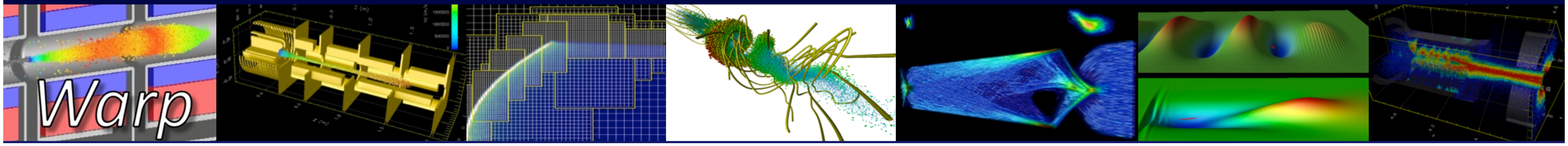
On Some Computational Challenges & Novel Solutions in the Kinetic Modeling of Beams and Plasmas

Novel Simulation Methods in the Particle-In-Cell Code-Framework Warp



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Computational Methods in High Energy Density Plasmas

Workshop I: Computational Challenges in Hot Dense Plasmas

IPAM, UCLA, Los Angeles, USA – March 26-30, 2012

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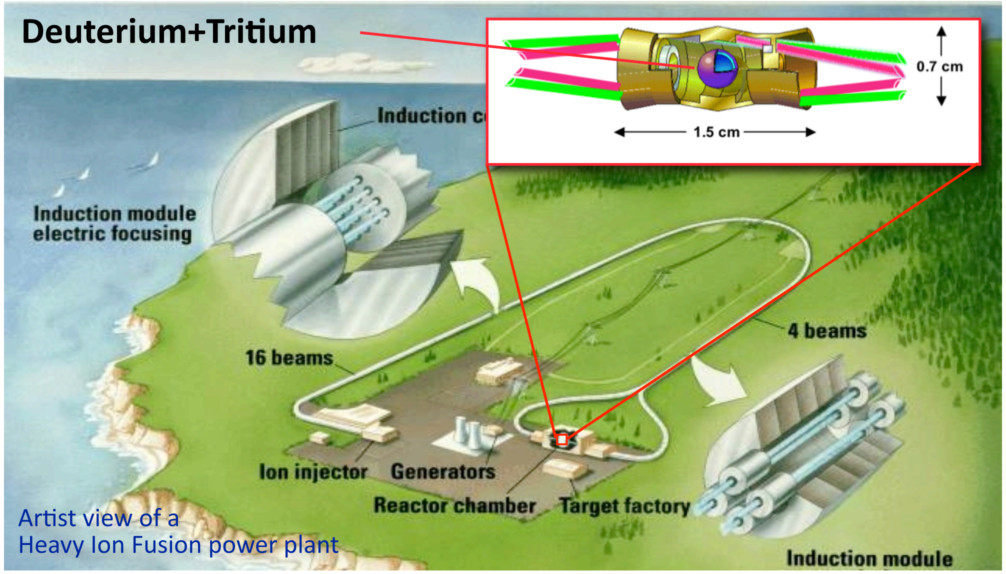
The Heavy Ion Fusion Science Virtual National Laboratory

Outline

- Warp overview
  - origins (Heavy Ion Inertial Fusion)
  - geometry, particle pushers, field solvers, etc
- Computational challenges - *novel algorithms*
  - large time-step in magnetic fields - *"Drift-Lorentz" particle pusher*
  - E+VxB cancellation in Boris pusher - *Lorentz invariant particle pusher*
  - spatial scale disparities - *Mesh Refinement for PIC*
  - time scale disparities - *boosted frame method*
  - numerical dispersion - *tunable EM field solver for PIC*
  - wideband filtering - *"strided" digital filters*
- Summary

The Heavy Ion Fusion Science Virtual National Laboratory

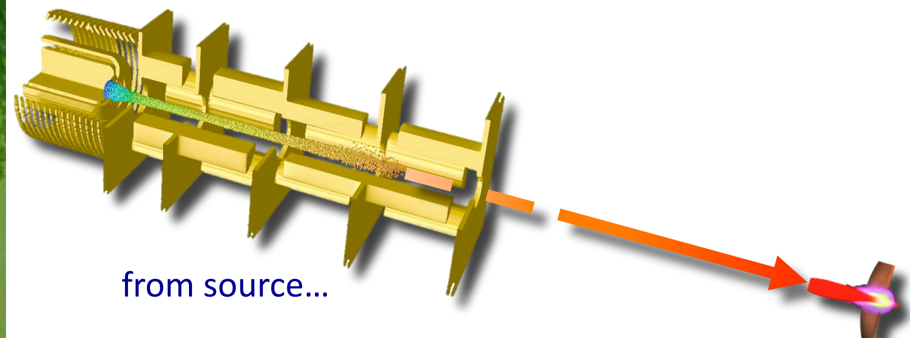
The Heavy Ion Inertial Fusion (HIF) program is studying the science of ion-heated matter, as well as drivers & targets for inertial fusion energy



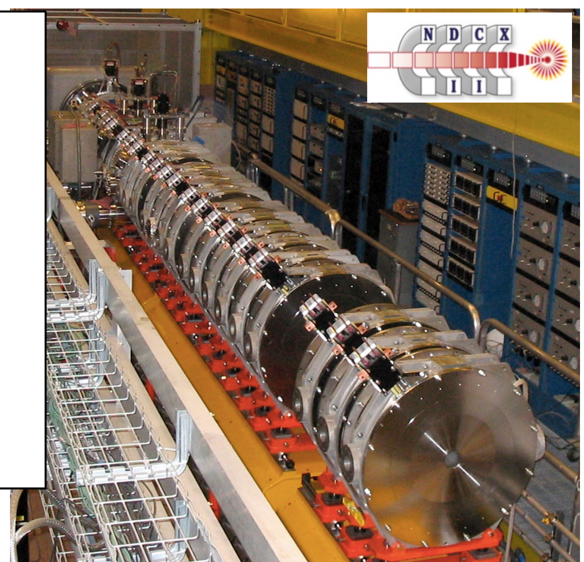
Artist view of a
Heavy Ion Fusion power plant

Space/time scales span 8 orders of magnitude:
from <mm to km>/<ps to 100 ms>

Simulation goal – integrated self-consistent predictive capability



NDCX-II is our new platform for studies of
-space-charge-dominated beams
-Warm Dense Matter physics
-beam-target energy coupling



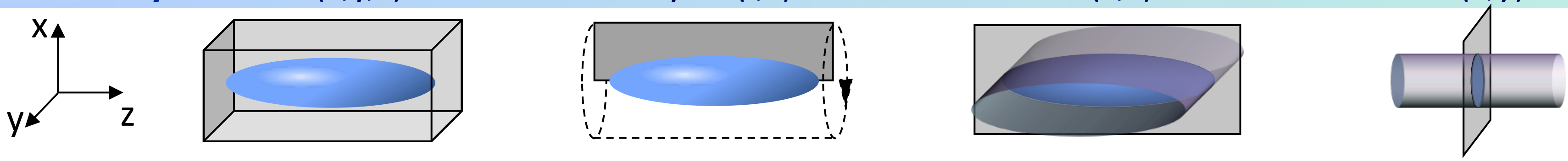
including:

- beam(s) generation, acceleration, focusing and compression along accelerator,
- loss of particles at walls, interaction with desorbed gas and electrons,
- neutralization from plasma in chamber,
- target physics and diagnostics.

=> Need large-scale multiphysics computing

Main code is Warp - a parallel framework combining features of plasma (Particle-In-Cell) and accelerator codes

- **Geometry:** 3-D (x,y,z) axisym. (r,z) 2-D (x,z) 2-D (x,y)



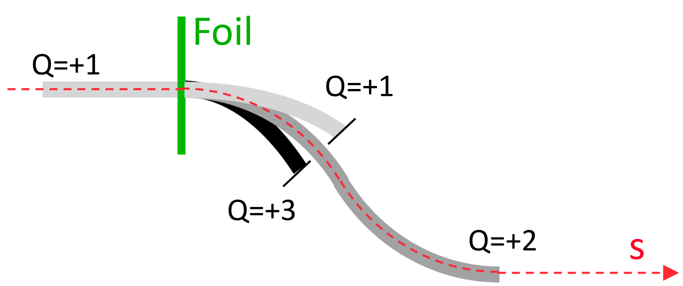
- **Reference frame:** **lab** **moving-window** **Lorentz boosted**

lab	moving-window	Lorentz boosted
z	z-vt	γ(z-vt); γ(t-vz/c^2)

