JC-106050

3. Implicit Multiscale PIC

Want to overcome limitations of "conventional" implicit PIC

- Advance each particle using a timestep that resolves the local field variations (assumed to be at scale of the grid spacing)
- Implicitness to:
  - Afford stability with $\Delta t > \tau_{plasma}$ and $\Delta x > \lambda_{Debye}$

    in *selected* regions of phase space where that physics is deemed unimportant

    … requires judgment on part of user, and/or smart controls
  - afford a time-centered, second-order-accurate scheme

The scheme builds upon direct-implicit PIC

- The field equation solved at every step is:

  $\nabla \cdot (1+\chi)\nabla\phi = \rho$, with $\chi(x) = \frac{1}{2}\omega_p^2 \Delta t^2$.

- By this method, the deposition of charge occurs *implicitly*, one step earlier than in an explicit code.

- We use this to let an infrequently-processed block (with associated timestep size $\Delta t = j\delta t$) deposit its information j time levels ahead of the current one.

- This information is then interpolated backward in time to yield the data needed to produce the field a single time level ahead.

- As particles move about, it is necessary to change their Δt's (move them from block to block), in order to preserve the accuracy of their orbits and the deposited charge density.

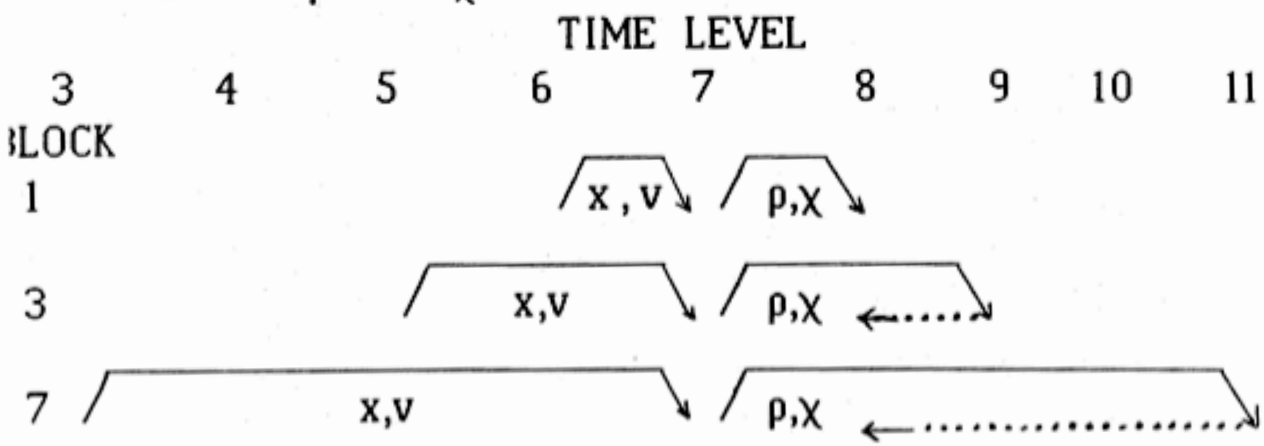
Timestep sizes are all multiples of some smallest "micro" step size; field-solve is done every micro-step

Particles are kept sorted into blocks. For every block k, there is an associated Δt_k; the large timestep used for particles in large cells should help suppress the finite-grid instability. The electron blocks might be:

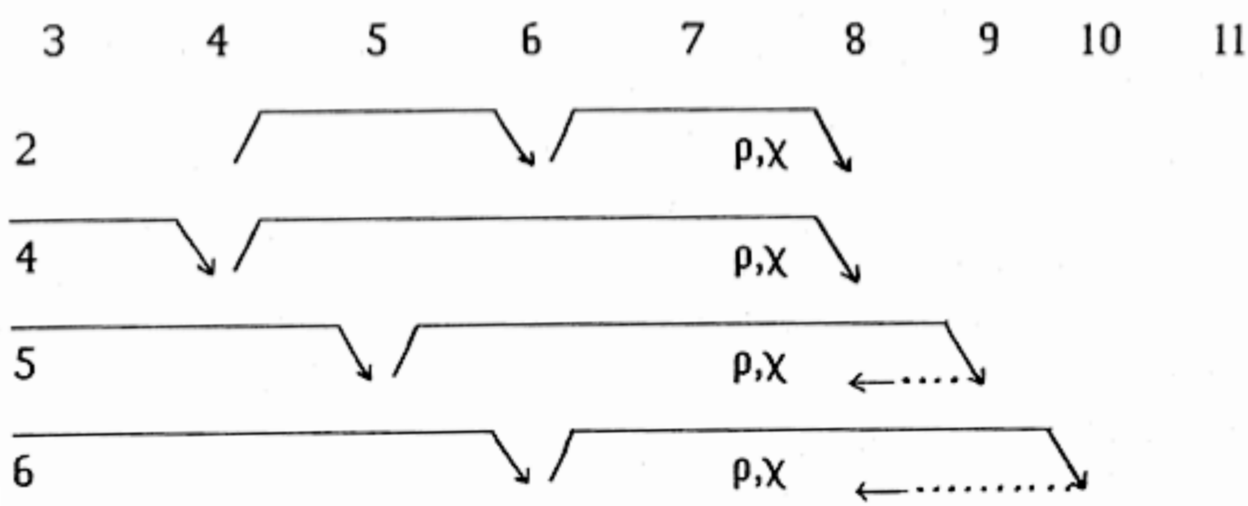
Block e1: push every step
Block e2: push on even-numbered steps
Block e3: push on odd-numbered steps
Block e4: push if (step number mod 4) = 0
Block e5: push if (step number mod 4) = 1
Block e6: push if (step number mod 4) = 2
Block e7: push if (step number mod 4) = 3

A timeline shows the procedure for both active and inactive blocks

- Dots with a back-arrow denote interpolation in time of ρ and χ.



The other blocks were advanced on earlier steps, and we need only interpolate their contributions to ρ,χ back to tl 8 before the field-solve:



To change step size, must generate new lag-averaged fields

For a particle that has moved to a point (x_n, v_n) where $\tau \equiv \Delta t(x_n, v_n) < \Delta t / r$, set $\bar{a}_{n-1} \Rightarrow (a + \bar{a}_{n-1})/2$, and set “new block” flag.

