New formulations of the semi-Lagrangian method for Vlasov-type equations

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Numerical methods for gyrokinetic model

- Most codes still based on Particle-In-Cell method and its variants.
- More codes now use phase-space grid. Such codes exist in Japan, USA and Europe.
- Most use eulerian methods from fluid dynamics.
- We have contributed to GYSELA code developed by V. Grandgirard which is based on semi-Lagrangian method.

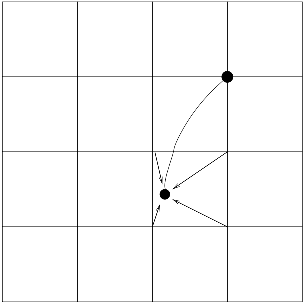
Outline

1. Classical semi-Lagrangian method

2. Conservative semi-Lagrangian method

3. Forward semi-Lagrangian method

The backward semi-Lagrangian Method



- f conserved along characteristics
- Find the origin of the characteristics ending at the grid points
- Interpolate old value at origin of characteristics from known grid values → High order interpolation needed

- Typical interpolation schemes.
  - Cubic spline (Cheng-Knorr)
  - Cubic Hermite with derivative transport (Nakamura-Yabe)

History of semi-Lagrangian schemes for Vlasov

- Cheng-Knorr (JCP 1976): splitting method for 1D Vlasov-Poisson. Cubic spline interpolation.
- ES-Roche-Bertrand-Ghizzo (JCP 1998): general semi-Lagrangian framework for Vlasov-type equations.
- Nakamura-Yabe (CPC 1999): semi-Lagrangian CIP method with Hermite interpolation
- Filbet-ES-Bertrand (JCP 2001) : semi-Lagrangian PFC method: positive and conservative
- N. Besse - ES (JCP 2003) : semi-Lagrangian solver on unstructured grids.
- Crouseilles-Mehrenberger-ES (2008): Equivalence of point based and conservative methods for Vlasov-Poisson + new class of positive filters.
- Crouseilles-Respaud-ES (2008): Forward semi-Lagrangian method.

Convergence of semi-Lagrangian schemes

- Filbet (SINUM 2001): PFC for Vlasov-Poisson
- N. Besse (SINUM 2003): semi-Lagrangian method with linear for Vlasov-Poisson.
- Campos Pinto - Mehrenberger (Numer. Math. 2008): adaptive SL method for Vlasov-Poisson
- N. Besse (SINUM 2008): Convergence of semi-Lagrangian method with cubic Hermite interpolation.
- N. Besse - Mehrenberger (Math of Comp 2008): SL method for different classes of high-order interpolators.

Computation of the origin of the characteristics

- Transport equation

$$\frac{\partial f}{\partial t} + \mathbf{a} \cdot \nabla f = 0,$$

- Characteristics

$$\frac{dX}{dt} = \mathbf{a}$$

- Computation of the origin of the characteristics :
  - Explicit solution if $\mathbf{a}$ does not depend on x
  - Else, numerical algorithm needed.

Splitting for exact computation of characteristics

- In many cases splitting can enable to solve a constant coefficient advection at each split step.
- E.g. separable Hamiltonian $H(\mathbf{q},\mathbf{p}) = U(\mathbf{q}) + V(\mathbf{p})$.
  - Vlasov equation in canonical coordinates reads

$$\frac{\partial f}{\partial t} + \nabla_p H \cdot \nabla_q f - \nabla_q H \cdot \nabla_p f = 0.$$

  - Split equations then become

$$\frac{\partial f}{\partial t} + \nabla_p V \cdot \nabla_q f = 0, \quad \frac{\partial f}{\partial t} - \nabla_q U \cdot \nabla_p f = 0,$$

    where U does not depend on $\mathbf{p}$ and V does not depend on $\mathbf{q}$ $\rightarrow$ characteristics can be solved explicitly.
  - Vlasov-Poisson falls into this category with $\mathbf{q} = \mathbf{x}$, $\mathbf{p} = \mathbf{v}$, $H(\mathbf{x},\mathbf{v}) = \frac{1}{2}m\mathbf{v}^2 + q\phi(\mathbf{x},t)$.