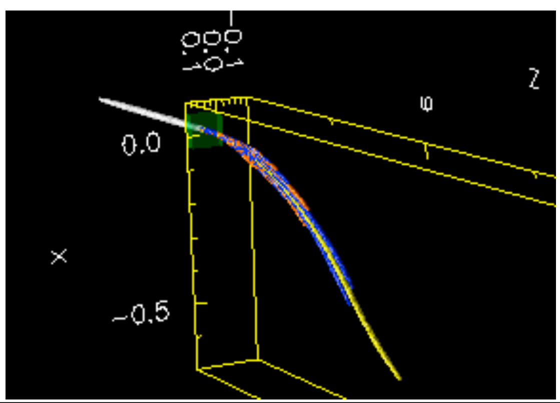
- **Bends:** "warped" coordinates (no "reference orbit")

see A. Friedman, D. P. Grote, and I. Haber, *Phys. Fluids B* **4**, 2203 (1992)

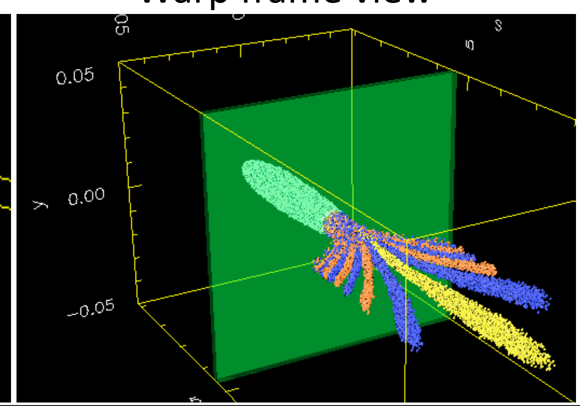
Example: beam stripping through a foil and charge selection in a chicane.



Lab frame view



Warp frame view

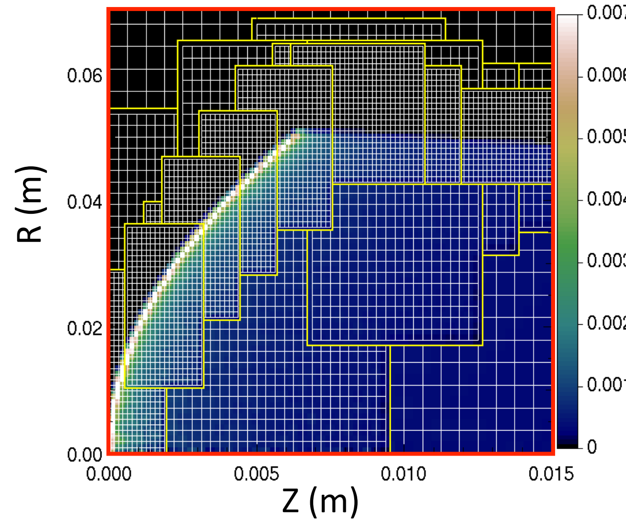


The Heavy Ion Fusion Science Virtual National Laboratory

SciDAC-II Compass

Field solvers based on Finite Difference methods

- **Field solvers**
  - Electrostatic/Magnetostatic - FFT, multigrid; AMR; implicit
  - Fully electromagnetic - Yee mesh, PML, MR



Automatic meshing around HCX ion beam source emitter from Warp (r,z) simulation

- "longitudinal Darwin" for ultra-relativistic beams* ($v_z >> v_x, v_y$)

$$\left.\begin{aligned}\frac{\partial^2\phi}{c^2\partial t^2}-\Delta\phi=\frac{\rho}{\varepsilon_0}\\ \frac{\partial}{\partial t}\approx v_z\frac{\partial}{\partial z}\end{aligned}\right\} \Rightarrow \frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial(\gamma z)^2}\approx-\frac{\rho}{\varepsilon_0} \Rightarrow \left\{\begin{aligned}\vec{E}\approx\left\{\frac{\partial\phi}{\partial x},\frac{\partial\phi}{\partial y},\left(1+\beta^2\right)\frac{\partial\phi}{\partial z}\right\}\\ \vec{B}\approx\left\{\frac{v_z}{c^2}\frac{\partial\phi}{\partial y},-\frac{v_z}{c^2}\frac{\partial\phi}{\partial x},0\right\}\end{aligned}\right.$$

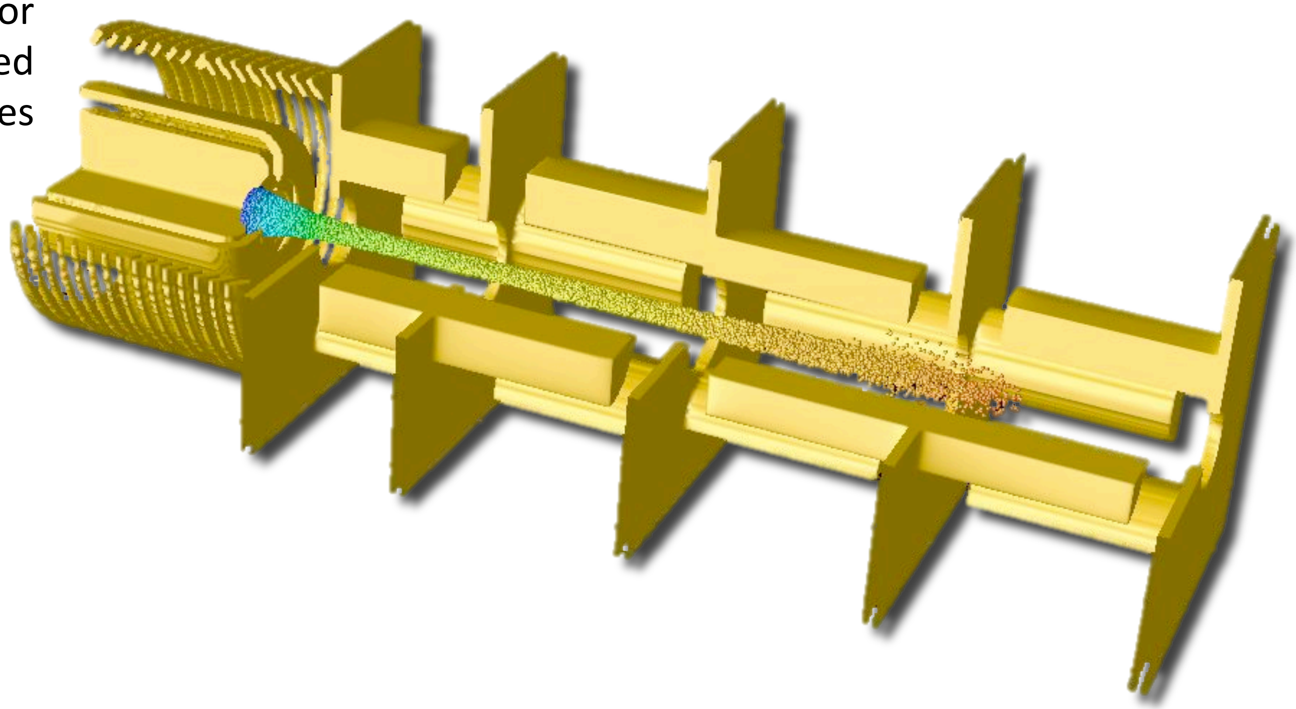
Only one Poisson solve with stretched z coordinate gives all E and B field components.

*J.-L. Vay, *Phys. Plasmas* **15**, 056701 (2008)

Support for internal conductors & accelerator lattice elements

- **Boundaries:** "cut-cell" --- no restriction to "Legos" for electrostatic solvers

Versatile conductor generator accommodates complicated structures



Modeling of HCX injector

- **Accelerator lattice:** general; non-paraxial; can read MAD files
  - solenoids, dipoles, quads, sextupoles, linear maps, arbitrary fields, acceleration.

Particle pusher based on leapfrog method

- **Position push**

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

- **Velocity push (u=γv)**

$$u^{n+1} = u^n + \frac{q}{m} f\left(E^{n+1/2}, B^{n+1/2}, u^n, u^{n+1}, \Delta t\right)$$

Four options

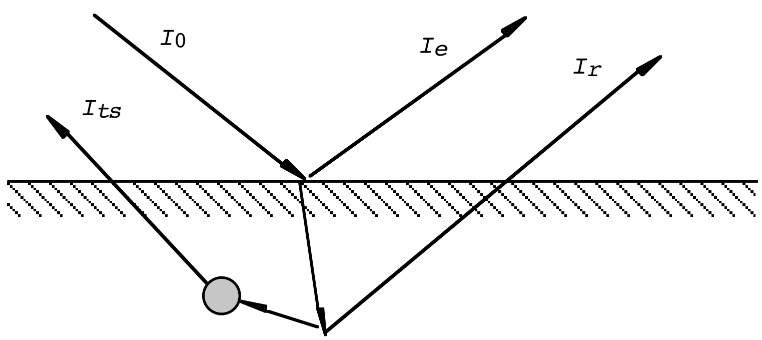
- standard Boris,
- Boris with "tan(α)/α" rotation angle correction,
- "drift-Lorentz"[1] (for taking large time steps > cyclotron period),
- Lorentz invariant[2] (provides proper treatment of self **E**+**v**×**B** for relativistic particles).