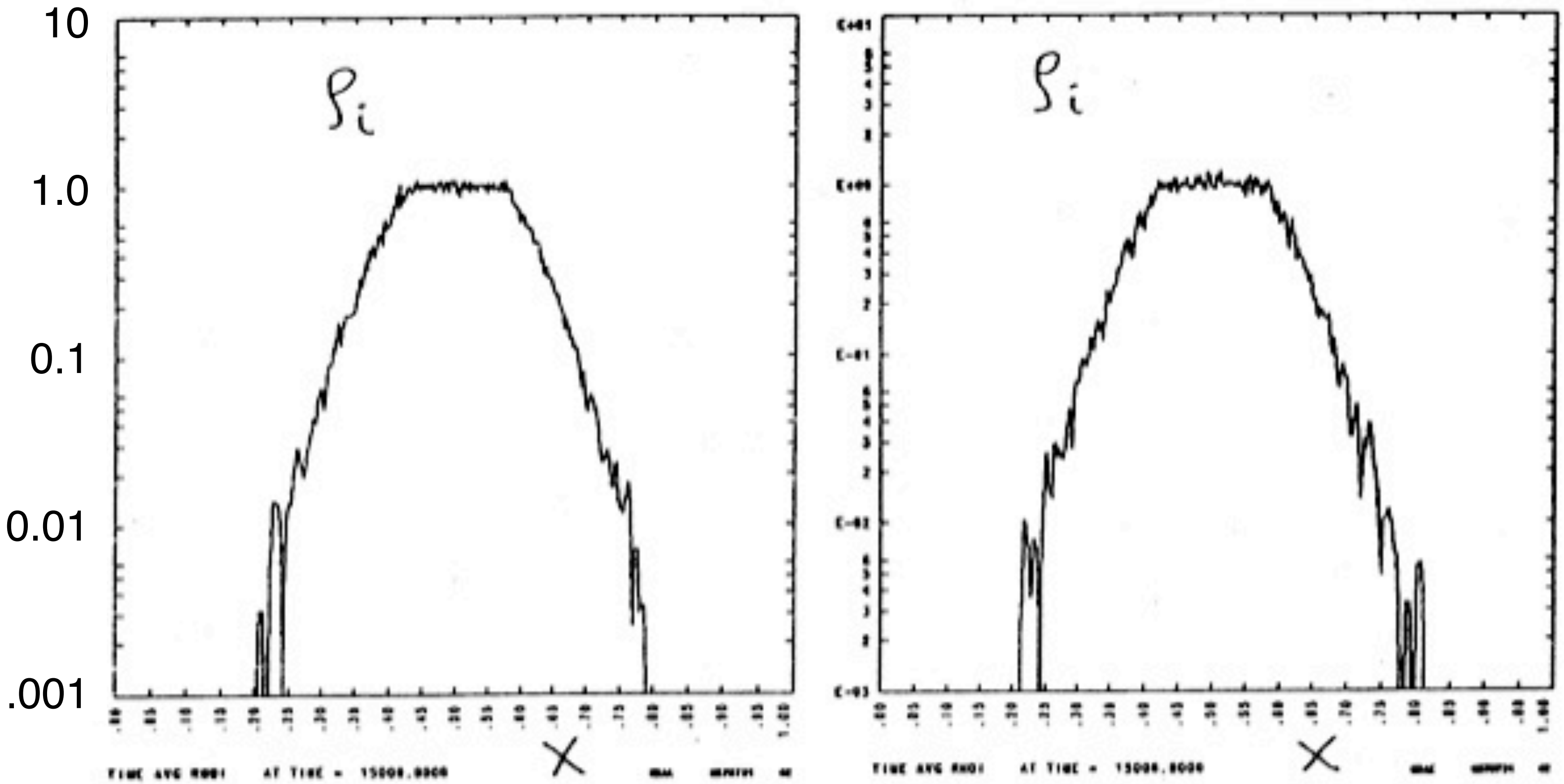
For particles that have moved to a point (x_n, v_n) where $\tau \equiv \Delta t(x_n, v_n) > r\,\Delta t$, set $\bar{a}_{n-1} \Rightarrow \bar{a}_{\mathrm{old}}$, and set “new block” flag.

We have used either $r = \sqrt{2}$ or $r = 2$; the latter offers useful hysteresis.

Our first tests* established method as a useful approach to “subcycling”

In a series of runs, free expansion of a plasma slab was studied

no subcycling — ions advanced every 8th step

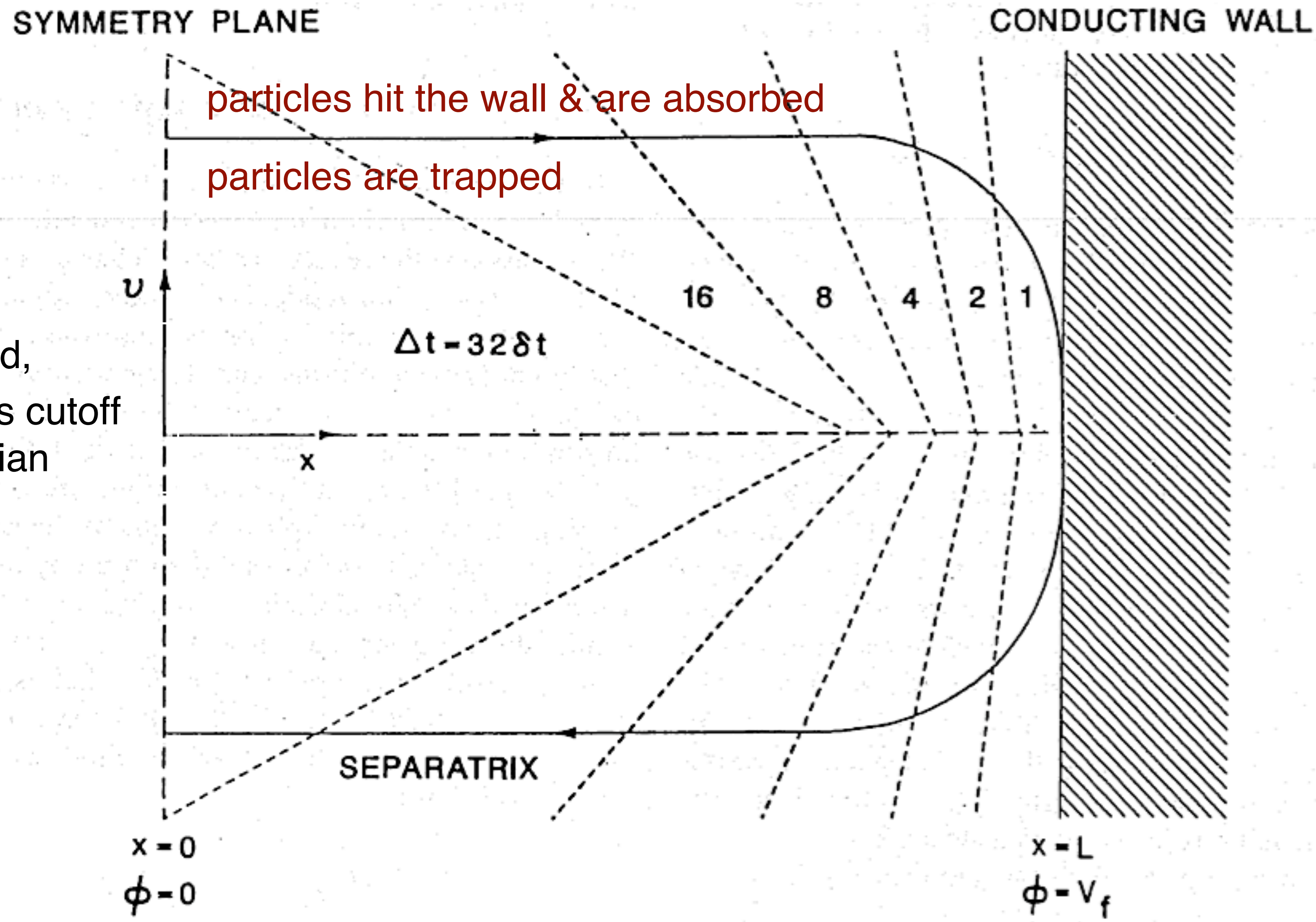


*A. Friedman, S. E. Parker, S. L. Ray, and C. K. Birdsall, “Multi-Scale Particle-in-Cell Plasma Simulation,” *J. Comp. Phys*. **96**, 54 (1991).

