First Steps towards a New Generation of High-Order PIC Methods based on DG-FEM Methods

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- Giovanni Lapenta (LANL)
- Tim Warburton (Rice)
- Eric Sonnendrucker (Strasbourg, France)

Kinetic Plasma Physics

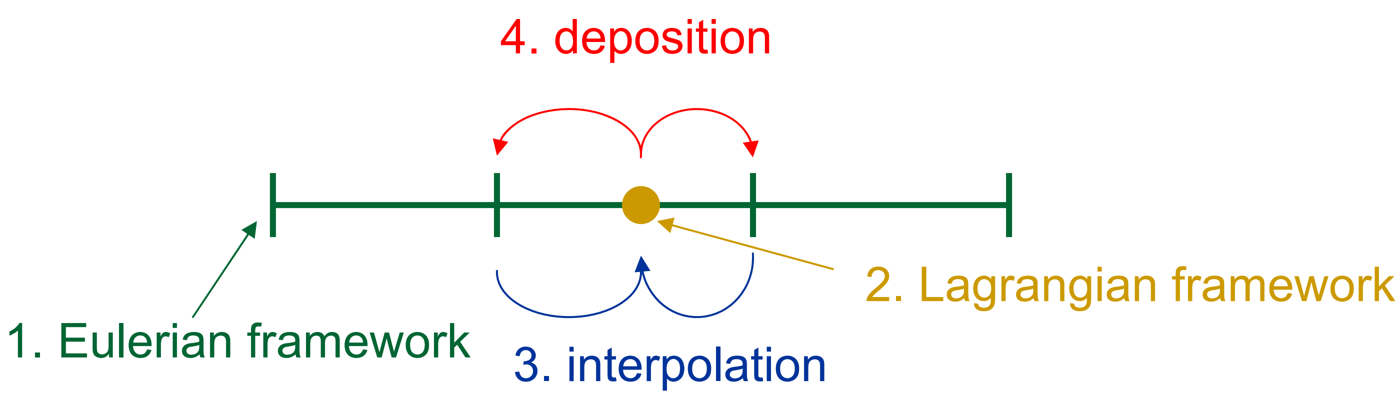
- Need to model strongly kinetic phenomena
  - Vlasov equation for f(x,v,t) - cost is high (6+1)
  - Particle in Cell methods - solution by sampling
- Typical applications
  - Microwave generators (magnetrons etc)
  - Particle accelerators/RF guns
  - Laser-matter interaction
  - Fusion applications
  - etc

Characteristics of the Problems

- Full coupling between particles and fields
- Electrically very large problems
- Time-dependent and highly dynamic
- Often complex interaction between particles, fields, and geometries
- Particles can be highly relativistic, requiring full EM modeling

Particle-in-cell methods

- PIC is a *particle-mesh* method that consists of four stages in a *Lagrangian-Eulerian* framework:
  - Solve continuum equations in Eulerian framework.
  - Track individual particles in Lagrangian framework.
  - Couple Eulerian->Lagrangian framework: interpolation.
  - Couple Lagrangian->Eulerian framework: deposition.



Governing equations in each stage

- Maxwell's equations:

$$\frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{H} + \boldsymbol{J} \quad , \quad \frac{\partial \boldsymbol{H}}{\partial t} = -\nabla \times \boldsymbol{E}$$

$$\nabla \cdot \boldsymbol{E} = \rho \quad , \quad \nabla \cdot \boldsymbol{H} = 0 \quad .$$

- Particle equations:

$$\begin{aligned} \frac{d\boldsymbol{x}_p}{dt} &= \boldsymbol{v}_p, \\ \frac{dm\boldsymbol{v}_p}{dt} &= q\left(\boldsymbol{E} + \boldsymbol{v}_p \times \boldsymbol{B}\right), \end{aligned}$$

- Lagrangian-> Eulerian:

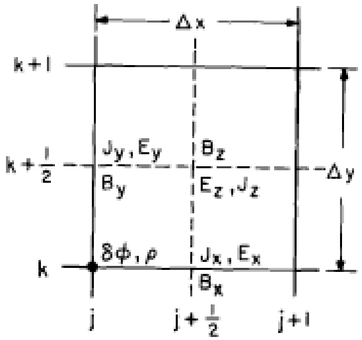
$$\begin{aligned} \rho(\boldsymbol{x}) &= \sum_{i=1}^{N_p} q_i S(|\boldsymbol{x}_p - \boldsymbol{x}|), \\ \boldsymbol{J}(\boldsymbol{x}) &= \sum_{i=1}^{N_p} q_i \boldsymbol{v}_i S(|\boldsymbol{x}_p - \boldsymbol{x}|). \end{aligned}$$

- Eulerian->Lagrangian:

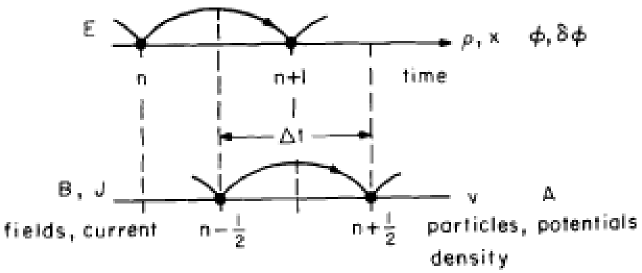
$$\boldsymbol{E}(\boldsymbol{x}_p), \quad \boldsymbol{B}(\boldsymbol{x}_p)$$

Explicit Finite Difference

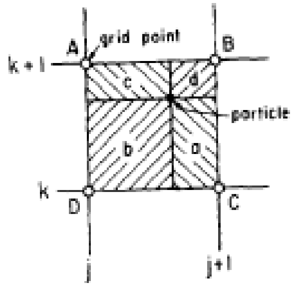
- Central Yee-Mesh in space



- Leap-frog in time



- Cloud-in-cell area weighing:
  - Charge conserving: [Villasenor, Buneman, *CPC, '92*]



- Interpolation
- Finite-difference Poisson solver
  - if necessary for divergence cleaning

[Birdsall and Langdon, '85]

Explicit Finite Difference Scheme: Typical Properties

- Established (30 years).
- Second order accurate in space and time.
- Energy conserving
- Very noisy.
- Structured grids.
- Staircase boundary fitting: first order.
- Stability criteria/issues.
- Significant dispersion errors if CFL < 1.0.
- Numerical Cherenkov radiation.

Limitations

- This will translate into modeling inaccuracies and excessive computational expense when
  - Problems are large
  - Problems require long time integration
  - Problems contain significant geometric complexity
  - When high density problems are considered
  - Etc.
- These are realistic regimes that need modeling
  - High-power microwave devices: Electro-magnetic pulse.
  - Fusion energy.
  - Accelerator modeling.
- New PIC algorithms
  - PIC algorithms other than the finite difference method have not received significant attention.
  - For pure electromagnetic simulation in these regimes, it is no longer the preferred method
  - Higher-order methods are superior.

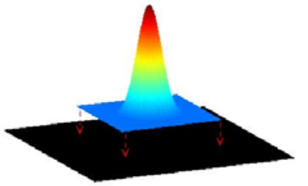
Project goals

- Based on a DG-FEM EM solver, develop a new family of PIC codes.
  - High-order, general grids, 3D parallel etc
- Identify and resolve key challenges
  - Divergence control, time-stepping, particle shapes, interaction with geometries, grid heating, Cherenkov radiation etc.
- Test, Test, Test
- Initial applications to the modeling of typical kinetic phenomena

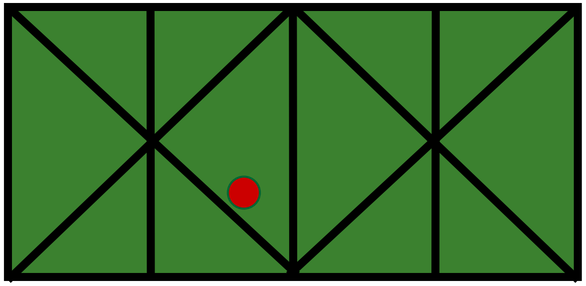
Development of high-order DG-PIC

Variable order Runge-Kutta schemes for time integration.

Update the particle position and velocity with Newton's law.



Weigh particle to grid through a smooth deposition function

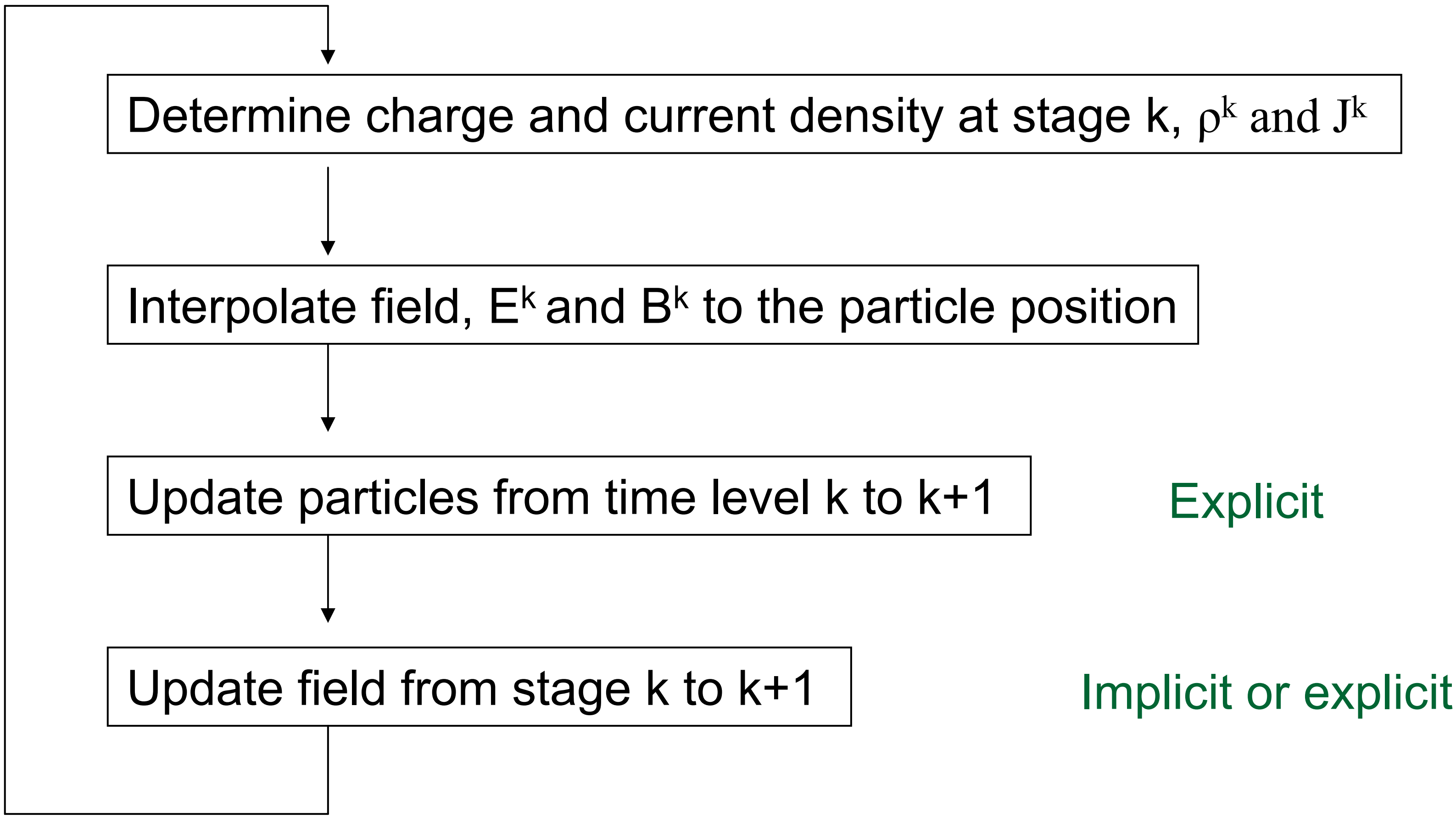


Use variable order interpolation to determine field at particle position.