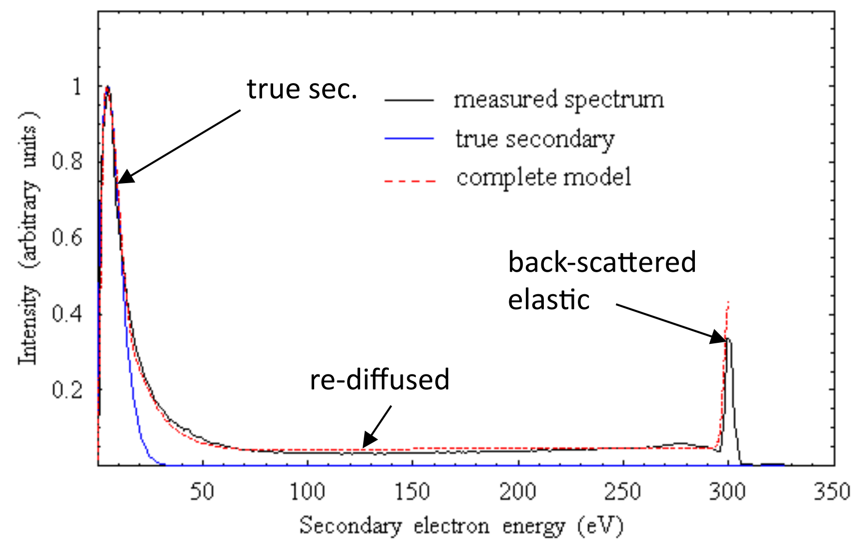
[1]R. Cohen et. al., *Phys. Plasmas* **12,** 056708 (2005)
[2]J.-L. Vay, *Phys. Plasmas* **15**, 056701 (2008)

Surface/volume physics

- **Particle emission:** space charge limited, thermionic, hybrid, arbitrary

- **Secondary electrons:** Monte-Carlo with energy and angular dependence (Posinst; M. Furman)





- **Ion impact- or photo-induced electron emission**

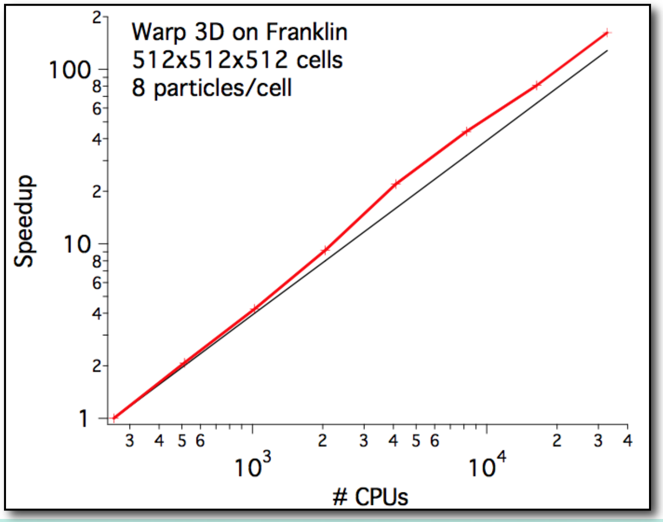
- **Ion impact-induced gas emission, tracking**

- **Monte Carlo Collision:** ionization, capture, charge exchange

Warp is parallel, combining modern and efficient programming languages

- **Parallellization:** MPI (1, 2 and 3D domain decomposition)

Parallel strong scaling of Warp 3D PIC-EM solver on Franklin supercomputer (NERSC)



- **Python and FORTRAN*:** "steerable," input decks are programs

From warp import *	Import Warp modules and routines in memory
…	
nx = ny = nz = 32	Sets # of grid cells
dt = 0.5*dz/vbeam	Sets time step
…	
initialize()	Initializes internal FORTRAN arrays
step(zmax/(dt*vbeam))	Push particles for N time steps with FORTRAN routines
…	

*http://hifweb.lbl.gov/Forthon (wrapper supports FORTRAN90 derived types)

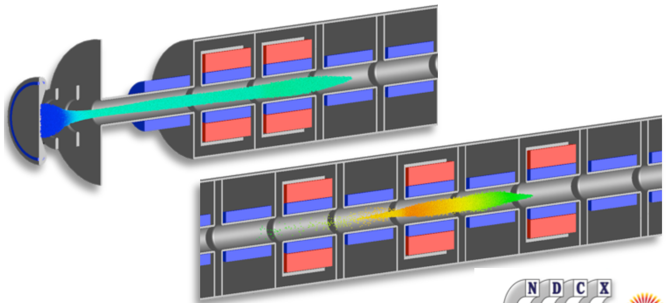
Warp's versatile programmable framework allows great adaptability

Standard PIC

Moving window

Example:

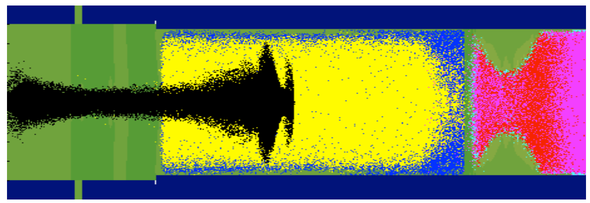
Beam generation & transport



Laboratory frame

Example:

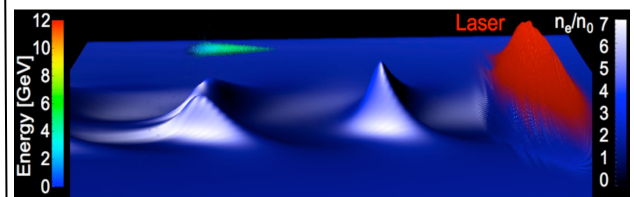
Beam neutralization in plasma



Lorentz Boosted frame

Example:

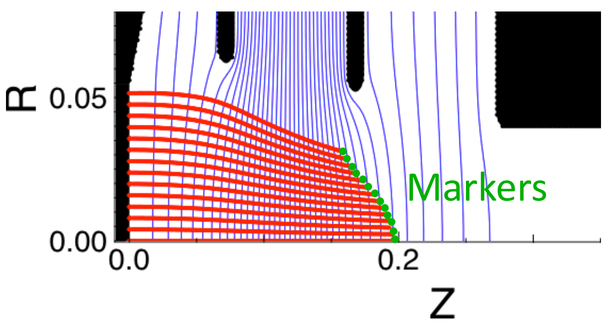
Laser plasma acceleration



Non-standard PIC

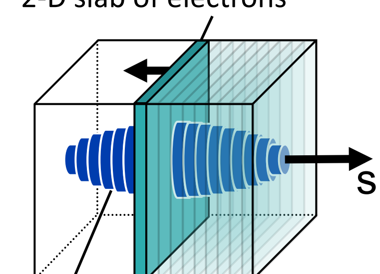
Steady flow

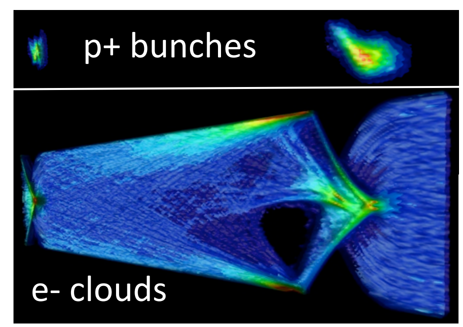
Example: Injector design



Quasi-static

Example: electron cloud studies





SPS - CERN

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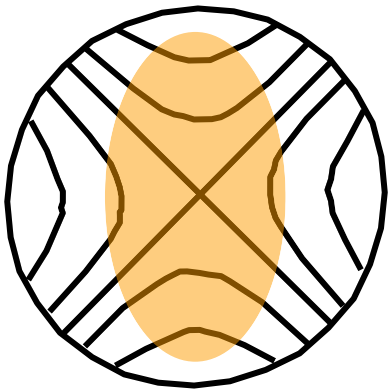
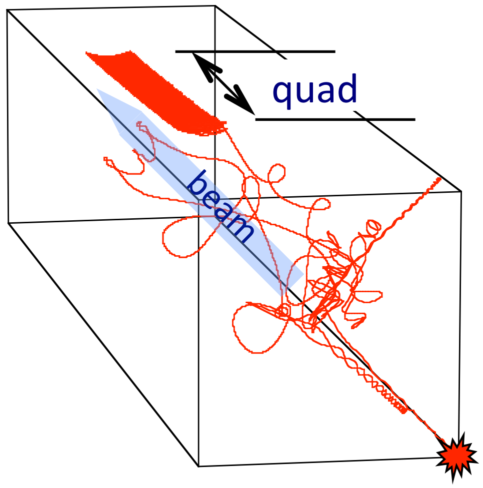
"Drift-Lorentz" particle pusher* relaxes the problem of short electron timescales in magnetic field