First order computation of characteristics

- Consider general case. Characteristics defined by

$$\frac{d\mathbf{X}}{dt} = \mathbf{a}(\mathbf{X}, t).$$

- Backward solution: $\mathbf{X}^n$ is known and $\mathbf{a}^n$ known on the grid.
- Standard procedure to derive first order numerical method for EDO. Integrate on one time step and use quadrature formula for integral (left or right rectangle).

$$\mathbf{X}^{n+1} - \mathbf{X}^n = \Delta t\, \mathbf{a}^n(\mathbf{X}^n) \quad \text{or} \quad \mathbf{X}^{n+1} - \mathbf{X}^n = \Delta t\, \mathbf{a}^{n+1}(\mathbf{X}^{n+1}).$$

- No explicit solution:
  - Fixed point procedure needed in first case (e.g. Newton).
  - Predictor-corrector method on $\mathbf{a}$ needed in second case.

Second order method for Vlasov-Poisson (1/2)

Technique can be used for solving separable Hamiltonian Vlasov equations without splitting. We shall consider Vlasov-Poisson to illustrate this case.

- At time t_n: f^n and E^n are known at grid points. f^{n+1} and E^{n+1} need to be computed.
- Need to solve characteristics backward in time from t_{n+1} to t_n

$$\frac{dV}{dt} = E(X(t), t), \quad \frac{dX}{dt} = V.$$

- Main problem E^{n+1} needed and not known.

Second order method for Vlasov-Poisson (2/2)

A second order in time algorithm predictor-corrector algorithm is defined as follows:

1. Predict $\bar{E}^{n+1}$ using continuity equation.
2. For all grid points $x_i = X^{n+1}, v_j = V^{n+1}$ compute
   - $V^{n+1/2} = V^{n+1} - \frac{\Delta t}{2}\bar{E}^{n+1}(X^{n+1})$,
   - $X^n = X^{n+1} - \Delta t V^{n+1/2}$,
   - $V^n = V^{n+1/2} - \frac{\Delta t}{2}E^n(X^n)$.
   - Interpolate f^n at point (X^n, V^n).
3. Yields first approximation of $f^{n+1}(x_i, v_j) = f^n(X^n, V^n)$ that can be used to correct $\bar{E}^{n+1}$.

Iterate until $\bar{E}^{n+1}$ does not vary anymore.

At most a couple iterations required.

A two step second order method

- Solve characteristics defined by $\frac{d\mathbf{X}}{dt} = \mathbf{a}(\mathbf{X}, t)$.
- Centered quadrature on two time steps:

$$\mathbf{X}^{n+1} - \mathbf{X}^{n-1} = 2\Delta t\, \mathbf{a}^n(\mathbf{X}^n), \quad \mathbf{X}^{n+1} + \mathbf{X}^{n-1} = 2\mathbf{X}^n + O(\Delta t^2).$$

- Use fixed point procedure to compute $\mathbf{X}^{n-1}$ such that

$$\mathbf{X}^{n+1} - \mathbf{X}^{n-1} = \Delta t\, \mathbf{a}^n(\frac{\mathbf{X}^{n+1} + \mathbf{X}^{n-1}}{2}).$$

- Problem: compute f^{n+1} from f^{n-1}. Even and odd order time approximations become decoupled after some time. Artificial coupling needs to be introduced.

A one step predictor-corrector second order method

- Solve characteristics defined by $\frac{d\mathbf{X}}{dt} = \mathbf{a}(\mathbf{X}, t)$.
- Centered quadrature on one time step:

$$\mathbf{X}^{n+1} - \mathbf{X}^{n} = \Delta t\, \mathbf{a}^{n+\frac{1}{2}}(\mathbf{X}^{n+\frac{1}{2}}), \quad \mathbf{X}^{n+1} + \mathbf{X}^{n} = 2\mathbf{X}^{n+\frac{1}{2}} + O(\Delta t^2).$$

- Now $\mathbf{a}^{n+\frac{1}{2}}$ is unknown. Predictor-corrector procedure needed.
- Use fixed point procedure to compute $\mathbf{X}^{n}$ such that

$$\mathbf{X}^{n+1} - \mathbf{X}^{n} = \Delta t\, \bar{\mathbf{a}}^{n+\frac{1}{2}}\left(\frac{\mathbf{X}^{n+1} + \mathbf{X}^{n}}{2}\right).$$

- Both predictor-corrector and fixed point iterations needed.