Solve Maxwell equations on variable order unstructured grid.

[Jacobs and H., *JCP*, '06]

DG-PIC: one Runge-Kutta stage



No splitting! High-order RK scheme gives high-order accuracy!

DG-PIC: why?

- Support for high-order accuracy: four to six points per smallest wavelength.
- Flexible:
  - Order flexibility in space and time.
  - Geometric complexity through unstructured grids.
  - Decoupling of particle resolution and continuum Maxwell's equation resolution.
  - Local character, ease of parallel implementation.
  - Build in dissipative mechanism for noise control.
  - Better characteristics to avoid numerical Cherenkov radiation
- Very well validated for solving large scale Maxwell's equations
- Flexibility in particle shapes.

DG method on triangles: interpolant

The domain is decomposed into K *bodyconforming* elements, each supporting a *nodal basis* of the form

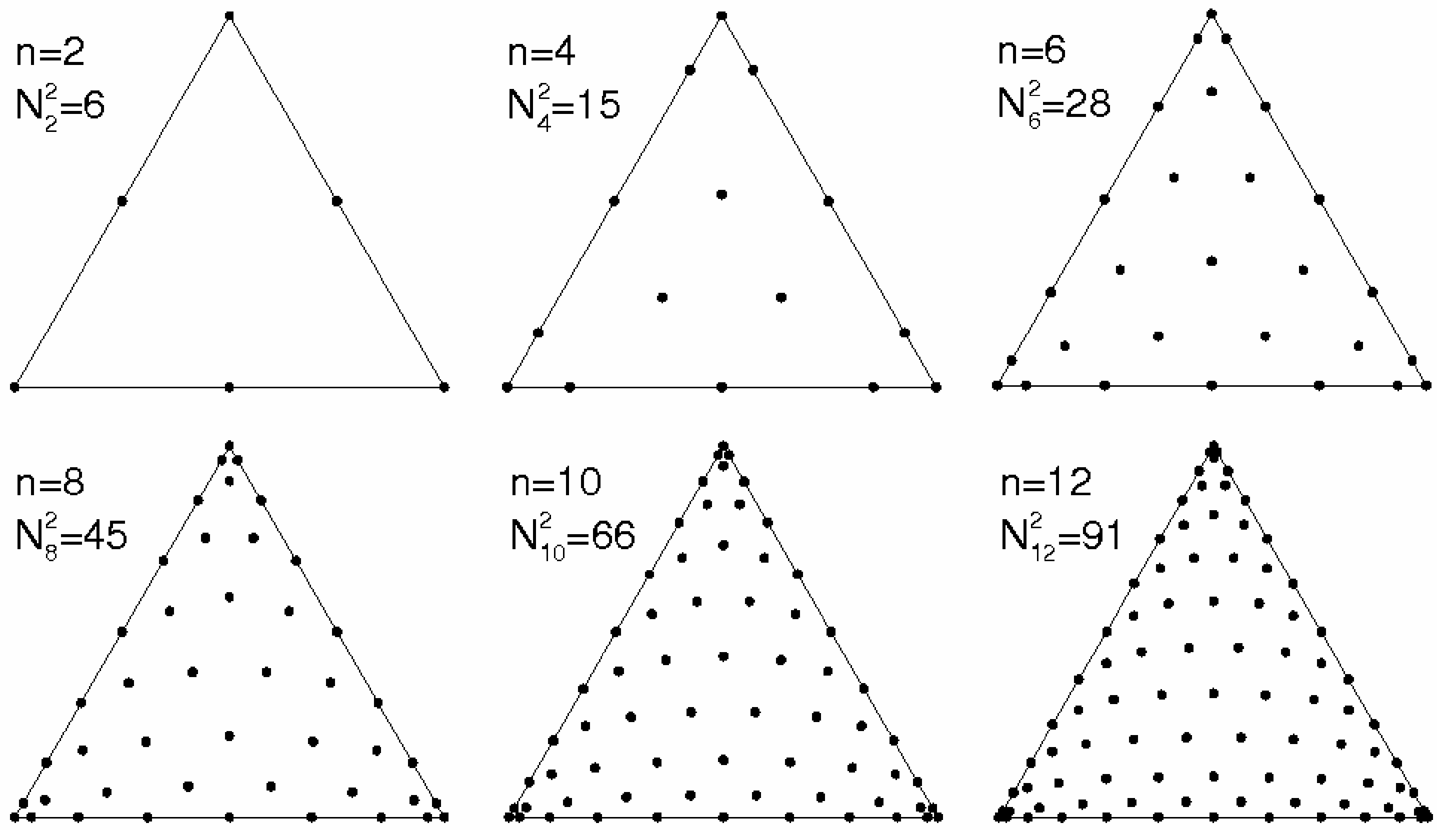
$$\boldsymbol{q}_N(\boldsymbol{x},t) = \sum_{j=1}^{N} \boldsymbol{q}(\boldsymbol{x}_j,t) L_j(\boldsymbol{x}) = \sum_{j=1}^{N} \hat{\boldsymbol{q}}_j(t) L_j(\boldsymbol{x})$$

Here:

- $L_j(x)$ is the multivariate Lagrange interpolating polynomial.
- q_j are nodal solutions at x_i

DG method on triangles: nodes

Electrostatic nodes:



[Hesthaven, *SIAM J. Num. Anal. '98*]

Nodal discontinuous Galerkin method

To recover the solution we require that q_N satisfies Maxwell's equations locally on D as,

$$\int_D \left(\frac{\partial \boldsymbol{q}_N}{\partial t} + \nabla \cdot \boldsymbol{F}_N - \boldsymbol{J}_N \right) L_i(\boldsymbol{x}) d\boldsymbol{x} = \oint_{\partial D} L_i(\boldsymbol{x}) \hat{\boldsymbol{n}} \cdot [\boldsymbol{F}_N - \boldsymbol{F}^*] \, d\boldsymbol{x}.$$

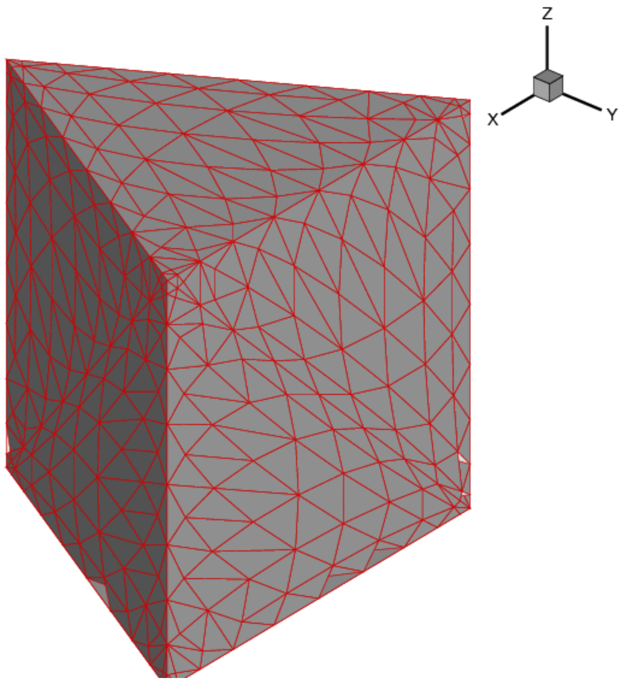
This yields the local element based scheme

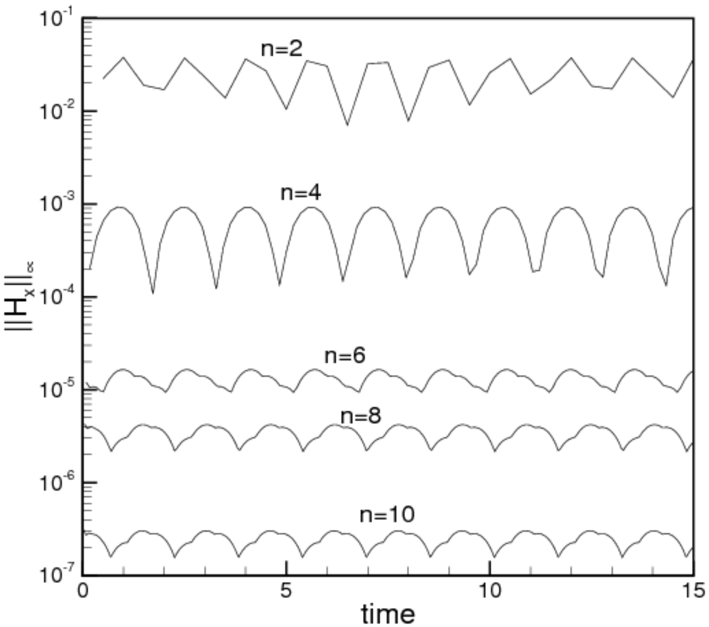
$$\hat{\mathrm{M}} \frac{d\hat{\boldsymbol{q}}}{dt} + \hat{\mathrm{S}} \cdot \hat{\boldsymbol{F}} - \hat{\mathrm{M}} \hat{\boldsymbol{J}} = \hat{\mathrm{F}} \hat{\boldsymbol{n}} \cdot \left[\hat{\boldsymbol{F}} - \hat{\boldsymbol{F}}^* \right],$$

The scheme is local, nodal, h/p adaptive, explicit/implicit depending on time scheme, parallel by construction. All operations are dense matrix-matrix multiplications.