Electron motion in Magnetic quadrupole





Sample motion

Problem: Electron gyro timescale

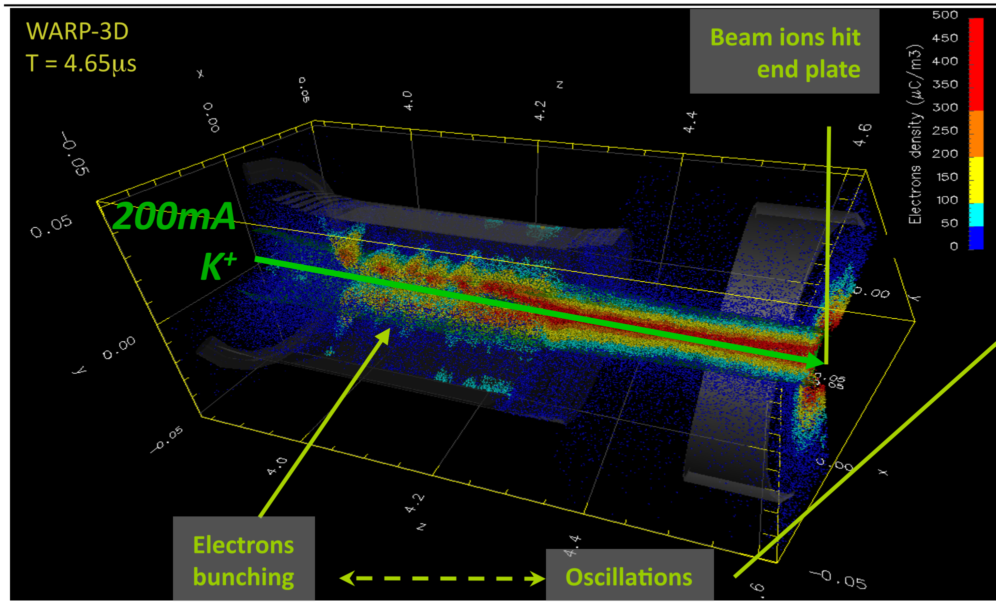
<< other timescales of interest

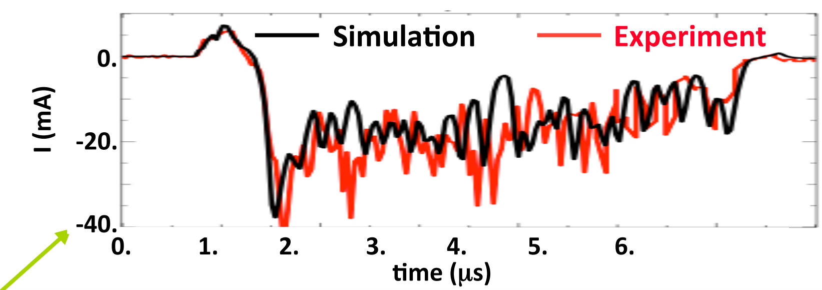
⇒ brute-force integration <u>very</u> slow due to small Δt

Solution*: Interpolation between full-particle dynamics ("Boris mover") and drift kinetics (motion along B plus drifts)

$$\vec{v}_{eff} = \vec{B}\left(\vec{B}.\vec{v}_L\right) + \alpha\vec{v}_{L,\perp} + \left(1-\alpha\right)\vec{v}_d$$

correct gyroradius with $\alpha = 1/\sqrt{1+\left(\omega_c\delta t/2\right)^2}$





Good agreement between sim. & exp.

Run time ~1 day with new electron mover (and MR). Would be ~10-20 days otherwise.

*R. Cohen et. al., *Phys. Plasmas* **12** (2005) 056708

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Lorentz invariant particle pusher

- Boris pusher introduces error in cancellation of self **E** and **v×B**
  - Velocity push: $$u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \boxed{\frac{u^{n+1}+u^n}{2\gamma^{n+1/2}}} \times B^{n+1/2}\right) \qquad u = \gamma v$$

issue: **E**+**v**×**B**=0 implies **E**=**B**=0 => large errors when **E**+v×**B**≈0 (e.g. relativistic beams).

- Solution
  - Velocity push: $$u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \boxed{\frac{v^{n+1}+v^n}{2}} \times B^{n+1/2}\right)$$

- Looks implicit but solvable analytically*

$$\begin{cases} \gamma^{i+1} = \sqrt{\dfrac{\sigma + \sqrt{\sigma^2 + 4(\tau^2 + u^{*2})}}{2}} \\ \mathbf{u}^{i+1} = [\mathbf{u}' + (\mathbf{u}'\cdot\mathbf{t})\mathbf{t} + \mathbf{u}'\times\mathbf{t}]/(1+t^2) \end{cases}$$

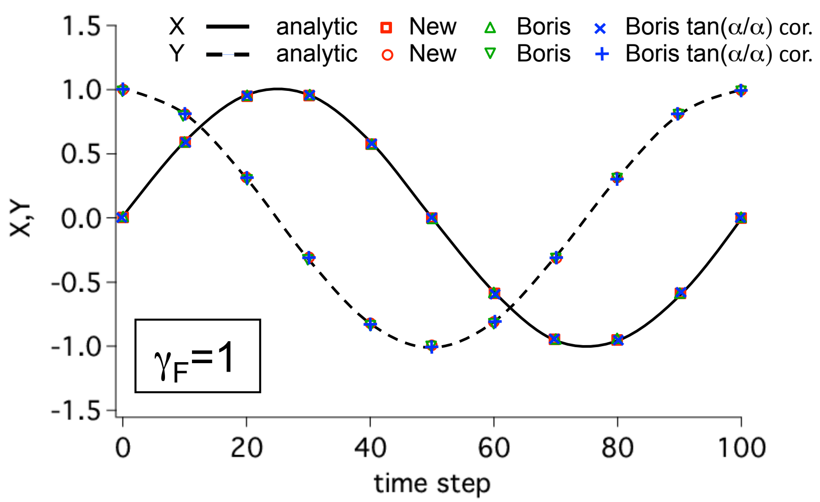
(with $\mathbf{u} = \gamma\mathbf{v}$, $\mathbf{u}' = \mathbf{u}^i + \frac{q\Delta t}{m}\left(\mathbf{E}^{i+1/2} + \frac{\mathbf{v}^i}{2}\times\mathbf{B}^{i+1/2}\right)$, $\boldsymbol{\tau} = (q\Delta t/2m)\mathbf{B}^{i+1/2}$,
$u^* = \mathbf{u}'\cdot\boldsymbol{\tau}/c$, $\sigma = \gamma'^2 - \tau^2$, $\gamma' = \sqrt{1+u'^2/c^2}$, $\mathbf{t} = \boldsymbol{\tau}/\gamma^{i+1}$).

*J.-L. Vay, *Phys. Plasmas* **15**, 056701 (2008)