Our later work* examined a sheath near a "floating" wall

ions fixed,

electrons cutoff Maxwellian



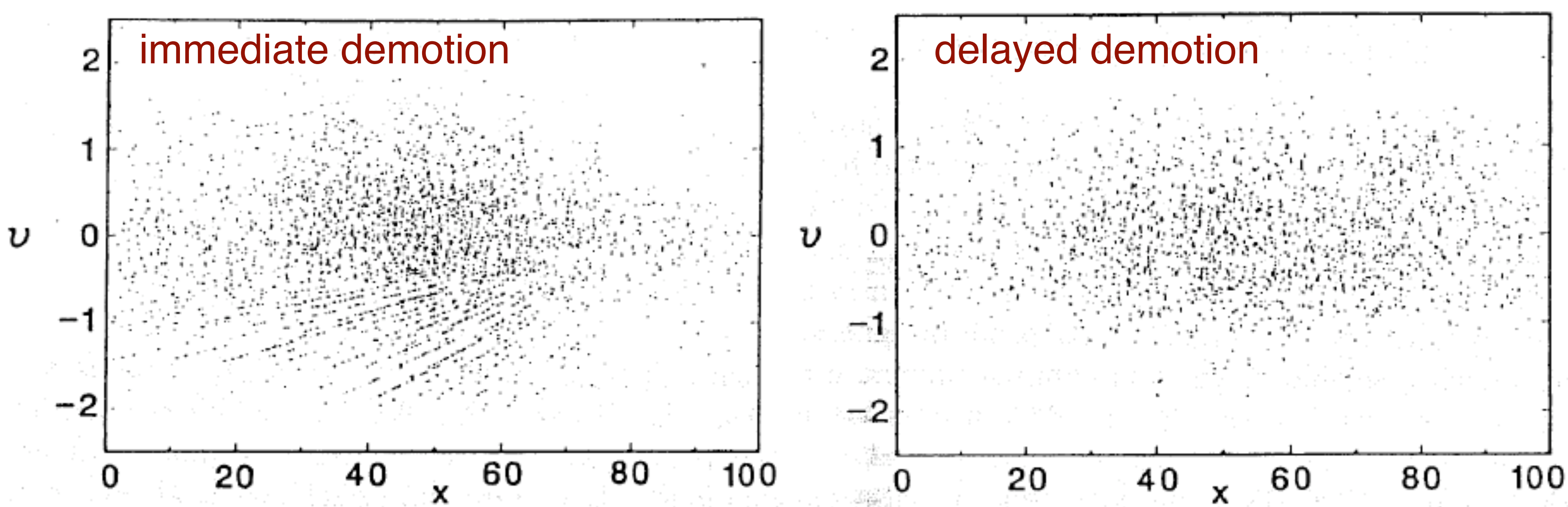
* S. E. Parker, A. Friedman, S. L. Ray, and C. K. Birdsall, "Bounded Multi-Scale Plasma Simulation: Application to Sheath Problems," *J. Comp. Phys*. **107**, 388 (1993).

Timestep size control is an “art” as much as a “science”

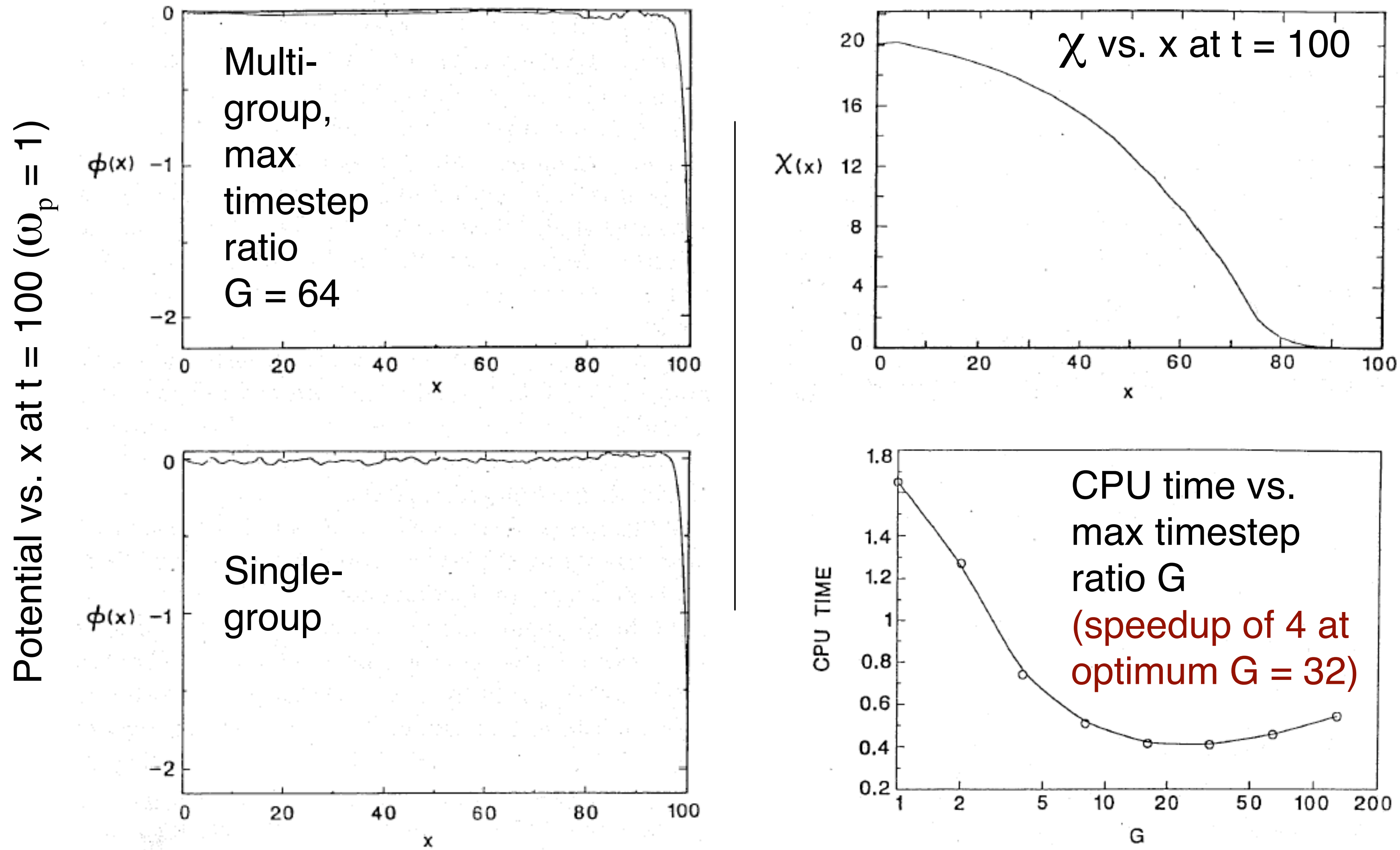
- Seek to control truncation error
  - Static control associates *ab initio* a step size τ with each location in phase space
  - Dynamic control sets τ based on evolving gradients, etc.
- In the sheath application, particle travel through the sheath (∂_xE), rather than the time-dependent variation of E, is most limiting
  - Would like to limit $|kv\Delta t| < \varepsilon_1$, where $k \sim \partial_x$E/E . However, if E and ∂_xE are fluctuating about zero (as is often the case), then where E ~ 0 there may be spuriously large values of k
  - It’s somewhat easier to limit $\omega^2_{\mathrm{trap}}\,\Delta t^2 \equiv (q/m)|\partial_x E|\Delta t^2 < \varepsilon_2$ by computing $|\partial_x E|$ on the grid
  - For our sheath work we used static control