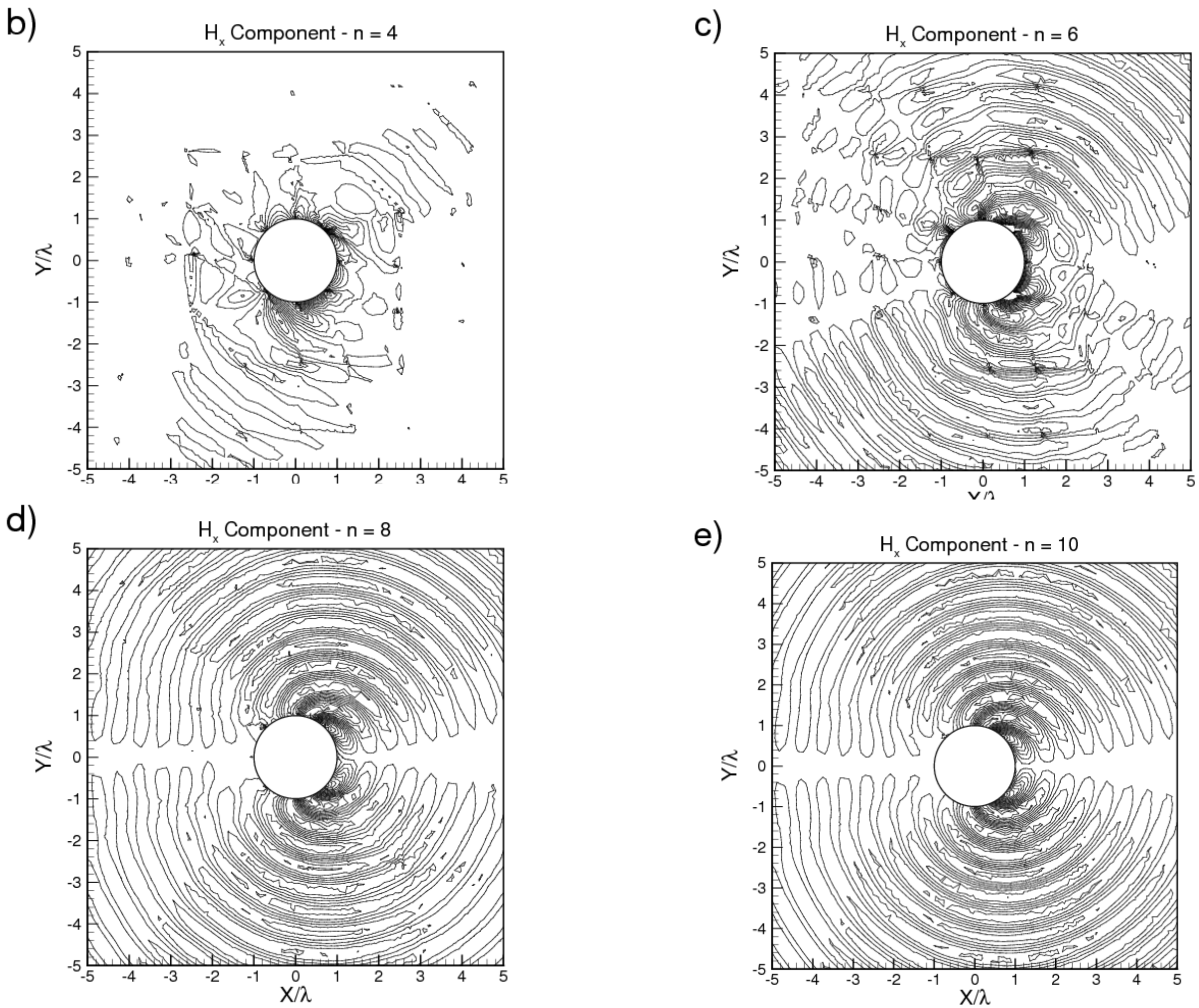
[H. and Warburton, *JCP '02*]

A Few EM results



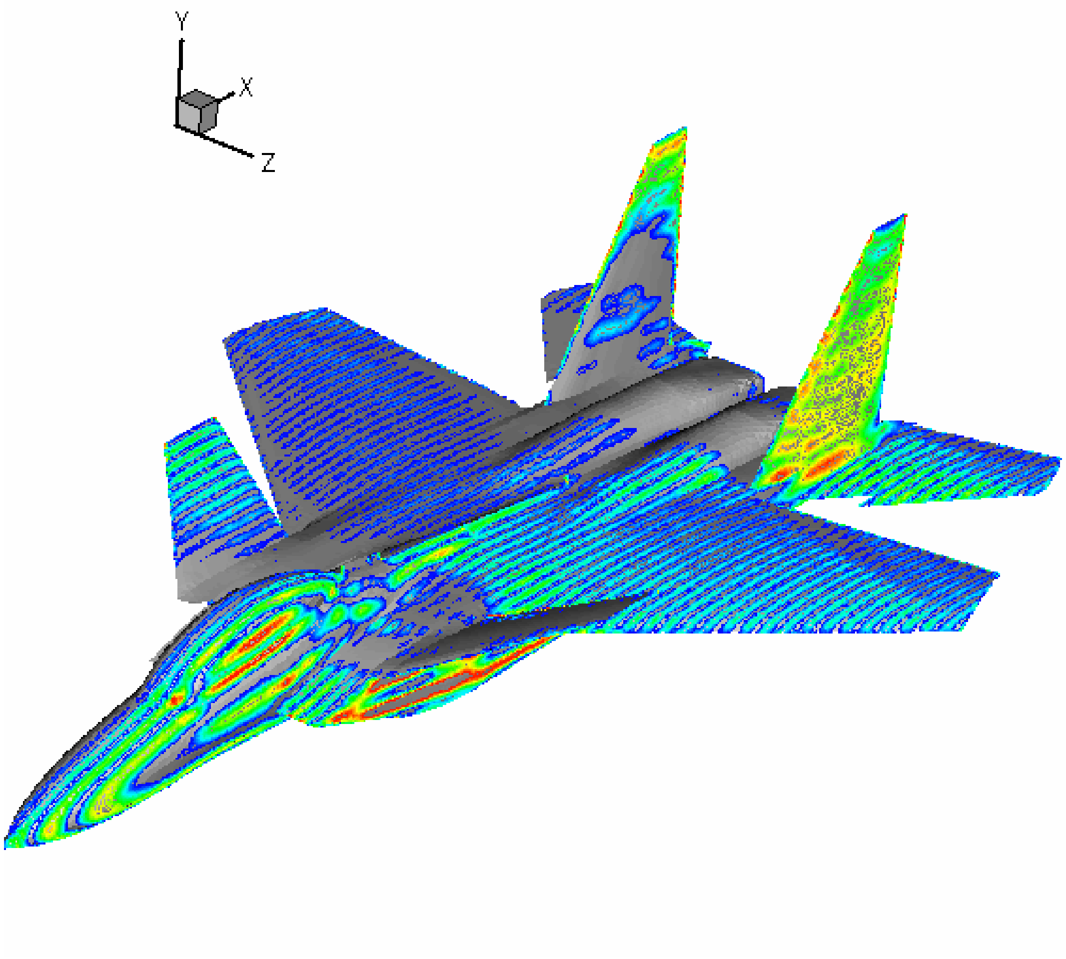


EM Results



b)
H x Component - n = 4
c)
H x Component - n = 6
d)
H x Component - n = 8
e)
H x Component - n = 10
Y/λ
X/λ

EM Results



EM Overview

- DG-FEM schemes for EM have been developed both for time-domain and frequency domain.
- Strong theoretical support
- Extensive validation have been performed, confirming benefits of high-order, general/nonconforming grids
- Highly efficient on parallel computers
- Other efforts include time-stepping, adaptivity/error control, reduced basis methods etc
- DG-FEM now used by several groups worldwide for EM modeling, incl defense and commercial use.
- USEMe and SLEDGE++ libraries available

Back to the Plasma Problem…

- This is a much harder problem … as you all know !
  - Divergence control/charge conservation
  - Particle movers
  - Particle/geometry interactions
  - Coupling between particles and grids
  - Numerical Cherenkov radiation
  - … and many other issues
- We will discuss some of these issues in the following -- we have not reached 'steady-state' yet !

Divergence cleaning.

- Divergence cleaning (satisfying Gauss laws).
  - Most methods: solve the Poisson equation for a correction potential φ that correct E to be divergence free.

$$\nabla^2\phi = \nabla\cdot\boldsymbol{E}^* - \rho \qquad \boldsymbol{E} = \boldsymbol{E}^* - \nabla\phi,$$

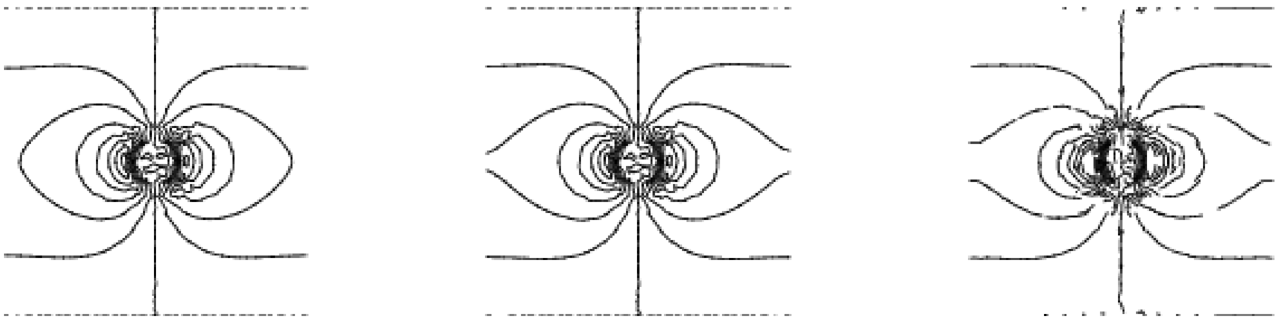
  - Potential reduction of accuracy in DG
  - DG-PIC: Hyperbolic cleaning: solves modified Maxwell's equations that sweep divergence errors out of the domain. No reduced accuracy, but stiff!

$$\frac{\partial E}{\partial t} = \nabla\times H + J - \chi\nabla\phi \qquad \frac{\partial\phi}{\partial t} + \chi\nabla\cdot E = \rho - \phi$$

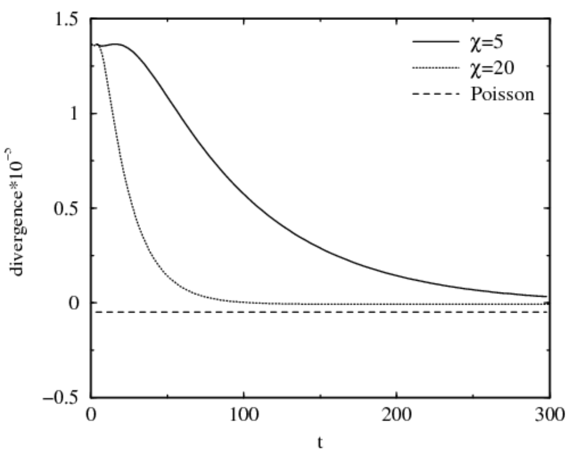
$$\frac{\partial H}{\partial t} = -\nabla\times E - \chi\nabla\psi \qquad \frac{\partial\psi}{\partial t} + \chi\nabla\cdot H = -\psi$$

[Jacobs and H., *JCP*, 06]

A Brief Comparison of the Two



χ=5 χ=20 Poisson



Which one to choose ?