Single particle test of Lorentz invariant pusher

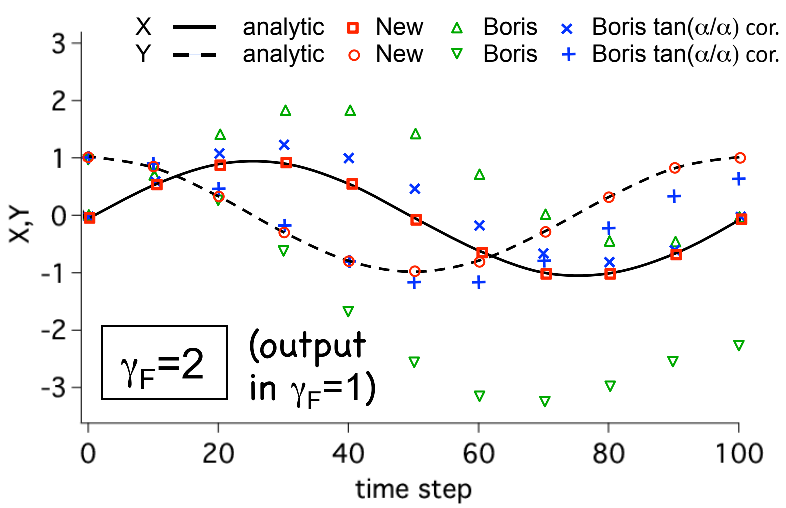
Lab frame

particle cycling in constant B field



Boosted frame γ=2

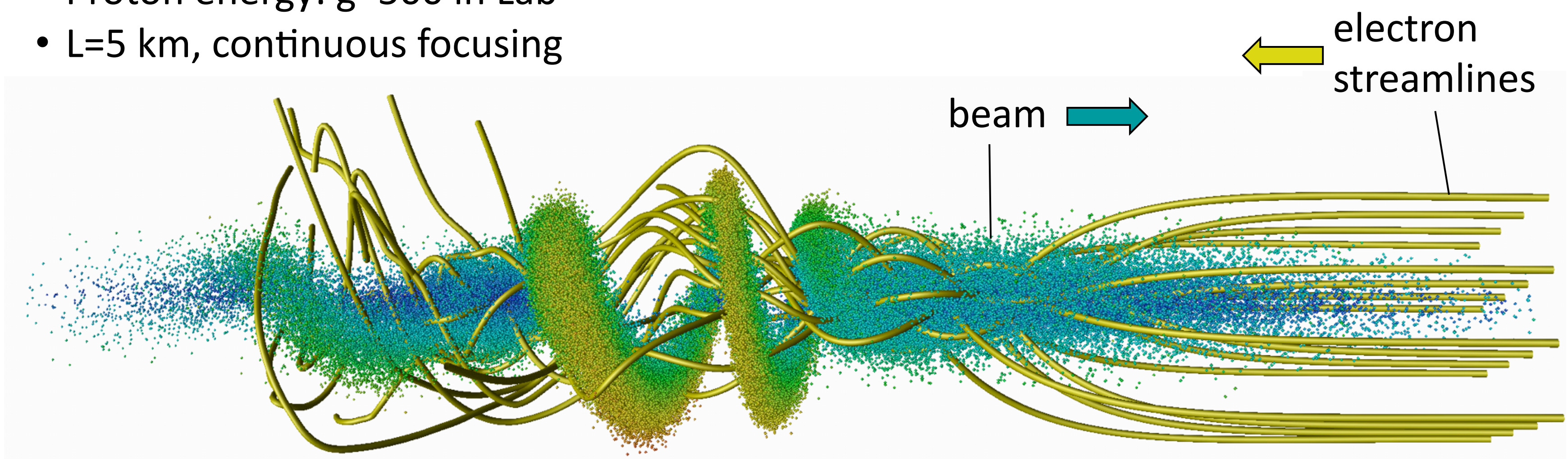
ExB drift adds to gyration



Example of application to LHC-like beam interacting with e-cloud

Calculation of e-cloud induced instability of a proton bunch*

- Proton energy: g=500 in Lab
- L=5 km, continuous focusing



- beam was lost after a few betatron oscillations with Boris pusher,
- accurate result was obtained with new pusher.

Pusher also used for modeling of

- astrophysical highly magnetized relativistic electron-ion flow (L. Sironi & A. Spitkovski, Princeton U.)
- particle trajectory integration in plasma with QED effects (N. Elkina, LMU, Germany)

*J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)

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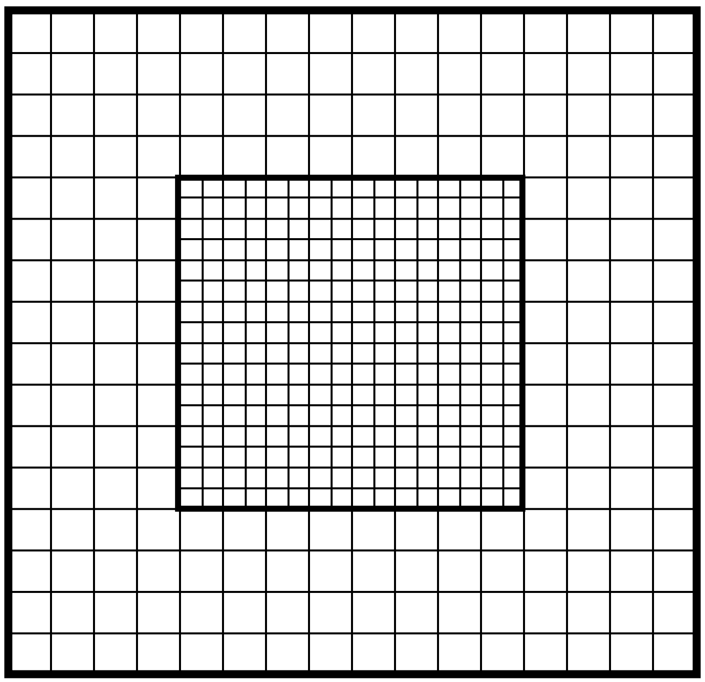
Coupling of AMR to PIC/Vlasov/MHD: issues

Mesh refinement implies a jump of resolution and some procedure for coupling the solutions at the interface.



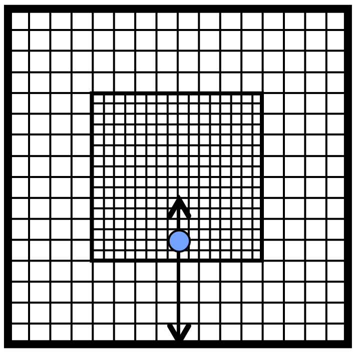
Consequences:

- loss of symmetry: self-force[1,2],
- loss of conservation laws[1,2],
- EM: waves reflection[3].

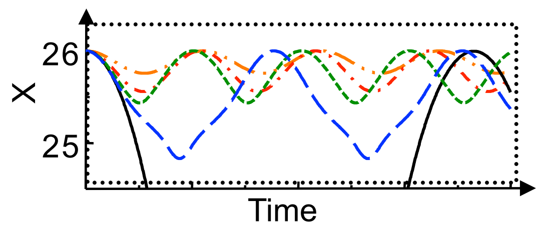
(1) Vay et al., *Laser Part. Beams* 20 (2002)
(2) Vay et al., *Phys. Plasmas* **11** (2004)
(3) Vay, *J. Comput. Phys.* 167 (2001)

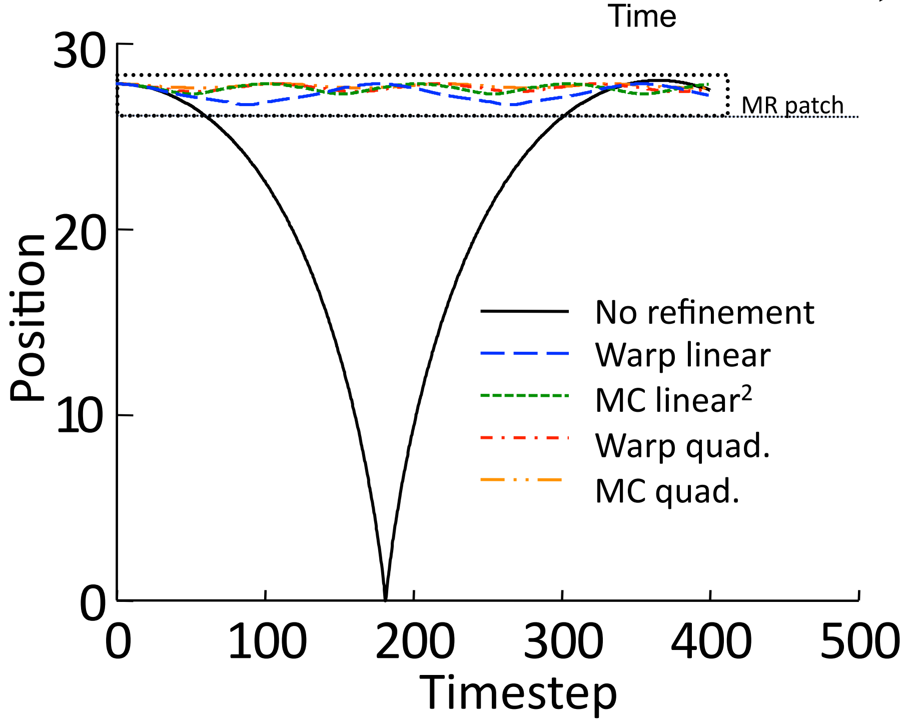
Electrostatic mesh refinement method: spurious self-force