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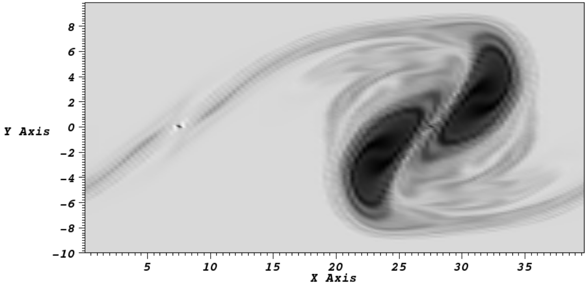
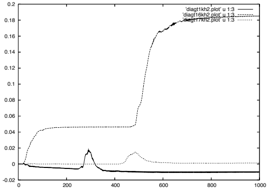
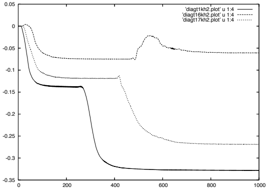
Problem with non conservative Vlasov solver

- When non conservative splitting is used for the numerical solver, the solver is not exactly conservative.
- Does generally not matter when solution is smooth and well resolved by the grid. The solver is still second order and yields good results.
- However: Fine structures develop in non linear simulations and are at some point locally not well resolved by the phase space grid.
- In this case a non conservative solvers can exhibit a large numerical gain or loss of particles which is totally unphysical.
- Lack of robustness.

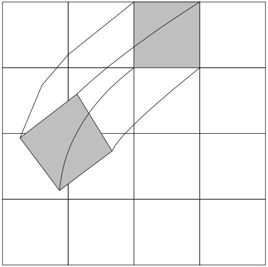
Vortex in Kelvin-Helmholtz instability







Conservative semi-Lagrangian method



- Start from conservative form of Vlasov equation

$$\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{a}) = 0.$$

- $\int_V f\, dx\, dv$ conserved along characteristics
- Three steps:
  - High order polynomial reconstruction.
  - Compute origin of cells
  - Project (integrate) on transported cell.
- Efficient with splitting in 1D conservative equations as cells are then defined by their 2 endpoints. A lot more complex for 2D (or more) transport.
- Splitting on conservative form: always conservative.

High order polynomial reconstruction

- We only use the method with 1D splitting with equations in conservative form.
- Unknowns are cell averages: $f_j = \frac{1}{\Delta x} f(x)\,dx$.
- At time step t_n let f_j^n known average value of f^n on cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$ of length $h_j = x_{j+\frac{1}{2}} - x_{j-\frac{1}{2}}$.
- Construct polynomial $p_m(x)$ of degree m such that

$$\frac{1}{h_j} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} p_m(x)\,dx = f_j^n.$$

- Reconstruction by primitive.

Choice of interpolation

- What interpolation should be chosen for primitive?
- Lagrange interpolation with centered stencil (used in PFC Filbet, ES, Bertrand JCP 2001).
- ENO type interpolation. Lagrange with varying stencil. Not efficient for Vlasov.
- Cubic spline interpolation: cubic polynomial on each cell, globally C^2 $\rightarrow$ reconstructed function is then locally a quadratic polynomial and globally C^1. Linked to cubic spline interpolation for classical semi-Lagrangian method.

Origin of cells and projection

- Compute cell origins:
    - In 1D cell and its origin determined by end points. Compute origin of end points like in classical semi-Lagrangian method.
    - Need to make sure end points do not cross → restriction on time step.
- Compute average value of f^{n+1} on cells using

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f^{n+1}(x)\,dx = \int_{X(t_n;x_{i-\frac{1}{2}},t_{n+1})}^{X(t_n;x_{i+\frac{1}{2}},t_{n+1})} f^n(x)\,dx,$$

where $f^n(x)$ is the high order reconstruction.