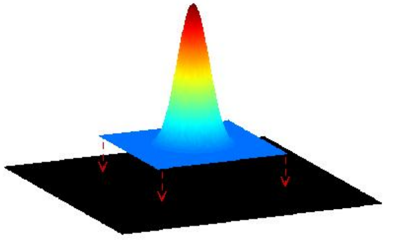
- Hyperbolic cleaning
  - Speed and simplicity
  - .. Only approximate but controllable with parameter.
  - Large parameter induces stiffness
  - Parallel performance is direct
- Projection
  - Exact charge conservation
  - Sole solver for low speed problems
  - Global solver - parallel efficiency still possible
  - Global exchange of information
  - Noise sensitive

Particle deposition: distribution function

- The elements that are influenced by the particle cloud are determined through a look up table.
- The particle influence area is constant
  - Ensures charge conservation
  - Makes # of elements within reach variable in space
- The following function

$$S_{po1l} = \frac{\alpha + 1}{\pi R^2} \left[1 - \left(\frac{r}{R} \right)^2 \right]^\alpha \qquad r = 0 \cdots R$$

- was found to be
  - flexible
  - computationally efficient



- Still options to be explored here (local particle vs not)

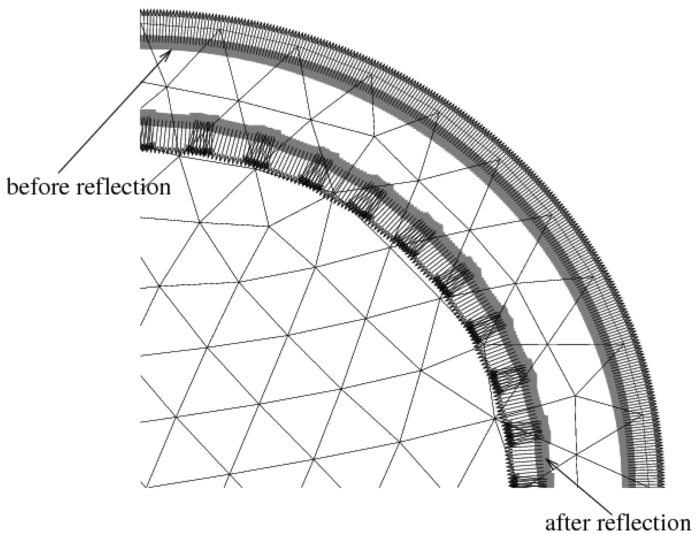
Particle tracking: complex particle-wall interaction

- For elastic collision, a levelset γ is pre-computed by solving the Hamilton-Jacobi equation

$$\frac{\partial \gamma}{\partial \tau} + \boldsymbol{w} \cdot \nabla \gamma, = sgn(\gamma_0) + \mu \Delta \gamma. \qquad \boldsymbol{w} = sgn(\gamma_0) \frac{\nabla \gamma}{|\nabla \gamma|}$$

- ($\gamma, \boldsymbol{w}$) yields (distance, normal) to boundary
- Pure reflection is now accomplished by a mirror principle
- This works for any geometry!
- Solve with explicit DG scheme in a pre-processing step.
- This also provides information that may be useful for other things, e.g., particle emission models

Particle-Wall Interactions

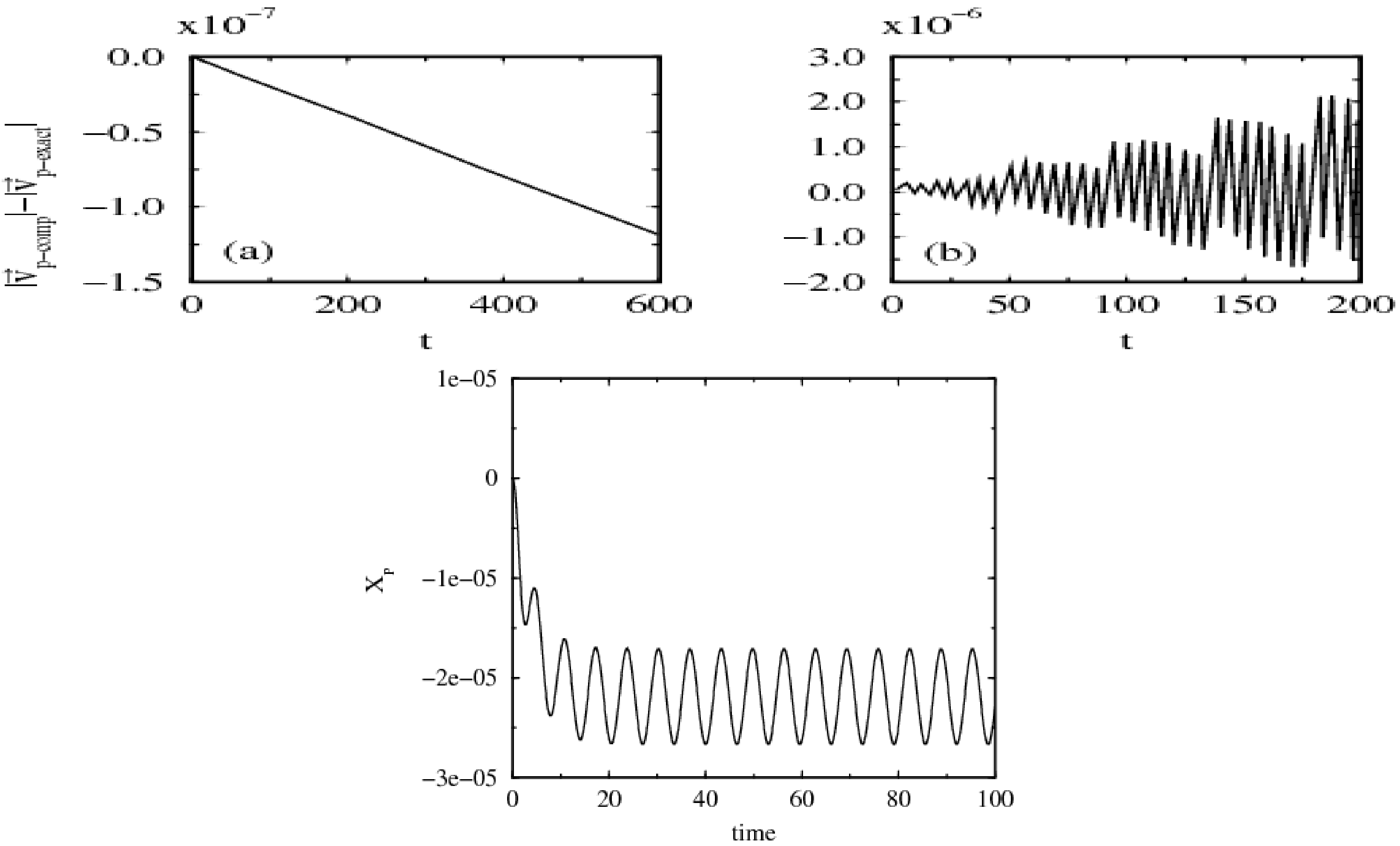


QuickTime™ and a
BMP decompressor
are needed to see this picture.

Verification: Testing the Components of the Algorithm

- Larmor particle track shows current Runge-Kutta tracking is slightly dissipative.
- Release of a single particle shows neglible self-force.
- Grid heating can be reduced with orders of magnitude by smoothening the particle shape.
- Plasma wave computations shows hyperbolic cleaning requires $\chi > 10$ for accurate prediction of plasma frequency and energy conservation.
- Plasma wave computations confirm fourth order accuracy of the Runge-Kutta scheme.
- Classic plasma wave, two-stream instability, and Landau damping compare well to established methods.

A Few Single Particle Tests



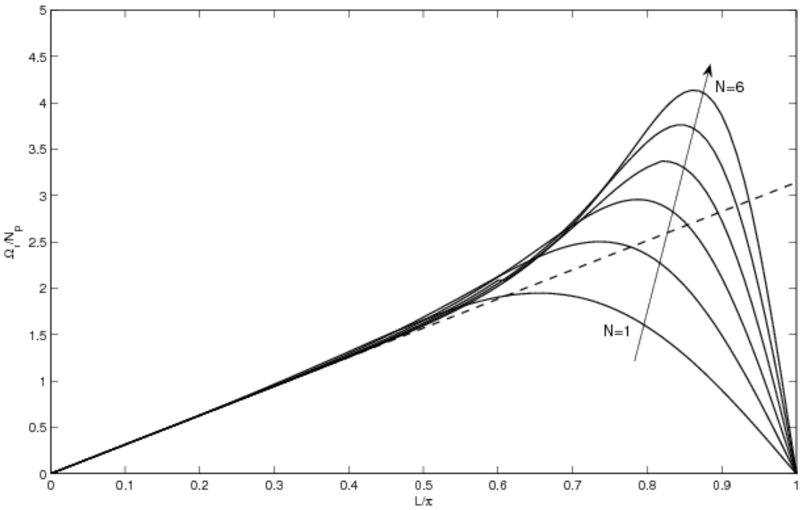
Grid Heating

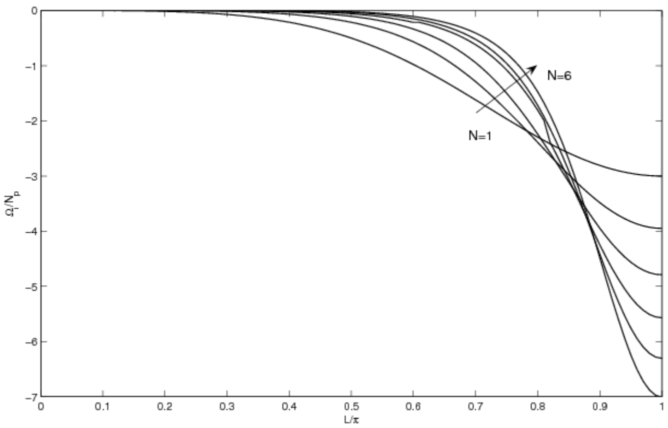
- This is related to a requirement of resolving the Debye length and is a big problem in dense plasma modeling.
- Typical solution -- increased resolution or some smoothing (implicit)
- Further options in this formulation
  - Large particles
  - Smoother particles
- … the problem is much better controlled, but it remains.

Numerical Cherenkov Radiation

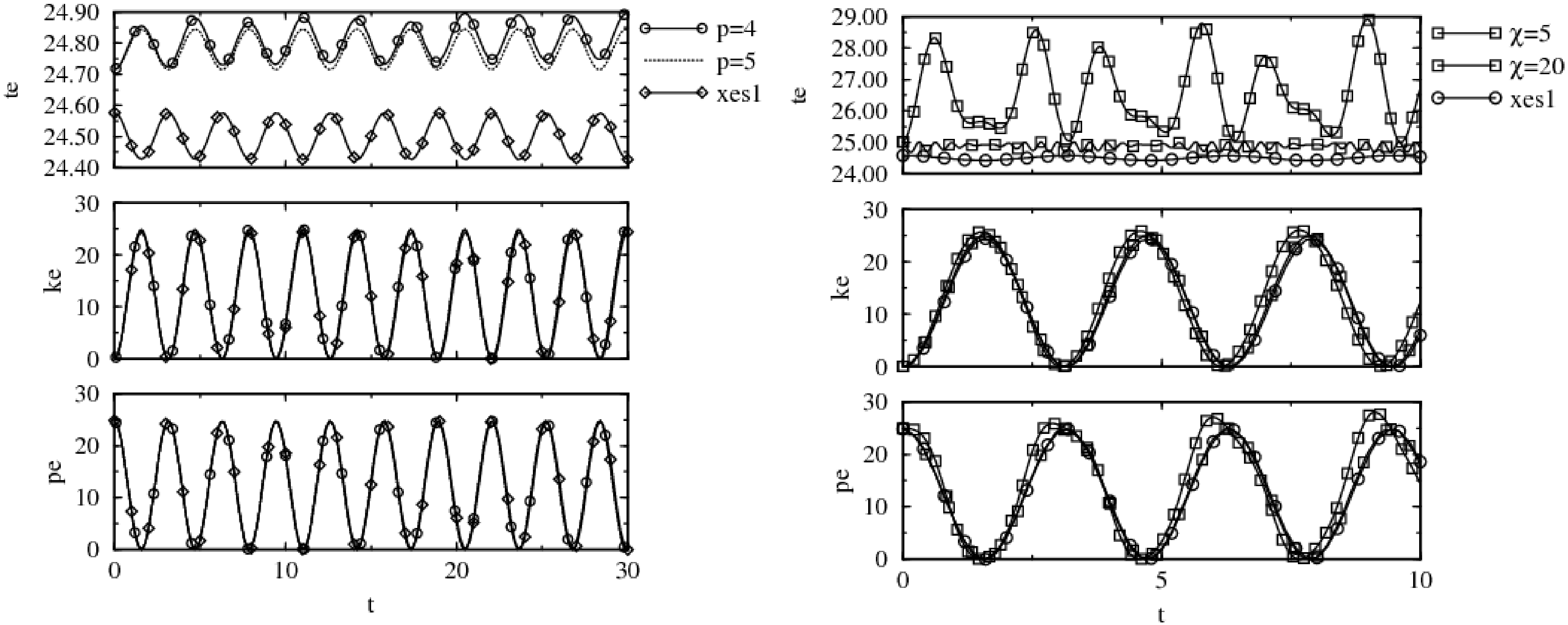
- This is directly associated with numerical properties of the field solver
  - High frequency waves propagate slower than speed-of-light
  - Fast particle are propagating faster than numerical speed-of-light
  - This creates numerical Cherenkov radiation -- which is a big problem in high-speed modeling.
  - Normal cure -- add dissipation to scheme.
- The DG-FEM solver does not cure this -- but the build in very slight dissipation helps to control it very nicely and the inherent dispersion relations are better than FDTD.