MR introduces spurious force[1]



particle feels its own field and can be trapped in patch

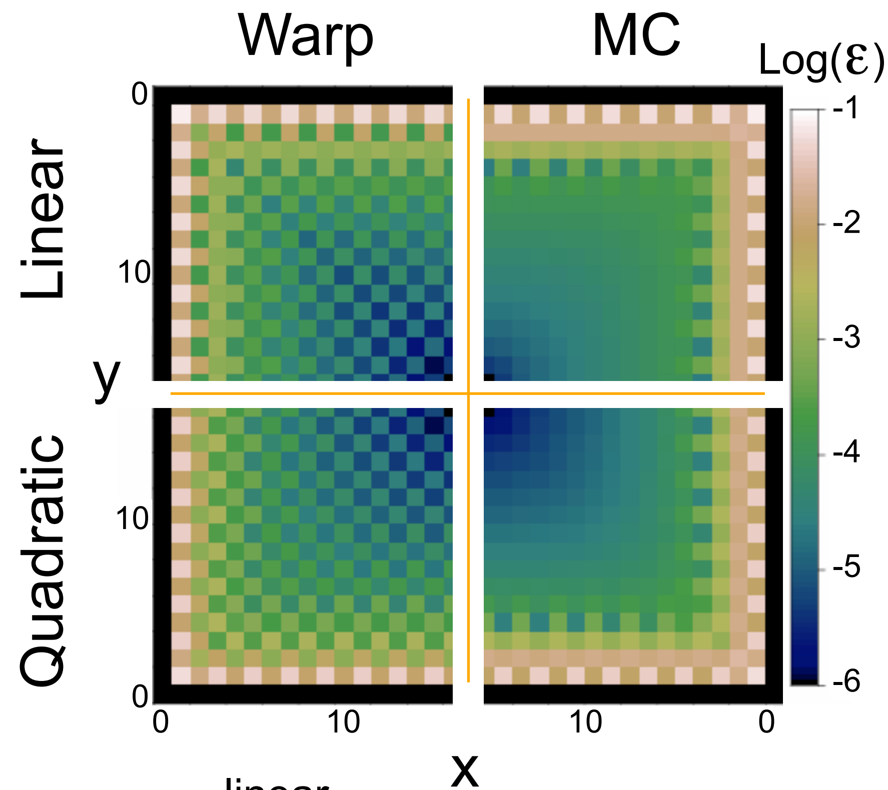


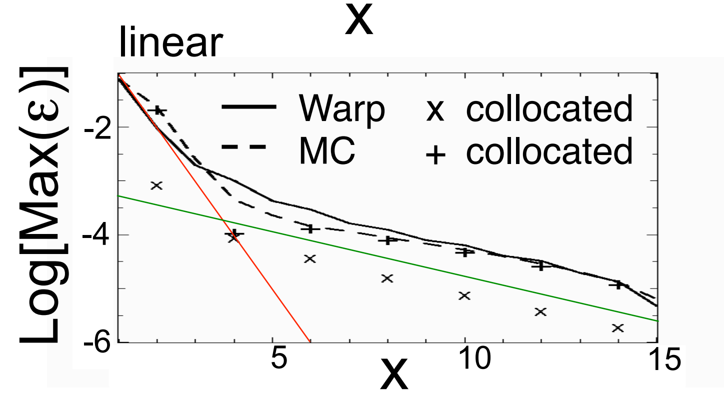


(1) Vay et al., *Laser Part. Beams* **20** (2002)

(2) McCorquodale et al., *J. Comput. Phys.* **201** (2004)

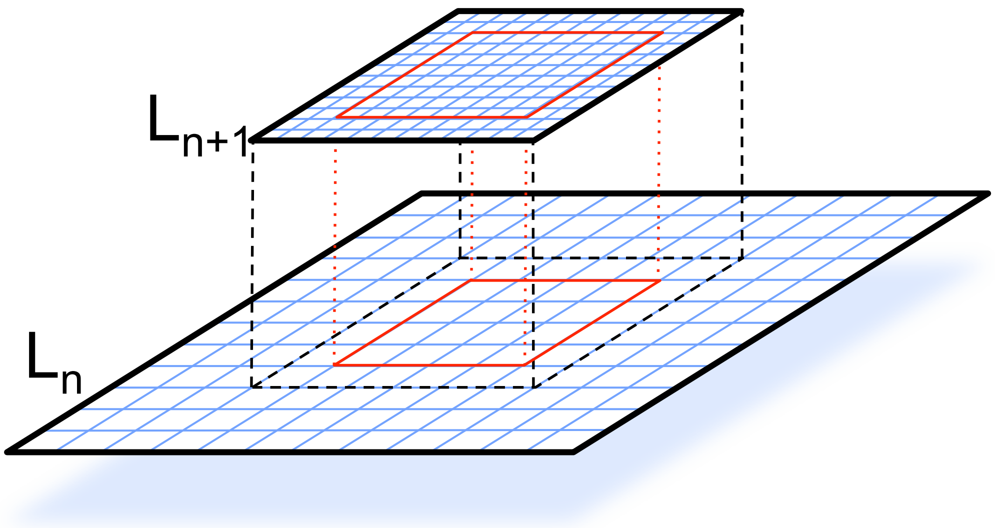
Spurious self-force decrease rapidly in patch





Spurious self-force mitigated in Warp using guard cells

Warp's electrostatic MR solver[1,2]

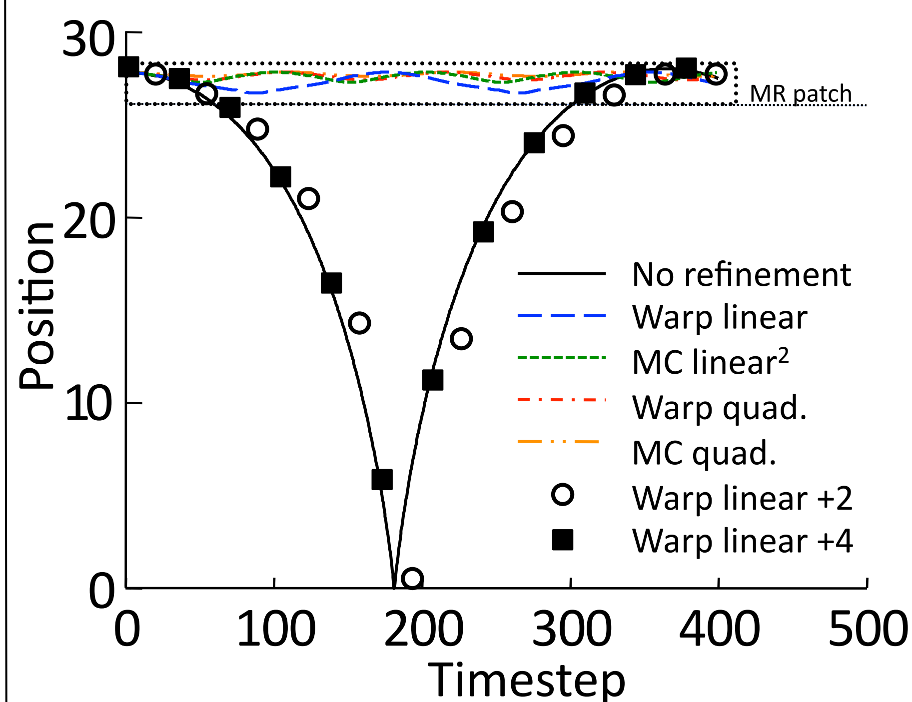


1 – solve on coarse grid,
2 – interpolate on fine grid boundaries,
3 – solve on fine grid,
4 – disregard fine grid solution close to edge when gathering force onto particles.

Guard cells provide user control of relative magnitude of spurious force[(2)].

(1) Vay et al., *Laser Part. Beams* **20** (2002)
(2) Vay et al., *Phys. Plasmas* **11** (2004)