Link between classical and conservative semi-Lagrangian methods

- For constant coefficient advections it can be shown that

$$\text{C-Lag(2d)} \Longleftrightarrow \text{SL-Lag(2d+1)}$$
$$\text{PSM} \Longleftrightarrow \text{SPL}$$

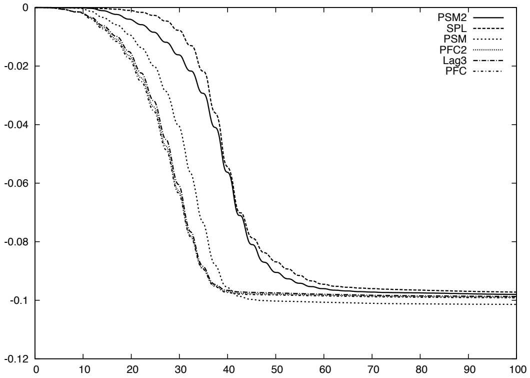
- Consequences :
  1. Classical and conservative semi-Lagrangian methods equivalent for constant coefficients split equations.
  2. The PFC method (Filbet-ES-Bertrand, JCP 2001) corresponds for the Vlasov-Poisson (or Vlasov-Maxwell) systems to a classical semi-Lagrangian method with cubic Lagrange interpolation.

Positive reconstruction

- Physical distribution function is always positive.
- High-order interpolation can lead to negative values in some zones.
- Reconstructed polynomial can be locally modified to remain positive.
- Performed for Lagrange reconstruction in PFC method.
- Introduces a little more dissipativity, but far less as monotonic reconstructions performed in fluid dynamics.

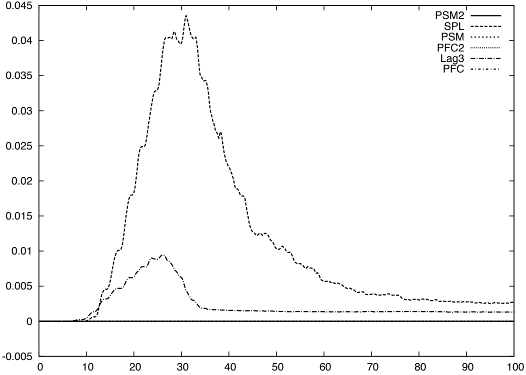
Simulations

Evolution of L^2 norm for $N = 128$ for SLD



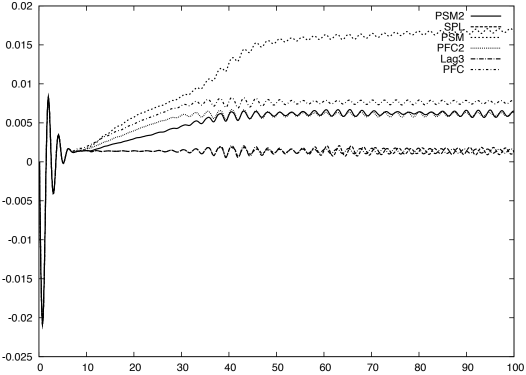
Simulations

Evolution of L^1 norm for $N = 128$ for SLD



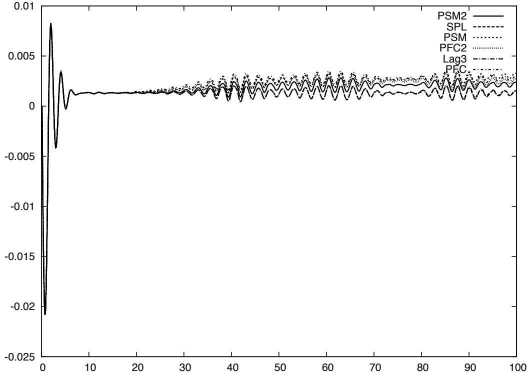
Simulations

Evolution of total energy for $N = 128$ for SLD



Simulations

Evolution of total energy for $N = 512$ for SLD



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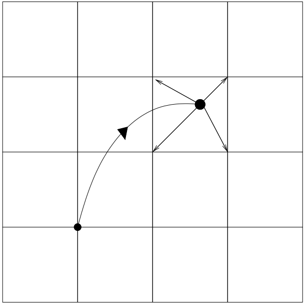
The forward semi-Lagrangian method



- f conserved along characteristics
- Characteristics advanced with same time schemes as in PIC method.
- Leap-Frog Vlasov-Poisson
- Runge-Kutta for guiding-center or gyrokinetic

- Values of f deposited on grid of phase space using convolution kernel.
- Identical to PIC deposition scheme but in whole phase space instead of configuration space only.
- Similar to PIC method with reconstruction introduced by Denavit (JCP 1972).