Numerical Cherenkov II

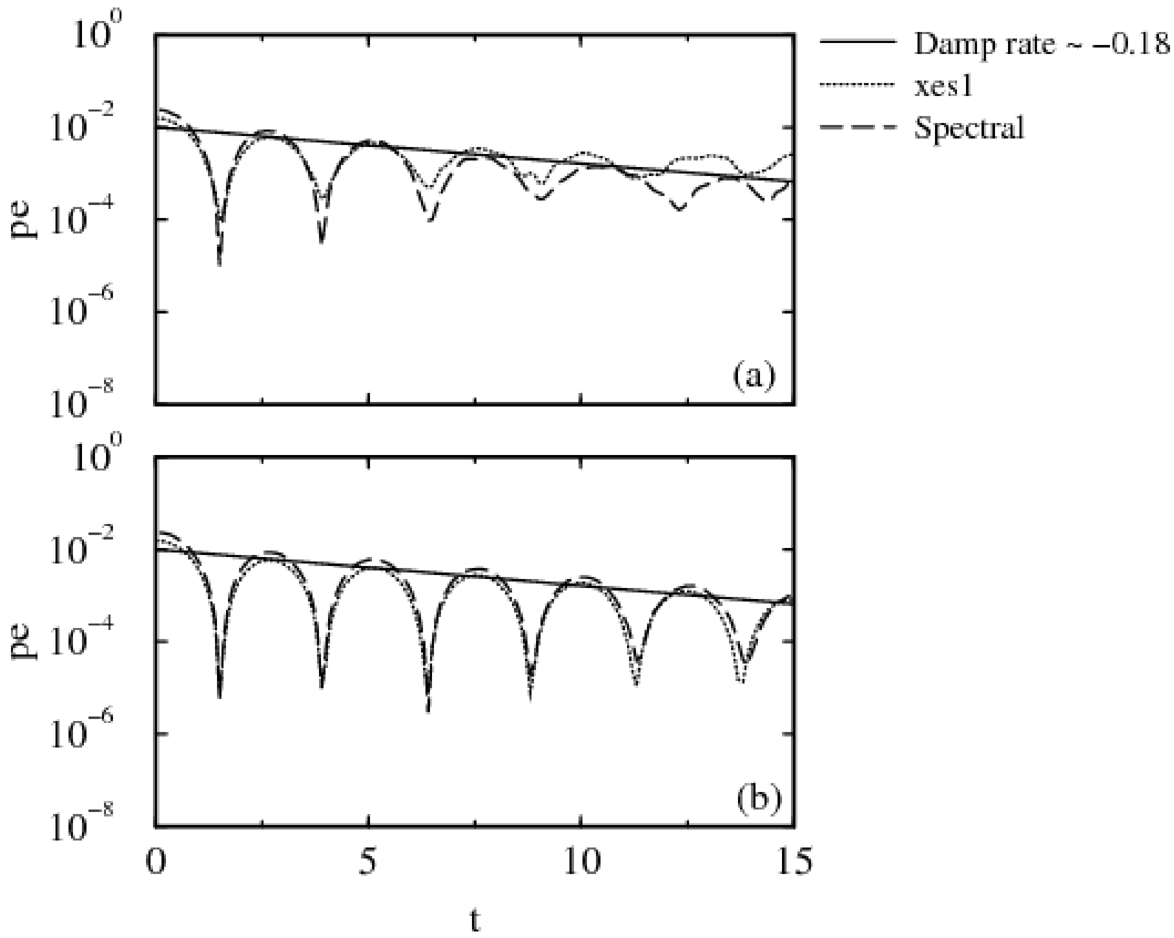




Plasma Waves



Landau Damping



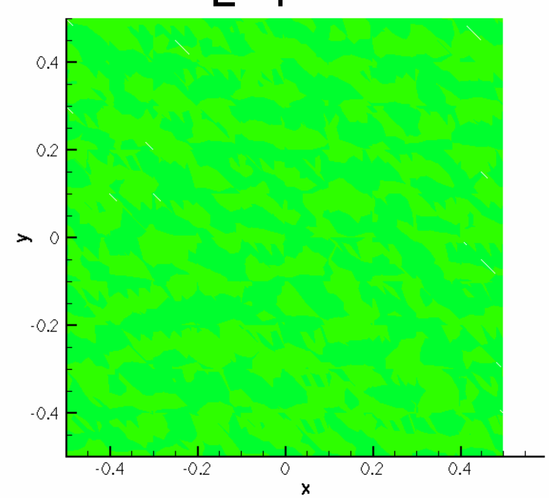
Weibel instability: computational model.

- Initial conditions:
  - Homogeneous plasma with zero net charge. Constant background ionic charge density.
  - Initial electron thermal velocities, u=0.25 and v=0.05.
  - Zero initial electric and magnetic field.
- From these initial conditions the two velocities will evolve towards one thermal velocity in time
- Weibel instability: unstable growth of transverse electromagnetic waves:

L=1

$$\omega_{pe} = 15\pi$$
$$u_{th} = 0.25$$
$$v_{th} = 0.05$$
$$\lambda_{De} = 0.0011$$

L=1



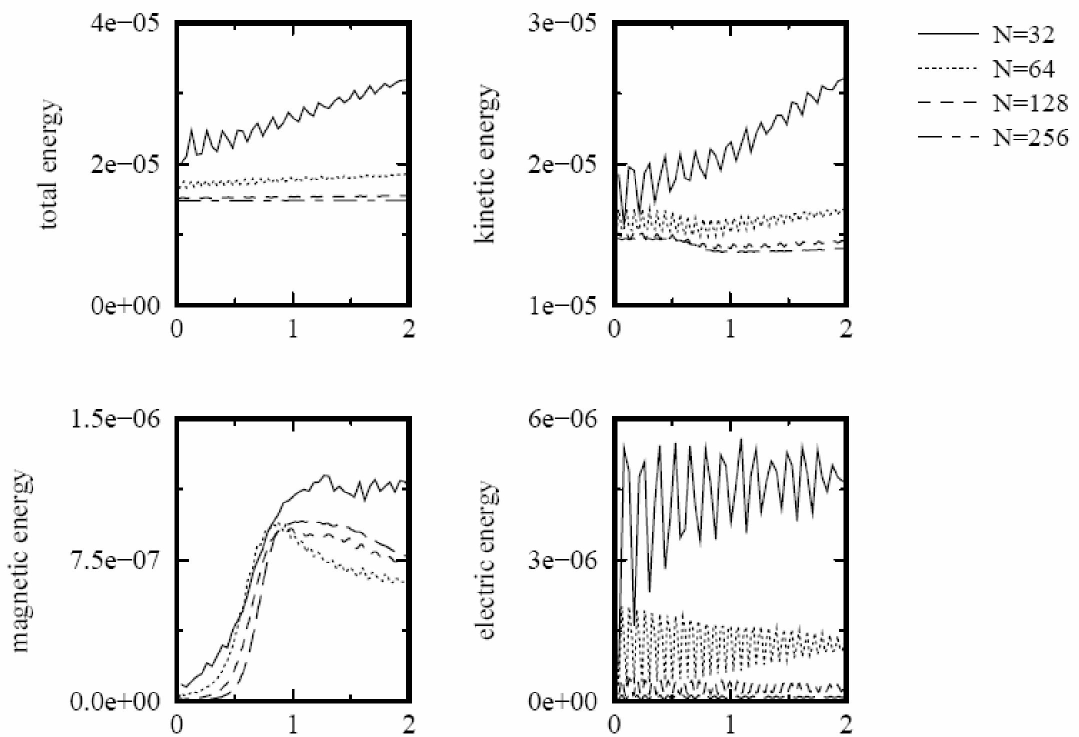
[Jacobs *et al., AIAA-2006-1171*]

Weibel instability: EFDTD simulation

- Convergence study establishes base result.
- Simulation parameters:
  - NxN grid cells, with N=32, 64, 128, 256
  - Initialized with N_p=36 particles per cell for all N.
  - At N=256 the smallest grid spacing is on the order of the Debye length, i.e. should be resolved.

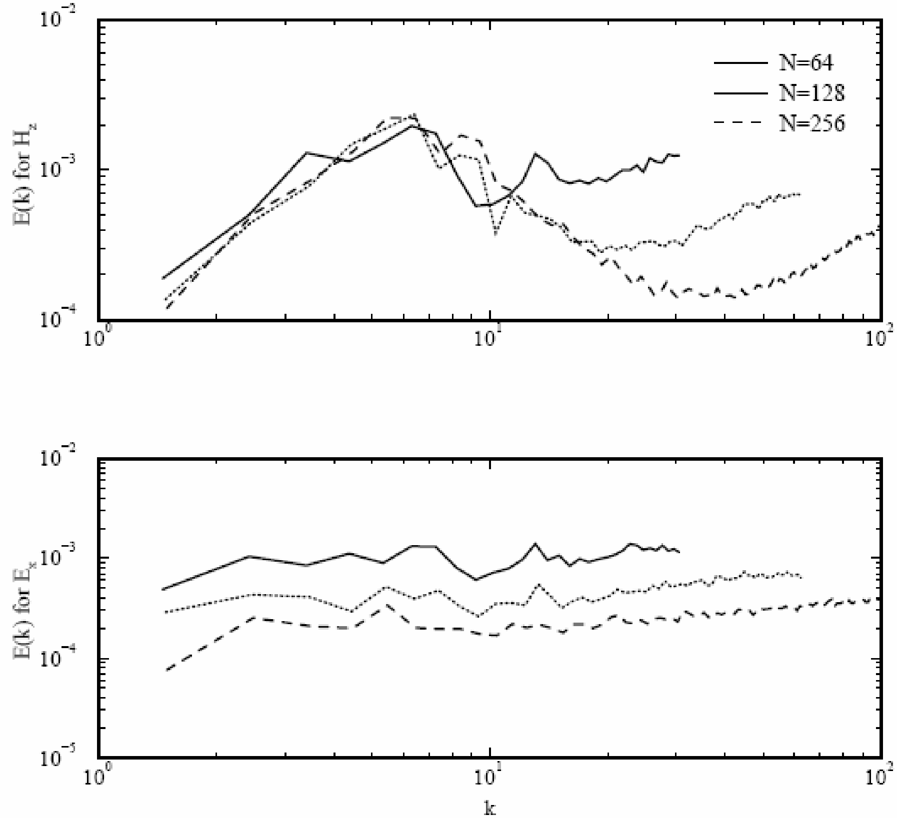
EFDTD results: energies versus time.