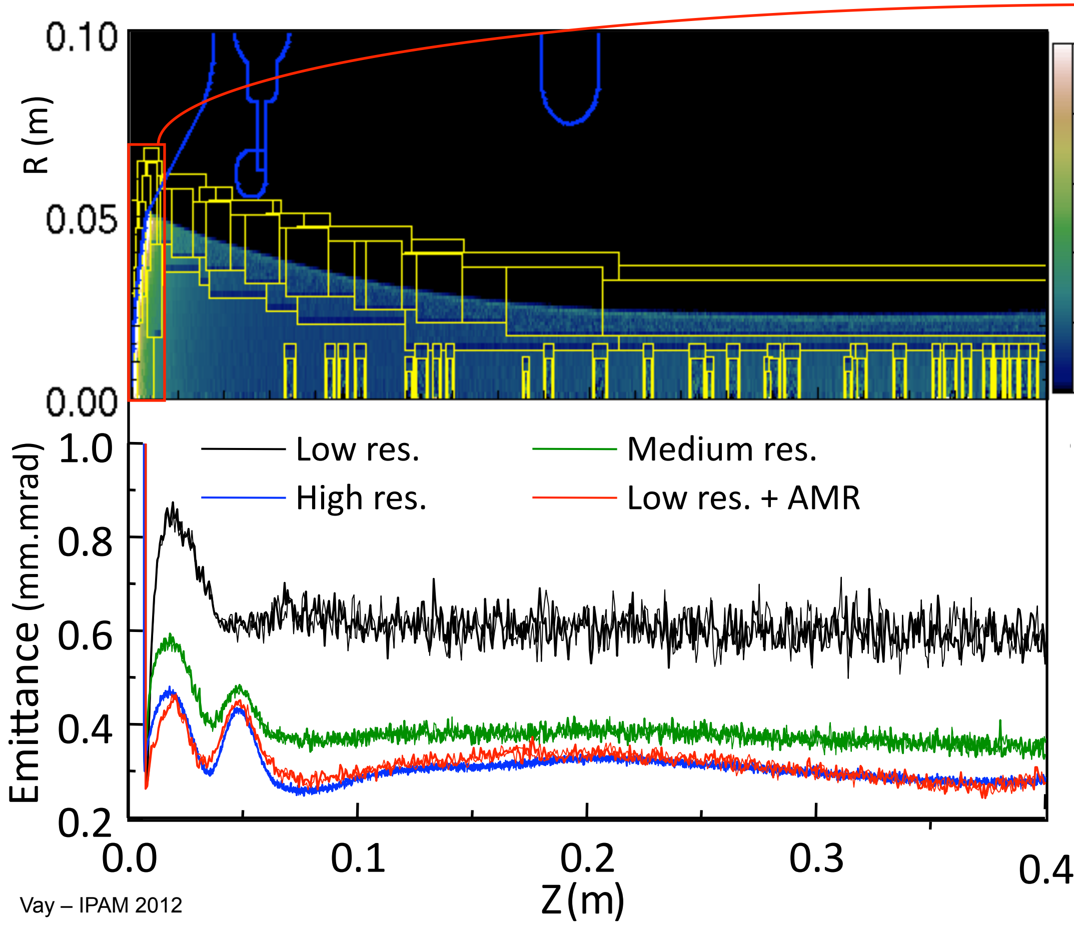
Example with 2 and 4 guard cells

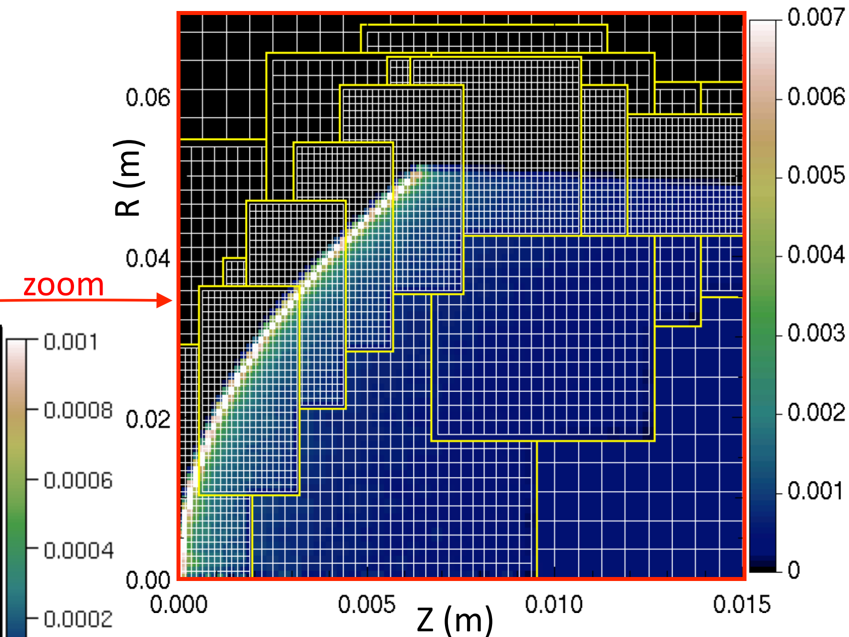


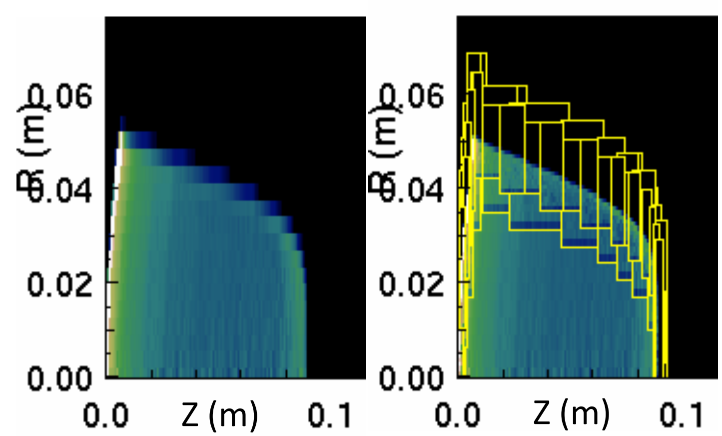
Example of application to AMR simulations of ion source

-- speedup from AMR x10

Run	Grid size	Nb particles
Low res.	**56 x 640**	**~1M**
Medium res.	**112 x 1280**	**~4M**
High res.	**224 x 2560**	**~16M**
Low res. + AMR	**56 x 640**	**~1M**

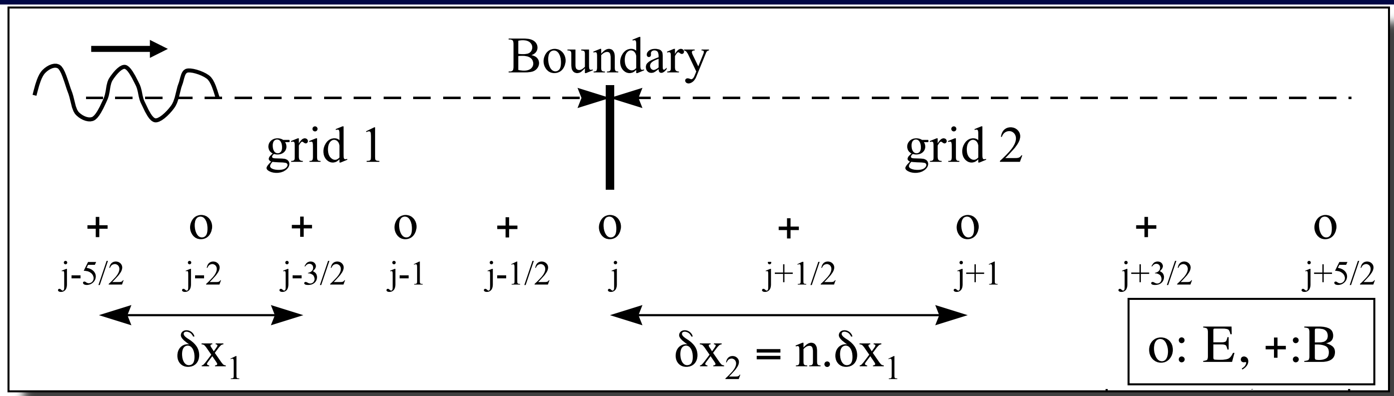


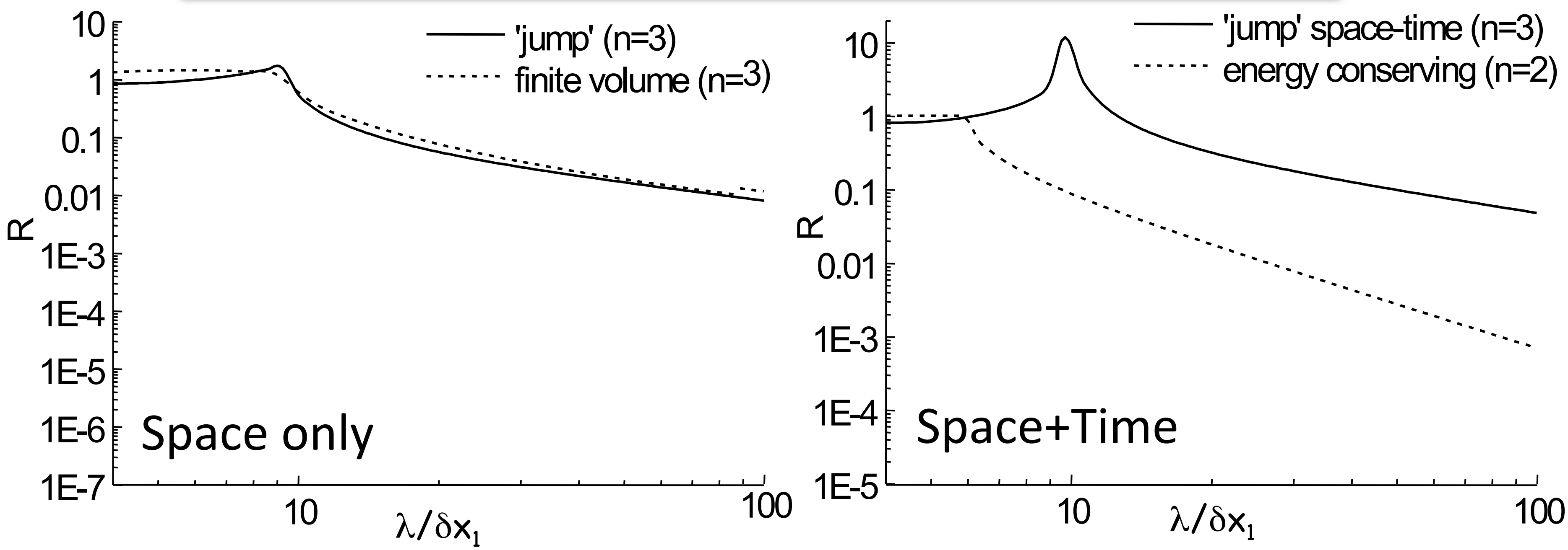




Automatic mesh refinement follows gradients: emitting area, beam edge and front.