Particle “promotion” to smaller Dt and “demotion” to larger Dt must be handled carefully

- Look ahead by $Cv\Delta t$, where C is a constant, and see if particle will enter a spatial region wherein $\omega^2_{\mathrm{trap}}\,\Delta t^2 < \varepsilon_2$. This produces lines in phase space with slope that are the boundaries between Δt groups.
- Choose $C > 2$ so that a particle will be promoted to smaller Δt soon enough to “keep up” with the constraint; can’t allow more than a halving of Δt in a single step.
- When “demoting” particles to larger Δt at a timestep boundary, an empty “wedge” in phase space is created; avoid by delaying demotion of half the particles by a step.



Application to sheath showed effectiveness of method



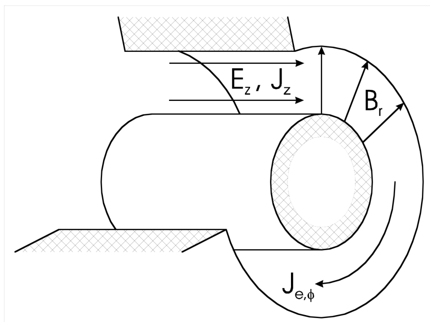
Another series of runs examined propagation of an ion acoustic shock front toward a conducting absorbing plate; see paper by Parker, *et al.*

4. Current related work

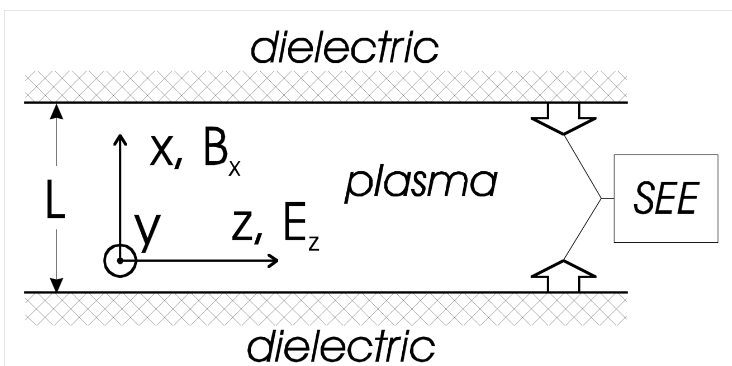
Simulations of secondary electron emission (SEE) effects in a plasma slab in crossed electric and magnetic fields

[Sydorenko, Smolyakov, 46th APS DPP, Savannah GA, 2004, NM2B.008]

Hall thruster, cylindrical geometry:



1D3V PIC simulations, plane geometry, approximation of accelerating region of a Hall thruster:



Motivation:

Electron temperature in the accelerating region of a Hall thruster (40 eV) is higher than the temperature of charge saturation of SEE in Maxwellian plasma (17 eV). [Staack, Raitses, Fisch, *Appl. Phys. Lett.* 84, 3028 (2004).]

Objective:

The investigation of modification of electron velocity distribution function by SEE effects.

Simulation requirements:

Both the sheath and the bulk plasma must be resolved.

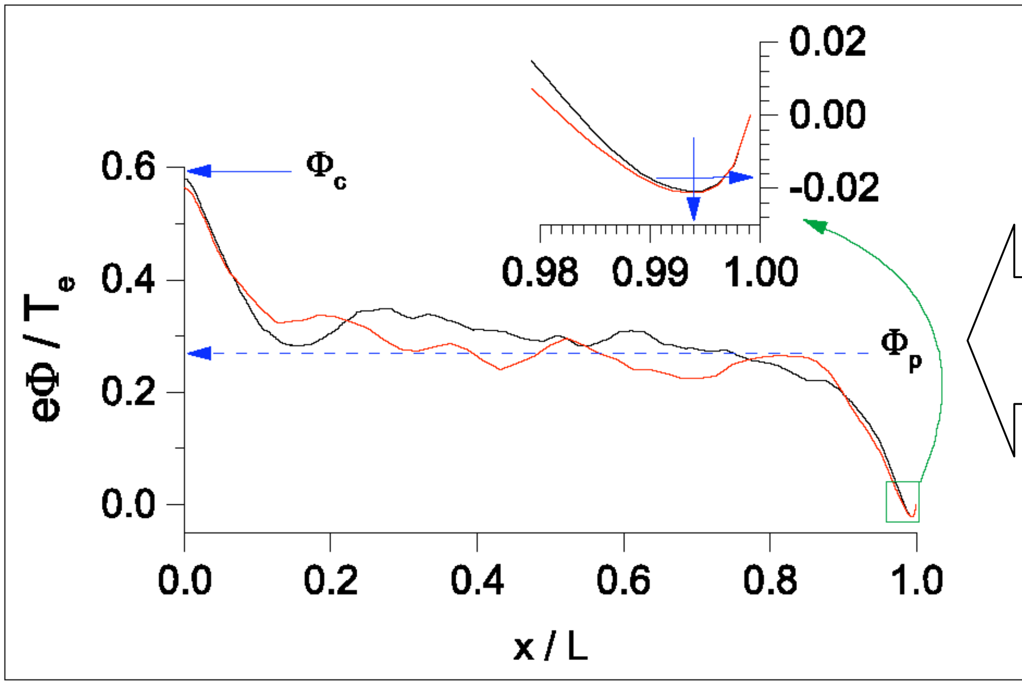
PIC code:

Electrostatic implicit multi-scale with non-uniform grid constant in time. [Friedman, Parker, Ray, Birdsall, *J. Comput. Phys.* 96, 54 (1991).] The external fields B_x and E_z are assumed constant.