- Total energy increase indicative of finite grid instability.
- At *N*=128 grid heating small enough to recognize trends.
- Initial exponential growth in magnetic energy predicted by linear theory.
- Electric energy mostly influenced by noise in the charge density through Gauss law.



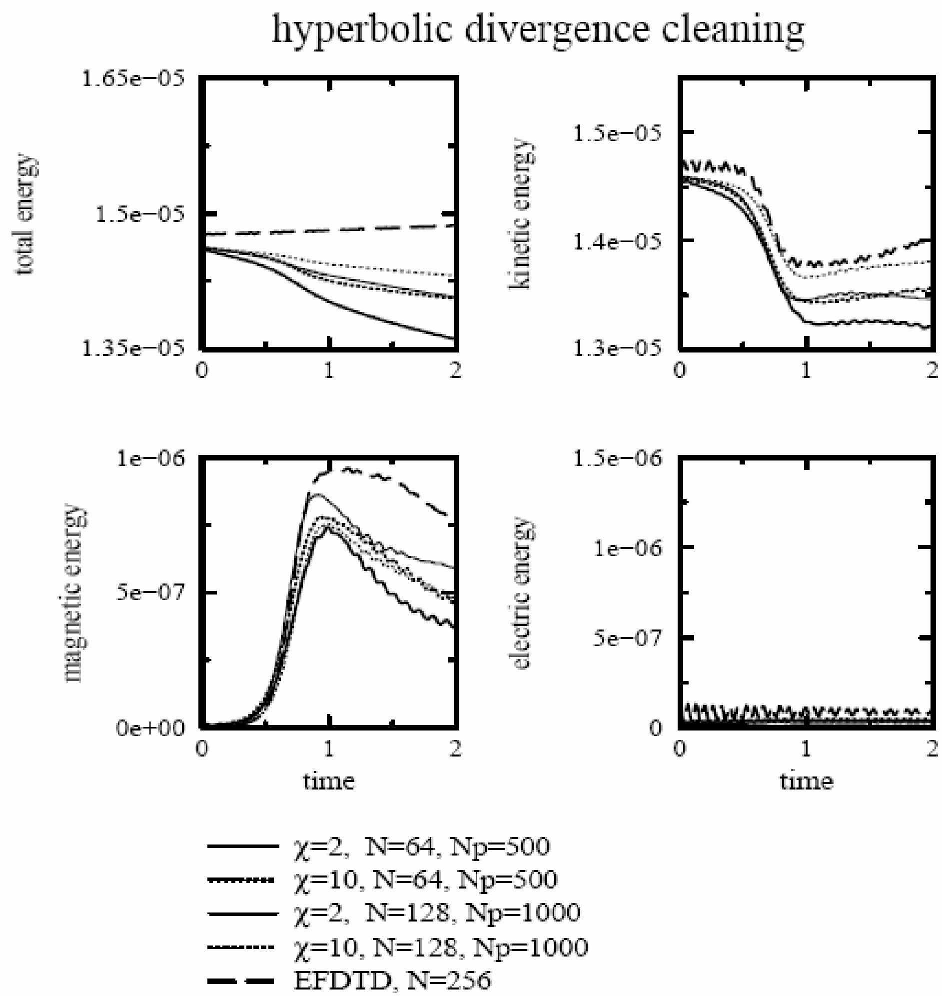
EFDTD: energy spectra.

- Highest resolved wave number k~ *N*/3. For larger k energy spectrum increases.
- Central scheme doesn't dissipate energy at high k.
- The electric field is dominated by noise, i.e. no drop in the energy spectrum at large k.



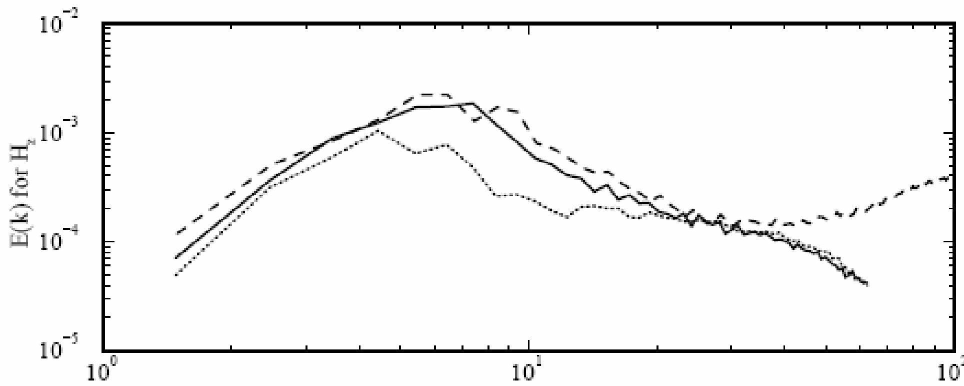
DG-PIC 2nd order: energies versus time.

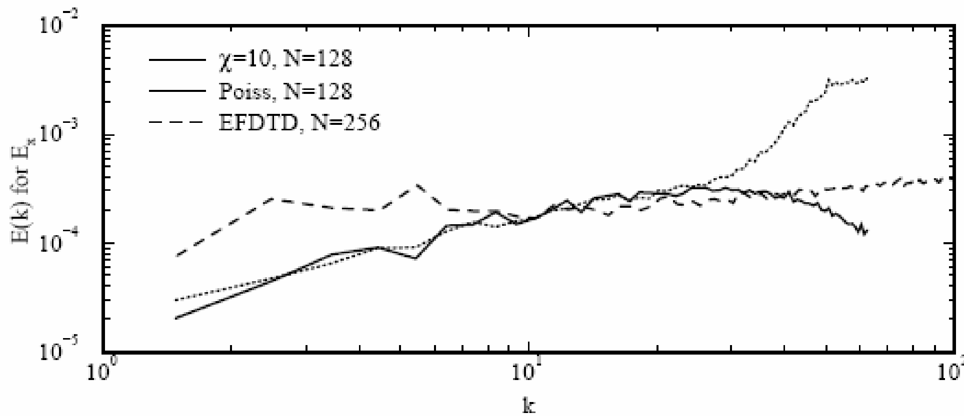
- The hyperbolic cleaning method is second order.
- At *N*=128, and χ=10, the energies are in good comparison.
- The peak magnetic energy is slightly less compared to IFDTD, perhaps a result from temporal damping in the DG-PIC method.



DG-PIC 2nd order: energy spectra.

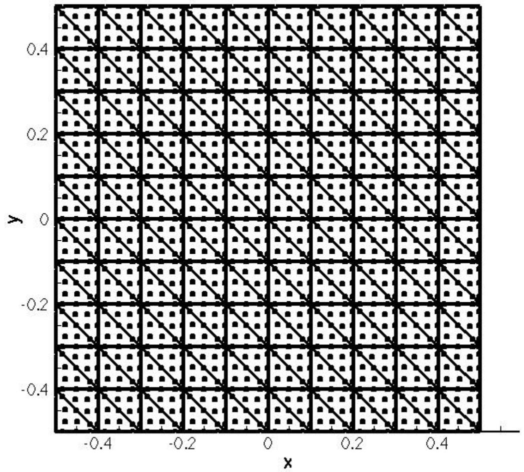
- Magnetic energy spectra compare well for hyperbolic cleaning.
- Energy spectrum at high k drops: the upwind nature of the interface matching results in damping of waves with high frequencies.





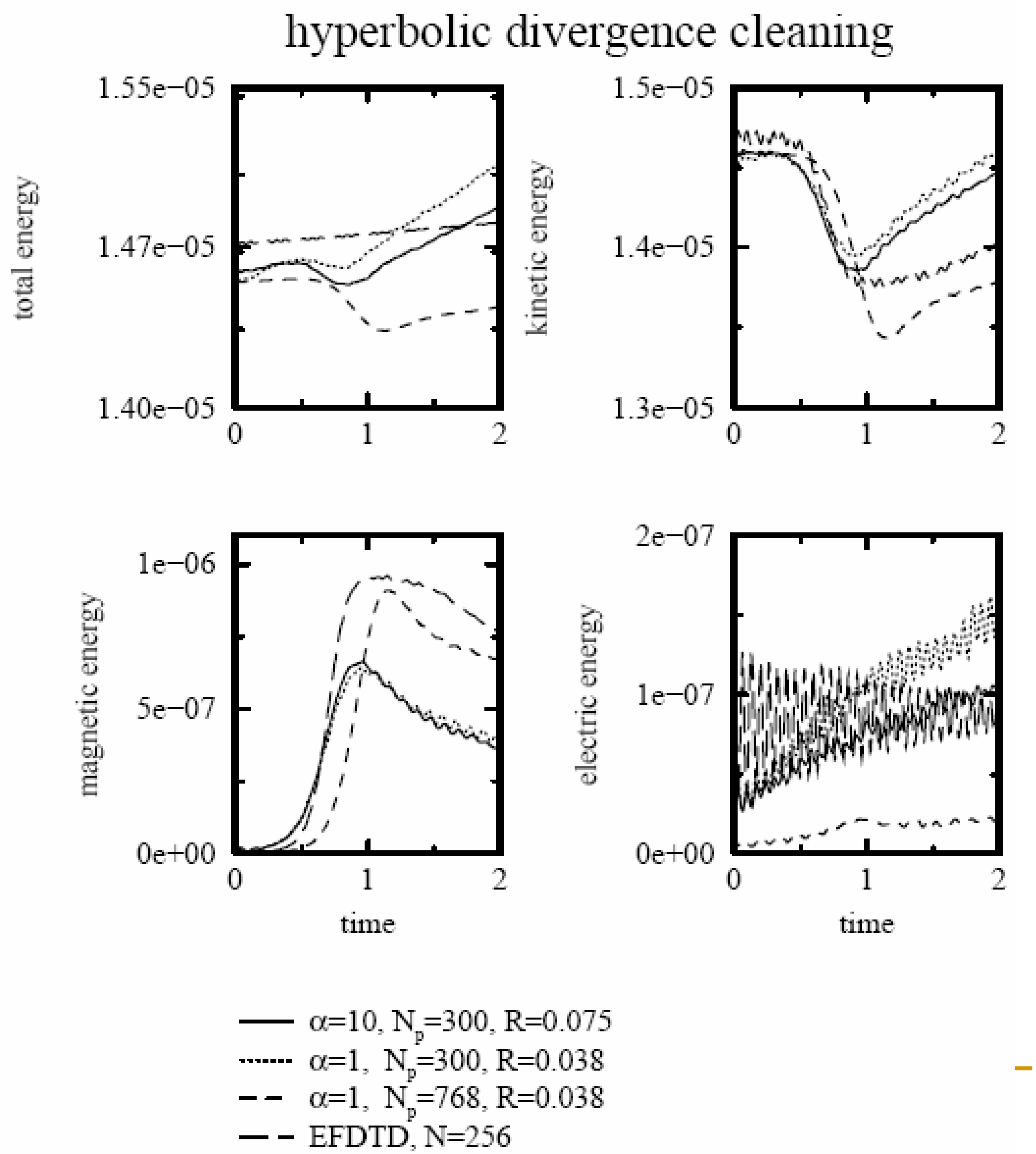
Weibel instability: DG-PIC 5th order simulation