Discrete distribution function

- Function projected on partition of unity basis for conservativity.
- Linear B-splines very diffusive. Not useful in practice.
- Good choice is cubic B-splines.
- f is reprojected on mesh at each time step.
- Between t_n and t_{n+1}

  $$f_h(x,v,t) = \sum_{i,j} w_{i,j} B(x - X(t;x_i,v_j,t_n)) B(v - X(t;x_i,v_j,t_n)).$$

  Weight $w_{i,j}$ associated to the particle starting from grid point (x_i, v_j) at t_n is coefficient of spline satisfying interpolation conditions

  $$f_h(x_k,v_l,t_n) = \sum_{i,j} w_{i,j} B(x_k - x_i) B(v_l - v_j).$$

- Projection on phase space mesh is obtained with formula

$$f^{n+1}(x_k,v_l) = \sum_{i,j} w_{i,j} B(x_k - X(t_{n+1},x_i,v_j,t_n)) B(v_l - V(t_{n+1},x_i,v_j,t_n)).$$

Time advance for Vlasov-Poisson

- As opposite to BSL, trajectories are advanced forward in time.
- Advection field is known at initial time. Standard ODE algorithms can be applied.
- For Vlasov-Poisson, we have $z(t^n) = (x^n, v^n)$, and $E(t^n, z^n) = E(t^n, x^n)$. Separable Hamiltonian.
- Natural scheme is Verlet algorithm, which is second order accurate in time

$$\text{Step1}: v^{n+\frac{1}{2}} - v^n = \frac{\Delta t}{2} E(t^n, x^n),$$

$$\text{Step2}: x^{n+1} - x^n = \Delta t \, v^{n+1/2},$$

$$\text{Step3}: v^{n+1} - v^{n+\frac{1}{2}} = \frac{\Delta t}{2} E(t^{n+1}, x^{n+1}).$$

Time advance for guiding-center

- Explicit Euler and Runge Kutta have been implemented.
- Second-order Runge Kutta method

$$\text{Step1}: X^{n+1} - X^n = \Delta t E^{\perp}(t^n, X^n)$$

$$\text{Step2}: \text{Compute } E^{\perp}(t^{n+1}, X^{n+1})$$

$$\text{Step3}: X^{n+1} - X^n = \frac{\Delta t}{2}\left[E^{\perp}(t^n, X^n) + E^{\perp}(t^{n+1}, X^{n+1})\right]$$

- Fourth order Runge-Kutta

$$\text{Step1}: k_1 = E^{\perp}(t^n, X^n)$$

$$\text{Step2}: \text{Compute } k_2 = E^{\perp}(t^{n+\frac{1}{2}}, X^n + \frac{\Delta t}{2} k_1)$$

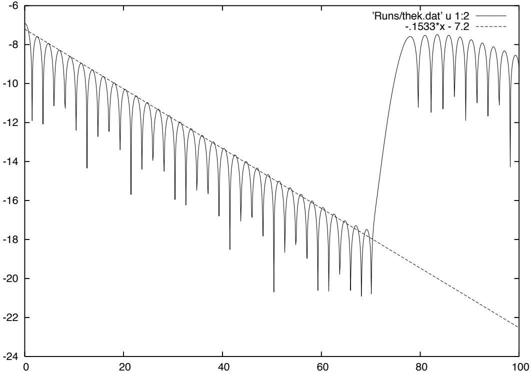
$$\text{Step3}: \text{Compute } k_3 = E^{\perp}(t^{n+\frac{1}{2}}, X^n + \frac{\Delta t}{2} k_2)$$