Simulations of SEE effects in a plasma slab …
Benchmarking of the multi-scale code

The code was applied to simulations of the region between the Maxwellian plasma source (x=0) and the wall with SEE (x=L). No collisions, zero external fields.

Such a problem was considered by Schwager [*Phys. Fluids* B 5, 631 (1993)]



Snapshots of profile of potential.

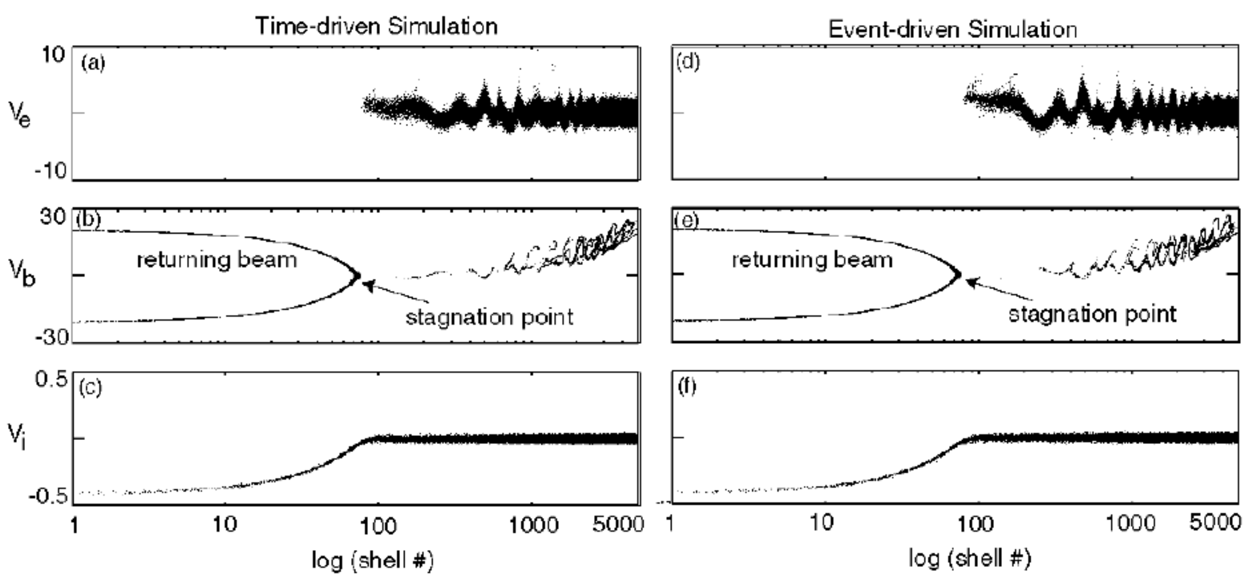
The insert figure zooms into the potential dip near the emitting wall.

- Blue arrows – Schwager's data.
- Black curves – uniform grid, $\Delta x = \lambda_{De}/32, \Delta t = 1/(4\omega_{pe})$
- Red curves – nonuniform grid, $\Delta x_{\min} = \lambda_{De}/32, \Delta x_{\max}/\Delta x_{\min} = 16;$ $\Delta t_{\min} = 1/(128\omega_{pe}), t_{\max}/\Delta t_{\min} = 64$

- The results of the single-scale and multi-scale simulations are close to each other and reproduce the results of Schwager.
- The multi-scale simulation is 8 times faster than the single scale simulation.

Discrete Event Simulation is an alternative approach

- DES PIC has similar goals to Implicit Multi-Scale PIC but differs fundamentally
  - Event-driven, not time-driven
  - Particle timesteps fully independent, asynchronous
  - Not (necessarily) implicit
- Builds on established discrete-event methodology
- Incremental field solution may be a challenge
- Successfully applied to spacecraft charging in 1D spherical geometry*:



*H. Karimabadi, J. Driscoll, Y. A. Omelchenko, and N. Omidi,to be publ. in *JCP*

Self-consistent e-i simulation of ion beams requires technique to bridge timescales*

- Need to follow electrons through strongly magnetized and unmagnetized regions ⇒ need to deal with electron cyclotron timescale, ~ 10^{-11} sec.
- Ion timescales 10^{-10} to > 10^{-8} sec.
- Parker & Birdsall (JCP '91) showed that standard "Boris" mover at large $\omega_c \Delta t$ produces correct **E**x**B** and magnetic drifts, but …
  - anomalously large "gyro" radius (~ $\rho\ \omega_c \Delta t$) [problematic for us]
  - anomalously small "gyro" frequency [OK for us]
- Our solution: interpolation between Boris mover and drift kinetics (motion along B, plus drifts).

$$\mathbf{v}_{new} = \mathbf{v}_{old} + \Delta t \left(\frac{d\mathbf{v}}{dt}\right)_{Lorentz} + (1-\alpha)\left(\frac{d\mathbf{v}}{dt}\right)_{\mu\nabla B}$$

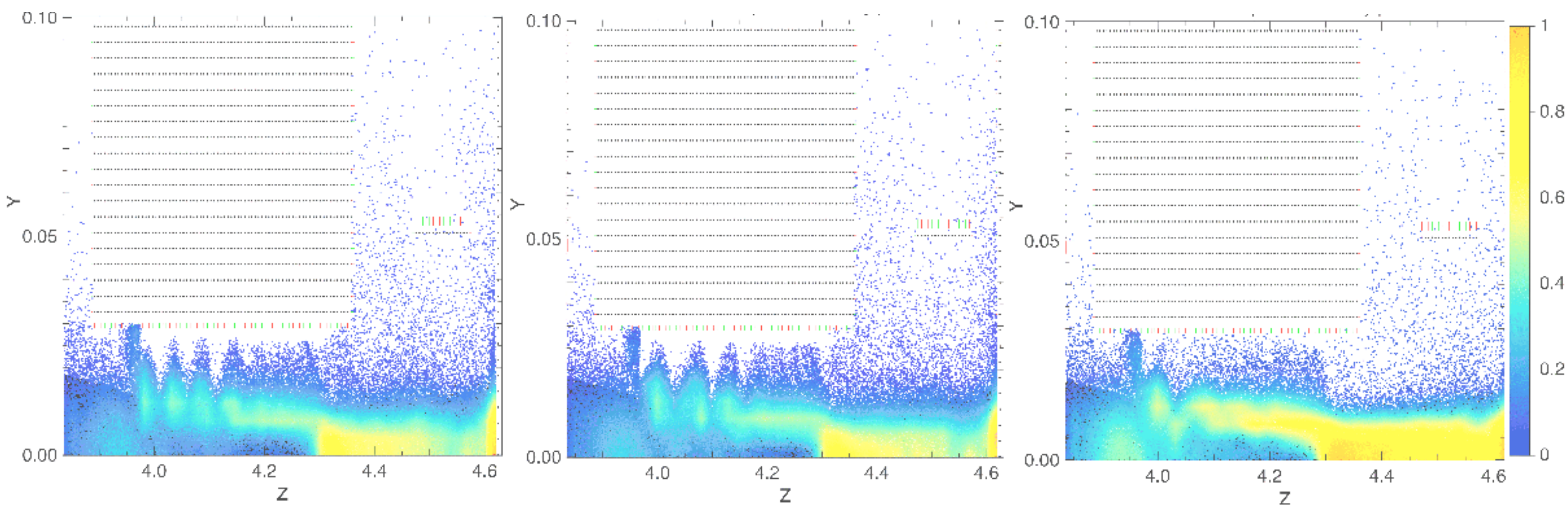
$$\mathbf{v}_{eff} = \mathbf{b}(\mathbf{b}\cdot\mathbf{v}) + \alpha\mathbf{v}_{\perp} + (1-\alpha)\mathbf{v}_d$$