- Investigate high-order DG-PIC discretization.
- Used both Poisson and hyperbolic divergence cleaning.
- Simulation parameters:
  - *NxNx2* grid cells, with *N*=10.
  - Initialized with $N_p=(300)^2$, and $(768)^2$ number of particles.
  - Approximation order 5.
  - Radius of particle R=0.075, and 0.038.
  - α=1 and 10. Power of distribution function: $S(r) = \frac{\alpha+1}{\pi R^2}\left[1-\left(\frac{r}{R}\right)^2\right]^\alpha$



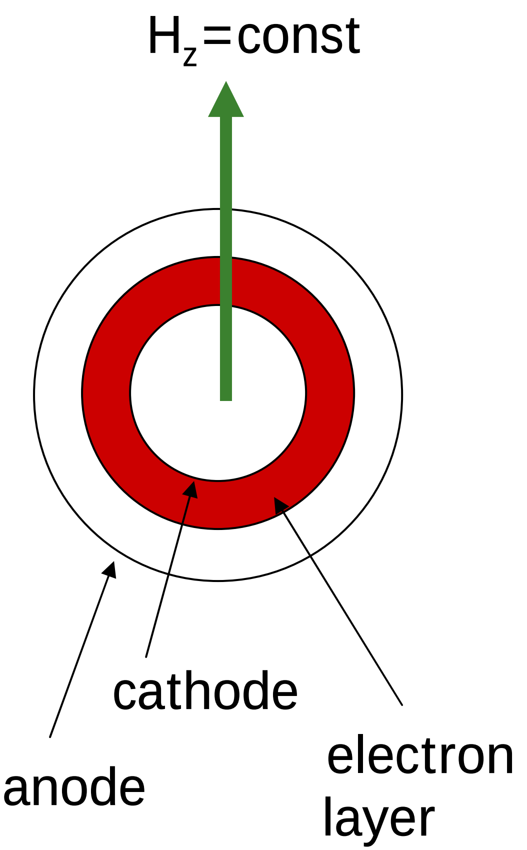
DG-PIC 5th order: energies versus time.

- Excellent stability properties, i.e. little grid heating.
- Increasing the number of particles leads a significant improved comparison to FDTD.



Smooth bore magnetron: Brillouin flow.

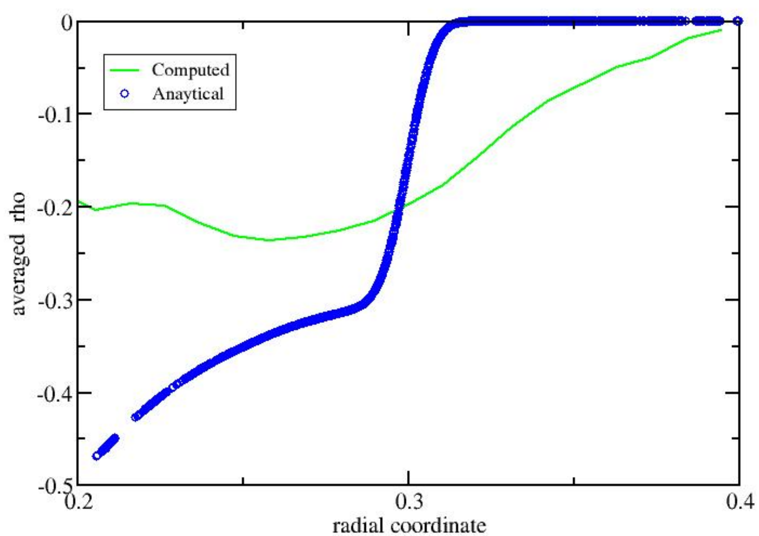
- Initial conditions:
  - Constant voltage.
  - Analytical solution of [Davidson *et al.*, *SPIE*, '89] for electric field and electron layer.
- The constant electric field rotate the electrons, while the voltage keeps the layer from reaching the anode.
- This flow is unstable, the mechanisms are unclear.



Smooth bore magnetron: results.

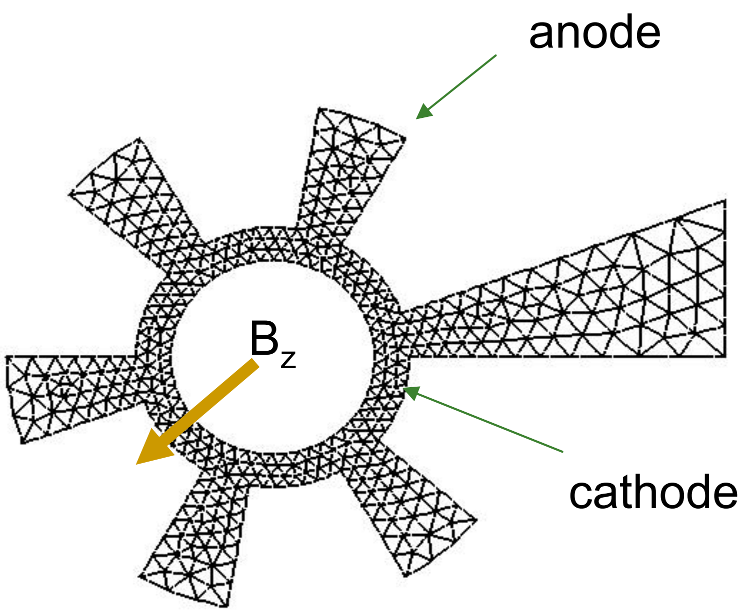
- The computation confirms the instability in the Brillouin flow.
- Low frequency particle spikes are also observed in finite difference simulations [Cartwright, *private communication*].
- Average shows the presence of an electron layer.

QuickTime™ and a
BMP decompressor
are needed to see this picture.



A6 Magnetron

- Initial conditions:
  - Brillouin flow.
  - Background electric (constant voltage) and magnetic field.
- Boundary condition: Conducting walls.
- Emission model: if electron leaves domain inject new one at cathode at random position.



[Palevski and Bekefi, *Phys. Fluids*,, ‘79]

A6 Magnetron: Prelimenary Results.

Particle show modes.

Radial electric field.

QuickTime™ and a
BMP decompressor
are needed to see this picture.

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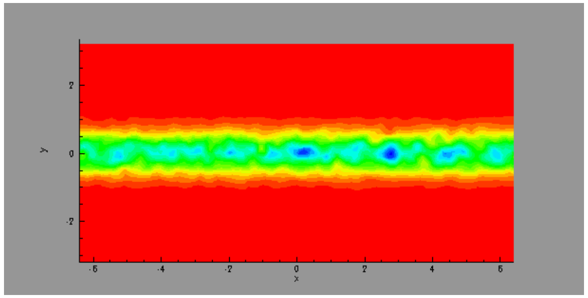
BMP decompressor
are needed to see this picture.

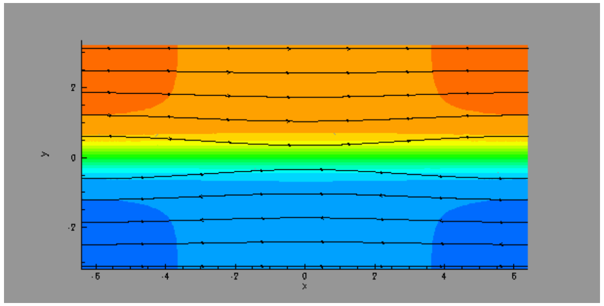
Magnetic Reconnection

- Initial conditions:
  - Harris current sheet.
  - Perturbed magnetic field.
- The magnetic field topology changes in time: magnetic reconnection.
- The reconnection is accompanied by a sharp drop in the magnetic potential energy and an increase in the kinetic energy. The flow exhibits dissipation without reconnection!

Out-of-plane current



Magnetic field lines and Hx contours



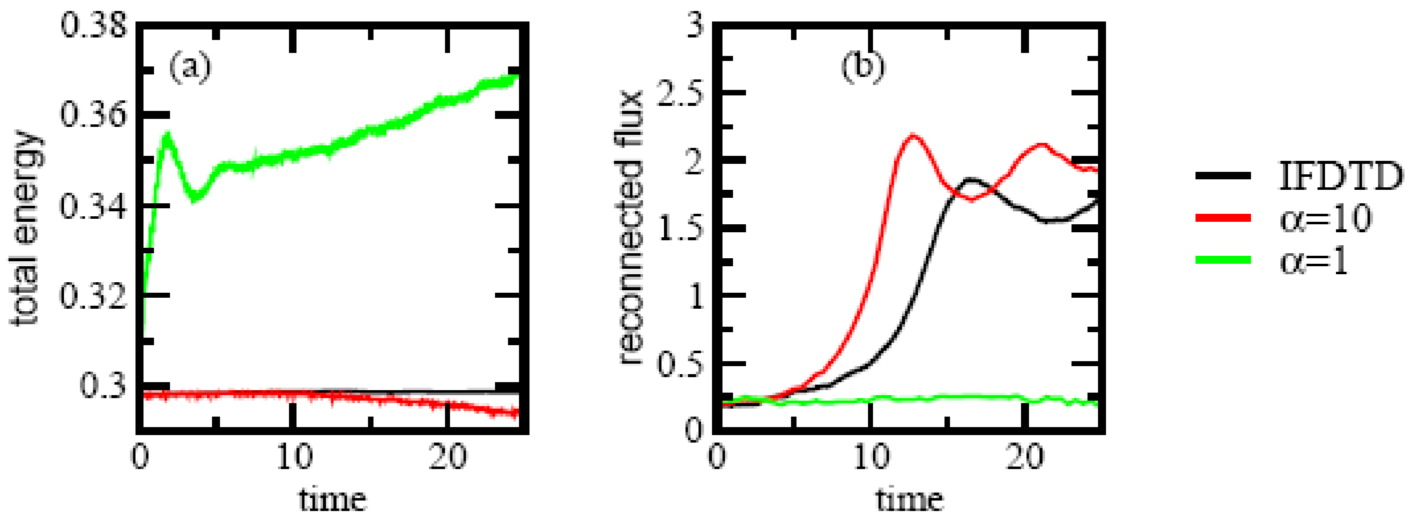
[Jacobs *et al.*, in preparation]

Magnetic reconnection: (in collaboration with G. Lapenta, LANL)

- IFDTD is reference simulation (ideally suited for magnetic reconnection simulation).
- IFDTD:
  - *N*x*N* grid cells, with N=32.
  - Initialized with N_p=25k particles.
- DG-PIC
  - 32x16x2 elements, fifth order.
  - Initialized with N_p=100k number of particles.
  - Radius of particle R=0.375=L_x/32 (32 grid spacings in length of domain).
  - $\alpha=10$, smooth distribution function.

Magnetic reconnection: shape function

- A smoother particle function reduces grid heating effects.
- A significant improvement of the results!



Current emphasis

- Improved temporal discretizations
  - IMEX-RK Methods
  - Fully implicit time-stepping
- Steps towards adaptive control of particle numbers
  - High-order local particle shapes.
  - Splitting/ coalesce strategies.
  - Kinetic error estimation.
  - Hybrid schemes.
- Alternative field solver formulations
- Validations

Temporal discretization.