$$\text{Step4}: \text{Compute } k_4 = E^{\perp}(t^{n+1}, X^n + \Delta t k_3)$$

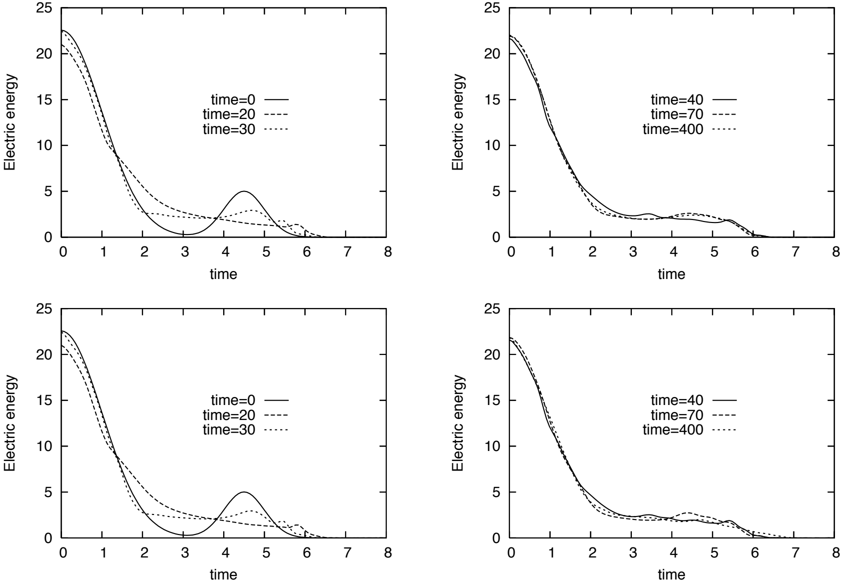
$$\text{Step5}: X^{n+1} - X^n = \frac{\Delta t}{6}[k_1 + 2k_2 + 2k_3 + k_4]$$

Landau damping

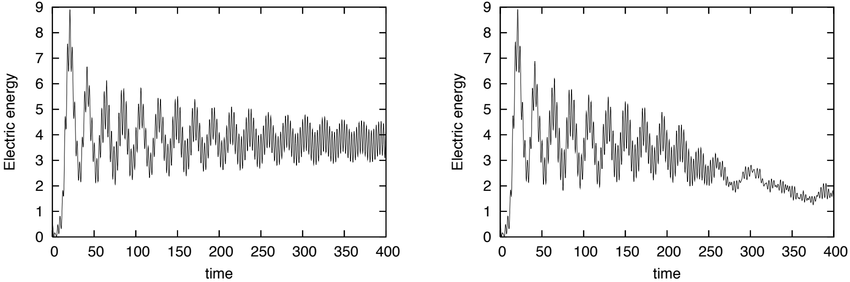
$$f_0(x, v) = (1 + 0.001 \cos(kx)) \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}, \quad L = 4\pi.$$



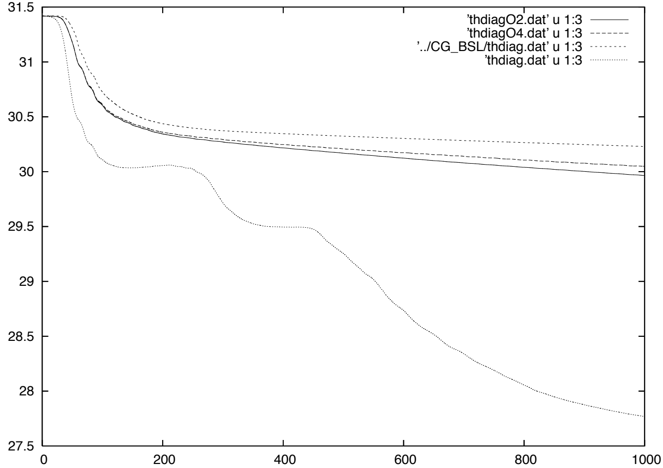
Bump on tail (BSL (top) vs. FSL (bottom))



Bump on tail: potential energy (BSL (left) vs. FSL (right))



Energy conservation for Kelvin-Helmoltz instability



FSL vs. BSL

- Forward semi-Lagrangian method very promising.
- Accurate description of whole phase-space in particular tail of distribution function and small perturbations.
- A little more diffusive than BSL. Better with smaller time steps.
- Some advantages: classical explicit EDO solver can be used, in particular high order if needed. No need for predictor-corrector or fixed point algorithm.
- Can benefit from charge conserving PIC algorithms (Villasenor-Buneman).