* R. H. Cohen, A. Friedman, M. Kireeff Covo, S. M. Lund, A. W. Molvik, F. M. Bieniosek, P. A. Seidl, J.–L. Vay, P. Stoltz and S. Veitzer, "Simulating Electron Clouds in Heavy-Ion Accelerators," to be published in *Phys. Plasmas*.

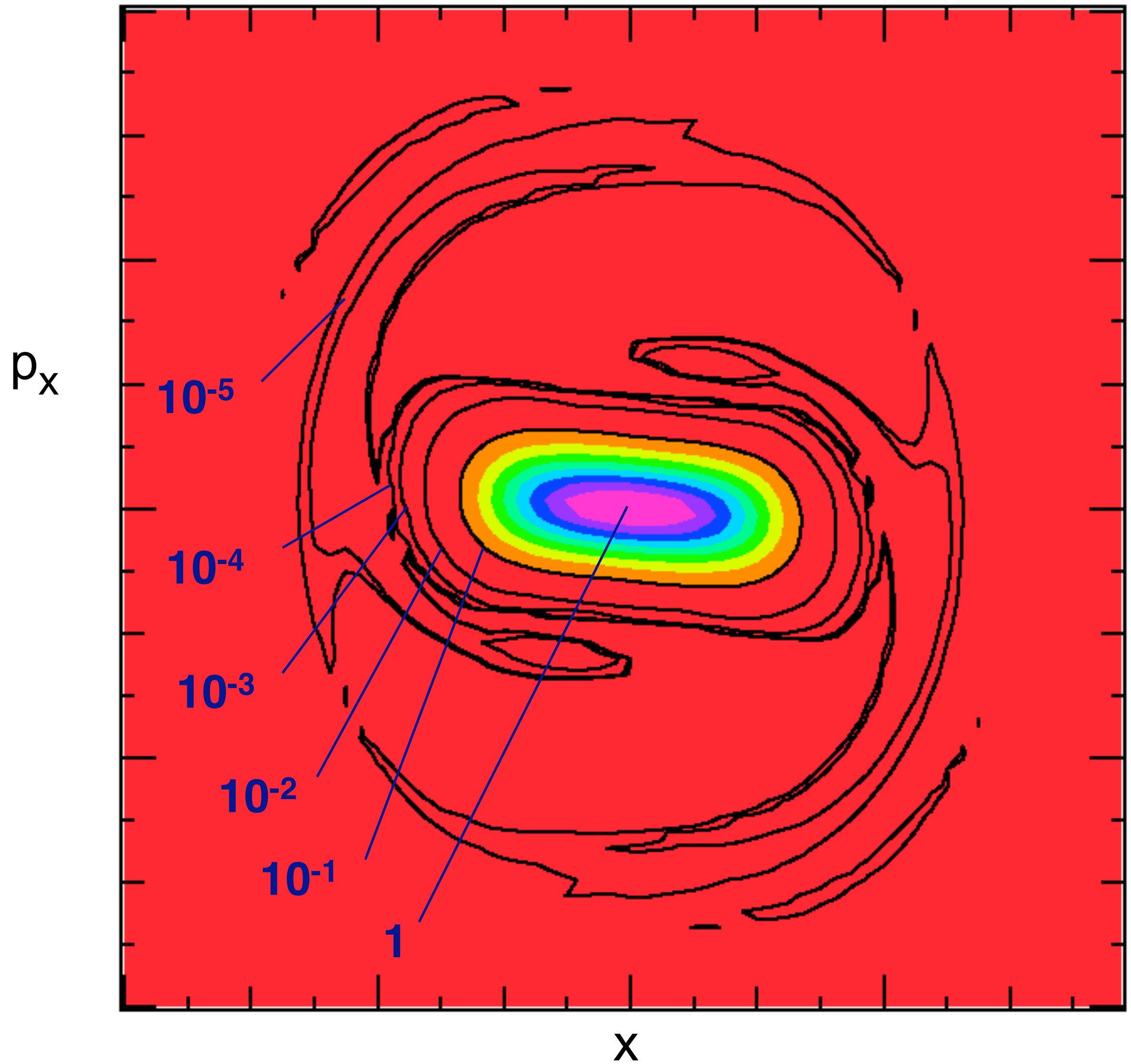
Interpolated mover enables bridging over electron cyclotron timescale

- The particular choice: $\alpha=1/[1+(\omega_c\Delta t/2)^2]^{1/2}$ gives
  - physically correct “gyro” radius at large $\omega_c\Delta t$
  - correct drift velocity and parallel dynamics
- Interpolated mover subjected to a number of tests and does well. e.g.: simulation of distribution of electrons in last magnetic quad of HCX:

small δt (1/10) interpolated mover Boris/Parker-Birdsall

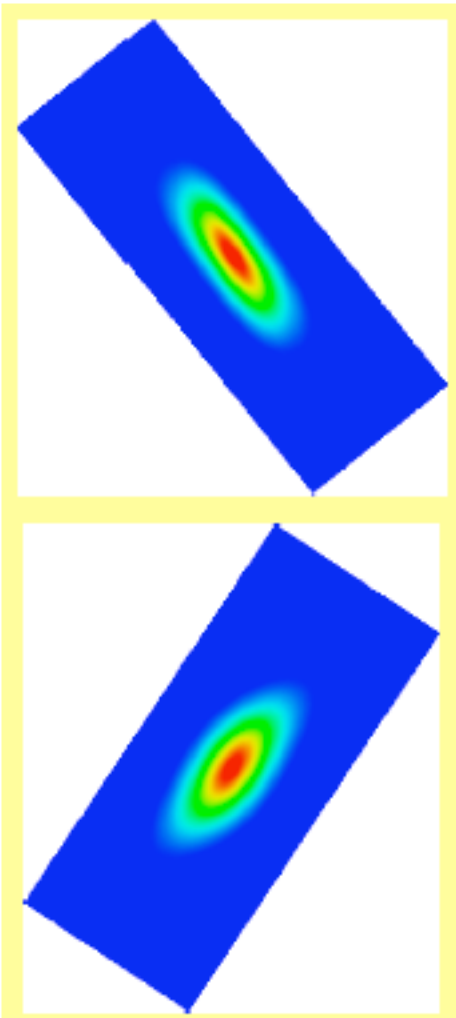


Solution of Vlasov equation on a grid in phase space offers low noise, large dynamic range for beam halo studies