- Explicit stability criteria restrict the maximum allowable time step.
  - CFL Condition
  - Implications of grid heating
  - Electron cyclotron frequency
- Often these criteria are more restrictive than they would need to be to get an accurate result.
- Solution is implicit temporal discretization:
  - Fully implicit particle-in-cell.
  - Partially implicit particle-in-cell
    - Explicit particles
    - Implicit field solver

Fully implicit particle-in-cell

- Simulating the whole system of particles and Maxwell's equation is very expensive.
- Update charge density and current density using the implicit moment method:

$$\rho_s^{n+1} = \rho_s^n - \Delta t \, \nabla \cdot \mathbf{J}_s^{n+1/2},$$

$$\hat{\mathbf{J}}_s = \sum_p q_p \hat{\mathbf{v}}_p W(\mathbf{x} - \mathbf{x}_p^n),$$

$$\mathbf{J}_s^{n+1/2} = \hat{\mathbf{J}}_s - \frac{\Delta t}{2} \boldsymbol{\mu}_s \cdot E_\theta - \frac{\Delta t}{2} \nabla \cdot \hat{\mathbf{\Pi}}_s$$

$$\hat{\mathbf{\Pi}}_s = \sum_p q_p \hat{\mathbf{v}}_p \hat{\mathbf{v}}_p W(\mathbf{x} - \mathbf{x}_p^n),$$

- First/second order.

- Combine with hyperbolic cleaning and DG-PIC discretization.

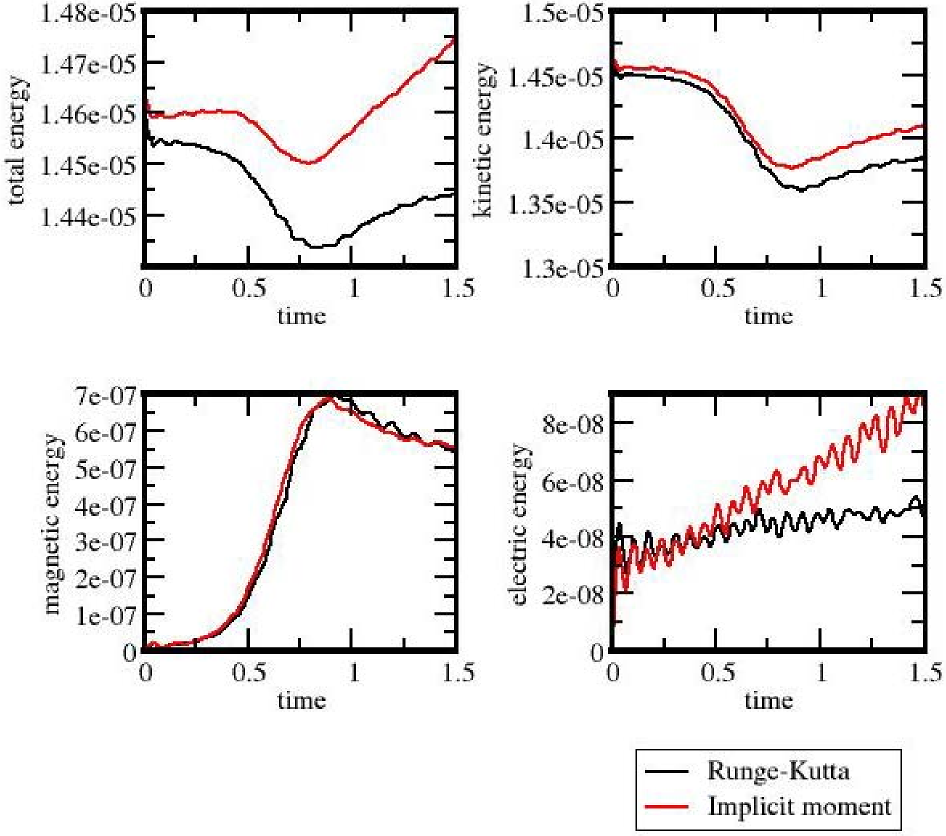
[Lapenta *et al.*, *Phys. Plasmas*, 06]

Partially implicit time scheme: IMEX Runge-Kutta.

- IMEX Runge-Kutta schemes:
  - Couple variable order explicit Runge-Kutta and implicit Runge-Kutta.
  - Any part of a system of equations can be solved with explicit or implicit scheme.
  - Any part of spatial regime can be solved with explicit or implicit scheme.
  - Singly diagonal implicit scheme, the global inverse can be re-used.
  - No low storage (yet). Fourth order ESDIRK scheme, requires 6N storage.
- Hyperbolic cleaning stiffens field equations:
  - Solve implicitly.

Time schemes: Weibel instability result.

- All temporal schemes can predict the Weibel instability.
- IMEX scheme is accurate for time steps that are χ (>10) times larger than explicit.
- The implicit moment scheme needs a time that is four times smaller than IMEX because of its lower order accuracy.

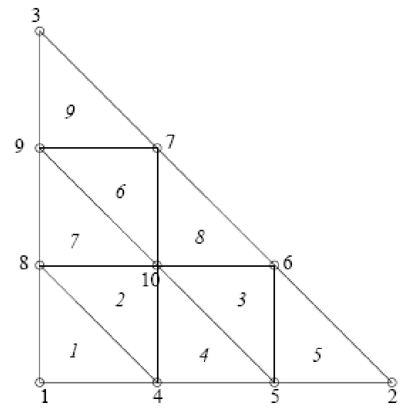


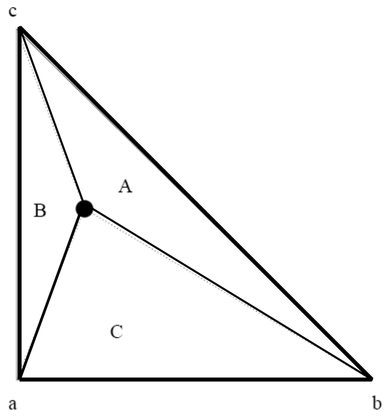
Adaptivity in Particle Numbers

- Why adaptivity in particles?
  - Large geometrical changes requires spatial adjustments of the particle.
  - Large physical changes require adaptivity of the particle in velocity phase space, i.e. adaptivity of the number of particles.
  - Particle dynamics is most expensive part
- How?
  - Variable radius of the deposition function.
  - Splitting and coalescence of particles
  - Error estimation for kinetic dynamics

Element based adaptivity: area weighing.

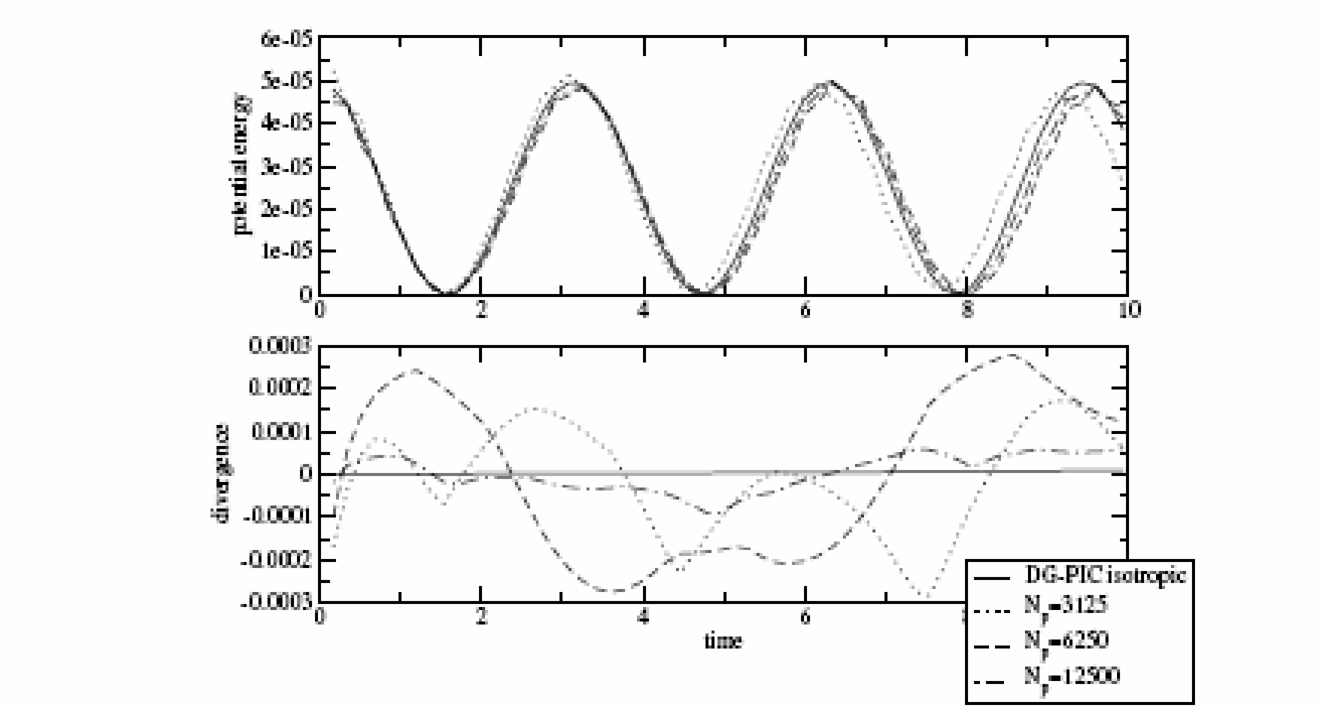
- Use equidistant basis on the triangle, as opposed to electrostatic basis.
- Do second order area weighing on the subtriangles.
- Particle splits triangle into three subareas that determine the relative weight to opposing corners.





Element based adaptivity: area weighing.

It works, but…..many particles.



Plasma wave simulation.

Error estimation - A Starting Point

- The development of a robust way to estimate the error in phase space is a significant challenge.
- We are pursuing the following approach
  - Solve along with the PIC, a fluid or df model to obtain the first few moments - compared to the particles, the cost is minimal.
  - Compare the computed dynamics, using non-parametric estimation, to the fluid-like model.
  - Act accordingly !
- DG-FEM is well suited for this approach as it solves the fluid equations without problems.
- It opens for a very natural way of doing hybrid modeling of fluid/kinetic systems.

Concluding remarks

- New PIC method based on a high-order DG-FEM
  - Decoupled particle resolution and field resolution.
  - High-order temporal schemes without splitting.
  - New divergence cleaning techniques.
  - 2D extensively tested, 3D exists but still prelimenary.
- Offers some advantages upon existing methods
  - Lower resolution requirements.
  - Complex geometry modeling.
  - Flexibility (order/locality/particle shapes etc)
  - Improved control of Cherenkov radiation and grid heating.
- Future developments
  - Particle adaptivity in phase-space and alternative formulations
  - Concrete evidence of advantage of high-order for particles
  - Parareal time-stepping using fluid equations
  - Hybrid modeling
  - Extensive 3D development and validation effort.

… and a bit of promotion

- SLEDG++ -- a DG discretization toolbox
  - Matlab style C++ operator building
  - General 2D/3D, high-order, unstructured grids etc
  - Support for refinement, coarsening, non-conforming etc
  - Integrated with solvers for parallel solution and matrix free form for time-advancement
  - A small but active user community
- Interested ? -- Jan.Hesthaven@Brown.edu

Thank you for your attention !