4D Vlasov testbed (with constant focusing) showed structure of the halo in a density-mismatched beam

New ideas: moving grid to model time-dependent applied field, AMR-Vlasov to resolve fine structures



moving phase-space grid, based on non-split semi-Lagrangian advance [E. Sonnendrucker, F. Filbet, A. Friedman, E. Oudet, J.-L. Vay, *CPC*, 2004]

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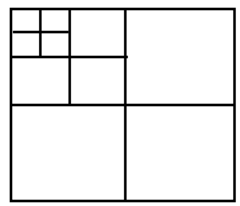

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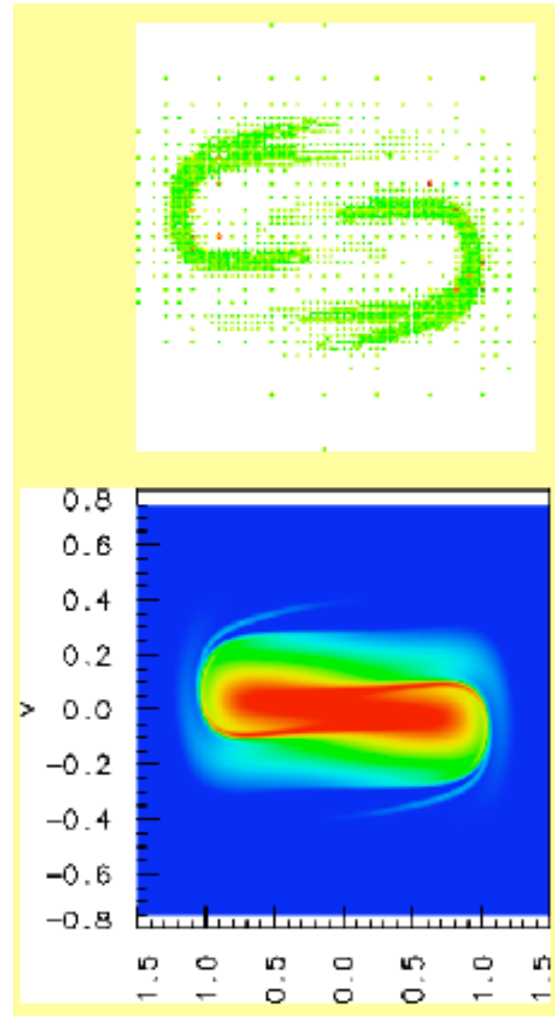

adaptive mesh [N. Besse, F. Filbet, M. Gutnic, I. Paun, E. Sonnendrucker, in *Numerical Mathematics and Advanced Applications, ENUMATH 2001,* F. Brezzi, A. Buffa, S. Corsaro, A. Murli (Eds), (Springer, 2003).]

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- A. Friedman, A. B. Langdon, and B. I. Cohen, "A Direct Method for Implicit Particle-in-Cell Simulation," *Comments on Plasma Physics and Controlled Fusion* **6**, 225 (1981).
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- B. I. Cohen, A. B. Langdon, and A. Friedman, "Smoothing and Spatial Grid Effects in Direct Implicit Plasma Simulation," *J. Comp. Phys.* **56**, 51 (1984).

<u>Tunably-damped particle mover and EM field advance (implicit and explicit)</u>

- A. Friedman, "A Second Order Implicit Particle Mover with Adjustable Damping," *J. Comp. Phys.* **90**, 292 (1990).
- A. D. Greenwood, K. L. Cartwright, J. W. Luginsland, and E. A. Baca, "On the Elimination of Numerical Cerenkov Radiation in PIC Simulations," *J. Comp. Phys*. **201**, 665 (2004).

<u>Implicit Multiscale PIC</u>

- A. Friedman, S. E. Parker, S. L. Ray, and C. K. Birdsall, "Multi-Scale Particle-in-Cell Plasma Simulation," *J. Comp. Phys*. **96**, 54 (1991).
- S. E. Parker, A. Friedman, S. L. Ray, and C. K. Birdsall, "Bounded Multi-Scale Plasma Simulation: Application to Sheath Problems," *J. Comp. Phys*. **107**, 388 (1993).

<u>Drift-kinetic / Newton "blend" mover (explicit)</u>

- R. H. Cohen, A. Friedman, M. Kireeff Covo, S. M. Lund, A. W. Molvik, F. M. Bieniosek, P. A. Seidl, J.–L. Vay, P. Stoltz and S. Veitzer, "Simulating Electron Clouds in Heavy-Ion Accelerators," to be published in *Phys. Plasmas*. A *J. Comp. Phys*. manuscript is in preparation.

IMSPIC works, but unanswered questions remain

Among them:

- How to achieve efficiency on problems that are not “embarassingly multiscale” (large “macro” regions, small “micro” regions)
- Relationship of implicit multiscale PIC to other methods

These slides are available at:

http://hifweb.lbl.gov/public/slides/Friedman-IPAM05.pdf

EXTRAS

Implicit "d1" advance is simple and popular

This version uses "integer time levels," allowing changes of Δt "between steps"

$$v_{n+1} = v_n + \Delta t\, [(3/2)a_{n+1} + (1/2)\bar{a}_{n-1}]/2$$

$$x_{n+1} = x_n + \Delta t\, [v_n + (\Delta t/2)a_{n+1}]$$

where:

$$\bar{a}_{n-1} = (1/2)a_n + (1/2)\bar{a}_{n-2} \qquad \text{(running sums)}$$

"Dispersion" at small timestep is:

$$\omega_r/\omega_0 = 1 - 11/24\, \omega_0^2 \Delta t^2 + \cdots$$

$$\gamma/\omega_0 = -1/2\, \omega_0^3 \Delta t^3 + \cdots$$

An analysis of the d1 mover in a "fixed" harmonic well suggests stability for any timestep size

$$\frac{1}{[(2/\omega_0\Delta t)\sin(\omega\Delta t/2)]^2} = \frac{2e^{-i\omega\Delta t}-1}{e^{-2i\omega\Delta t}}$$

with small timestep limits:

$$\omega_r/\omega_0 = 1 - 11/24\,\omega_0^2\Delta t^2 + \cdots$$
$$\gamma/\omega_0 = -1/2\,\omega_0^3\Delta t^3 + \cdots$$

- This expression, with stability for any Δt, obtains when the future field is interpolated at the true future positions
- However, it is usual to interpolate at the "~" positions; in that case the exact relation* replaces: $(\omega_0\Delta t)^2 \Rightarrow (W_0\Delta t)^2 = (\omega_0\Delta t)^2 / [1 - (\omega_0\Delta t)^2/2]$, and orbits are unstable *in a fixed well* for $(\omega_0\Delta t)^2 > 2.4$
- Electrostatic simulations with such codes are observed to be stable!

  This is a consequence of the implicit fieldsolver's reducing the restoring acceleration from $(-\omega_p^2 x)$ to $[-\omega_p^2 x / (1+\chi)]$, where $\chi = \omega_p^2\Delta t^2/2$

*A. Friedman, *J. Comp. Phys.* 90, 292 (1990)

Timestep limitations of “conventional” implicit PIC simulation

- A transit-time limitation: $kv_e\Delta t \lesssim 1$.
  Necessary for accuracy in a direct-implicit code.
  Necessary for stability in a moment-implicit code (?).

- A need to resolve trapping oscillations:
  Evaluation of δx at $\tilde{x}$ instead of at x_{n+1} leads to errors $\sim\delta x \cdot \nabla E$. The relative error is $(\omega_{trap}\Delta t)^2$, which must be small for the linearization to be valid; here $\omega_{trap} \equiv \sqrt{|\nabla a|}$. Numerical instability can result for many implementations if this condition is violated.

- The above condition can be rewritten as:
  $(kv_e\Delta t)^2 q\phi/T \lesssim 1$, so that if $kv_e\Delta t$ is $\lesssim 1$ there is the constraint: $q\phi \lesssim T$.

- In a grossly non-neutral region where $\rho_{net} \approx \rho_e$, the restriction on $(\omega_{trap}\Delta t)^2 \approx (\omega_{pe}\Delta t)^2 \rho_{net}/\rho_e$ implies that $\omega_{pe}\Delta t$ must be less than unity.

Explicit tunably-damped particle advances also exist

- They are obtained by extrapolating the electric component of the acceleration forward along the trajectory by one timestep: $a_{n+1} \Rightarrow 2a_n - a_{n-1}$
- At $\theta = 0$ the explicit scheme is just leapfrog
- Stability limits are slightly more severe than leapfrog when $\theta > 0$
- Damping at small Δt is identical to that of implicit scheme; real frequency shift is different:

$$\omega_r/\omega_0 = 1 - \omega_0^2 \Delta t^2 \left[\theta/4(2-\theta) - 1/24\right] + \cdots$$
$$\gamma/\omega_0 = -\theta/[2(2-\theta)^2]\omega_0^3 \Delta t^3 + \cdots$$

- These schemes are simpler than implicit and may have utility …

  … but I don't recall any examples

An explicit EM method has proven useful for noise reduction

- From [A. Friedman, *J. Comp. Phys.* **90**, 292 (1990)] :

$$\mathbf{E}_{n+1} = \mathbf{E}_n + c\,\Delta t\,\nabla\times\mathbf{B}_{n+1/2} - 4\pi\,\Delta t\,\mathbf{J}_{n+1/2}; \tag{34a}$$

$$\mathbf{B}_{n+3/2} = \mathbf{B}_{n+1/2} - c\,\Delta t\,\nabla\times\left[\left(1+\frac{\theta}{4}\right)\mathbf{E}_{n+1} - \frac{1}{2}\mathbf{E}_n + \left(\frac{1}{2}-\frac{\theta}{4}\right)\bar{\mathbf{E}}_{n-1}\right], \tag{34b}$$

where

$$\bar{\mathbf{E}}_{n-1} = \left(1-\frac{\theta}{2}\right)\mathbf{E}_n + \frac{\theta}{2}\bar{\mathbf{E}}_{n-2}. \tag{35}$$

On a one-dimensional spatial lattice with central differencing, a dispersion relation for a mode with spatial wavenumber k can be obtained. Defining $\Omega \equiv (c\,\Delta t/\Delta x)\sin(k\,\Delta x/2)$, one finds

$$\sin^2\left(\frac{\omega\,\Delta t}{2}\right) = \Omega^2\left[1 - \frac{2\theta\sin^2(\omega\,\Delta t/2)}{2e^{-i\omega\,\Delta t}-\theta}\right]. \tag{36}$$

For small $\omega\,\Delta t$, the damping is $\gamma\,\Delta t \approx -8\theta/(2-\theta)^2\,\Omega^4$, and so $\gamma \propto (k\,\Delta x)^4$.

- The method has attractive properties; see [Greenwood, *et al.*, *JCP* **201**, 665 (2004)]

The operations carried out at “timestep 7” are:

- Let us abbreviate "time-level" by "tl"; the code:

  Blocks 1: Advances x,v from tl 6 to tl 7;
  computes contribution to ρ,χ at tl 8.
  Blocks 3: Advances x,v from tl 5 to tl 7;
  computes contribution to ρ,χ at tl 9.
  Blocks 7: Advances x,v from tl 3 to tl 7;
  computes contribution to ρ,χ at tl 11.

- After the active particles have been pushed to tl 7 (and before their ρ and χ contributions have been accumulated), they are moved, if their (x,v) so dictate, to new blocks. Redistribution is always into a block which is active.

  For example, if at the end of the push phase of timestep 7 a particle that was in block e1 now is in a region where it should be pushed only every other step (or less often), it's moved into block e3 so that its next push will occur on timestep 9.

  Then the "pre-push" to tl 8 (or beyond) is performed, ρ and χ interpolated to tl 8 (for those blocks pre-pushed beyond 8), and the field equation solved for E_8.

IMSPIC algorithm advances particles over various intervals, but solves for E at every "micro" timestep

1. Carry out "final push" for all blocks, using Δt of the current block: $\Delta t = \Delta t_m$:

   Enforce particle boundary conditions

   For a particle that has moved to a point (x_n,v_n) where $\tau \equiv \Delta t(x_n,v_n) < \Delta t/r$, set $\bar{a}_{n-1} \Rightarrow (a + \bar{a}_{n-1})/2$, and set "new block" flag.

   (Here we have used either $r = \sqrt{2}$ or $r = 2$; the latter offers useful hysteresis)

   For particles that have moved to a point (x_n,v_n) where $\tau \equiv \Delta t(x_n,v_n) > r\Delta t$, set $\bar{a}_{n-1} \Rightarrow \bar{a}_{\mathrm{old}}$, and set "new block" flag

2. Exit "final push." For each active block, copy $\rho^{\sim}$ array into $\rho^{\sim}_{old}$, then set $\rho^{\sim}$ to 0

3. Sort flagged particles into new blocks, inject any new particles into the right blocks

4. Carry out "pre-push": compute $x^{\sim}$ positions and use them to compute the $\rho^{\sim}$ array associated with each block at its future time level

5. Exit "pre-push." Calculate field quantities:

   For all necessary blocks, interpolate $\rho^{\sim}$ and χ to time level n+1

   Perform the field-solve to obtain E_{n+1}