1-D AMR-EM: illustration of instability*



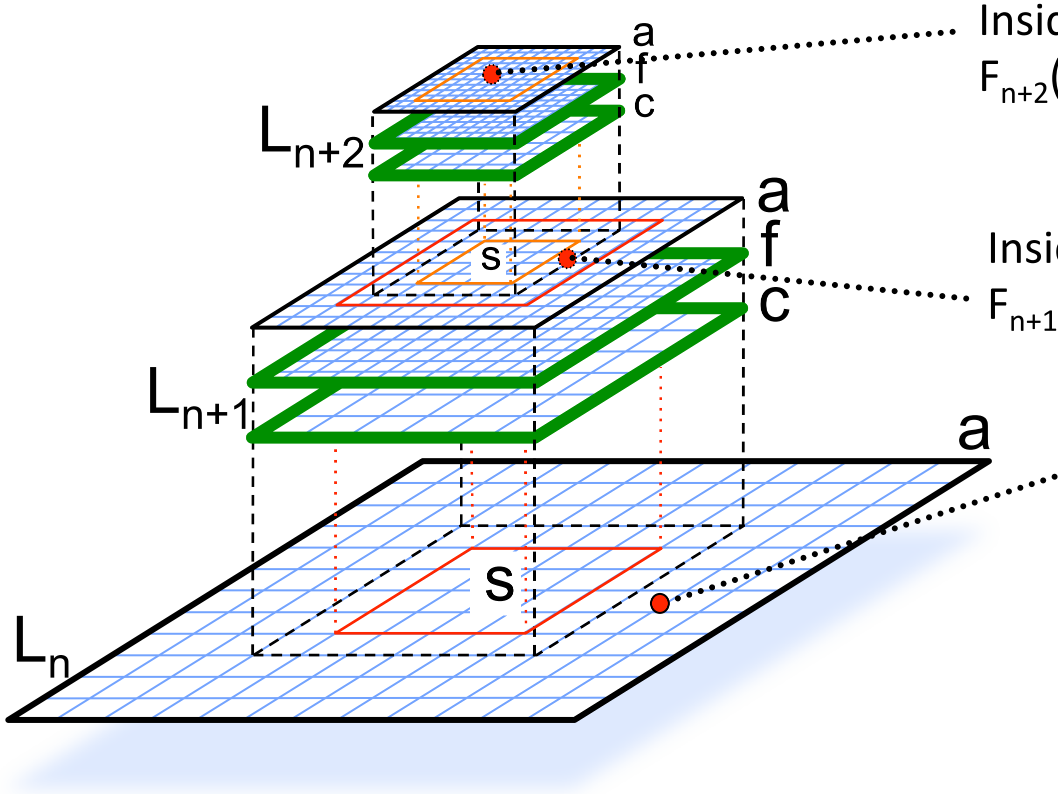


*J.-L. Vay, *J. Comput. Phys.* 167, 72 (2001)

Warp's Electromagnetic MR uses PML & substitution to prevent reflections

Warp's electromagnetic MR solver

- Termination of patches with PML avoids spurious reflections
- Guard cell used for mitigating spurious self-force



Inside patch at L_{n+2}:
$F_{n+2}(a) = I[F_{n+1}(s)-F_{n+2}(c)]+F_{n+2}(f)$

Inside patch at L_{n+1}:
$F_{n+1}(a) = I[F_n(s)-F_{n+1}(c)]+F_{n+1}(f)$

Main grid: $F_n(a)$

absorbing layer (PML)
a = auxilliary
f = fine
c = coarse

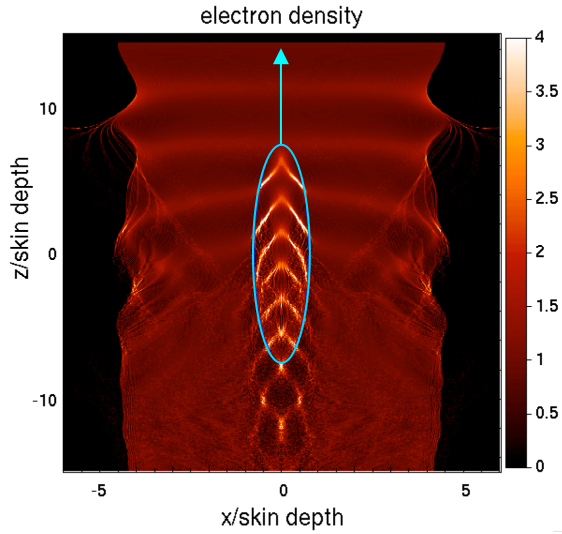
*Vay, Adam, Heron, *Comp. Phys. Comm.* 164 (2004)

Electromagnetic MR simulation of beam-induced plasma wake

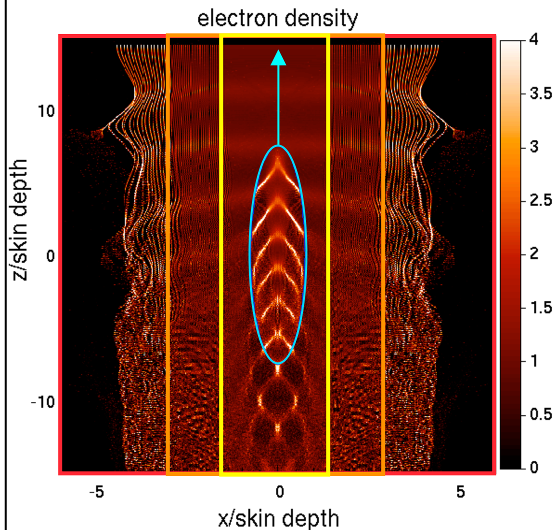
no refinement

2 levels of mesh refinement (MR)

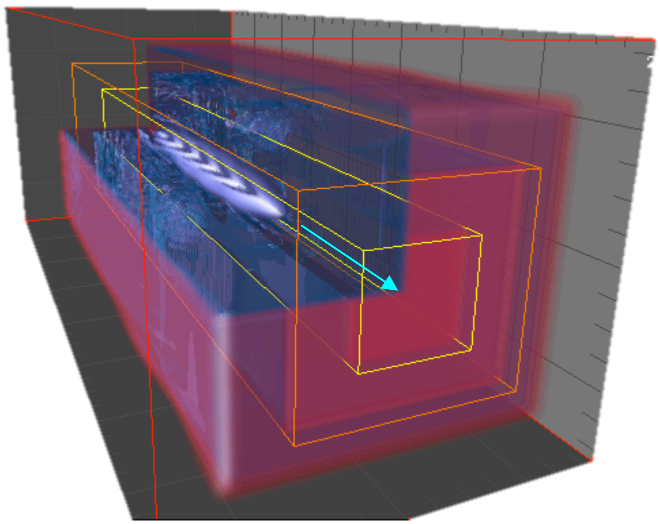
2-D high resolution



2-D low resolution + MR



3-D



Speedup x10 in 3D (using the same time steps for all refinement levels).

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- Summary

Berkeley Lab Laser Accelerator (BELLA) under construction

Laser Plasma Accelerators (LPAs) promise acceleration over short distances

10 GeV stages

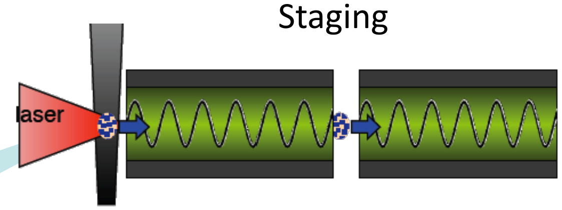
Energy spread &
Emittance preservation

BERKELEY LAB

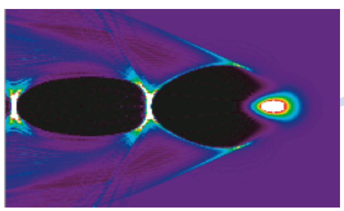
BELLA

PW laser
40 J / 40 fs

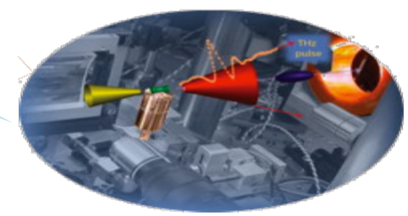
Staging



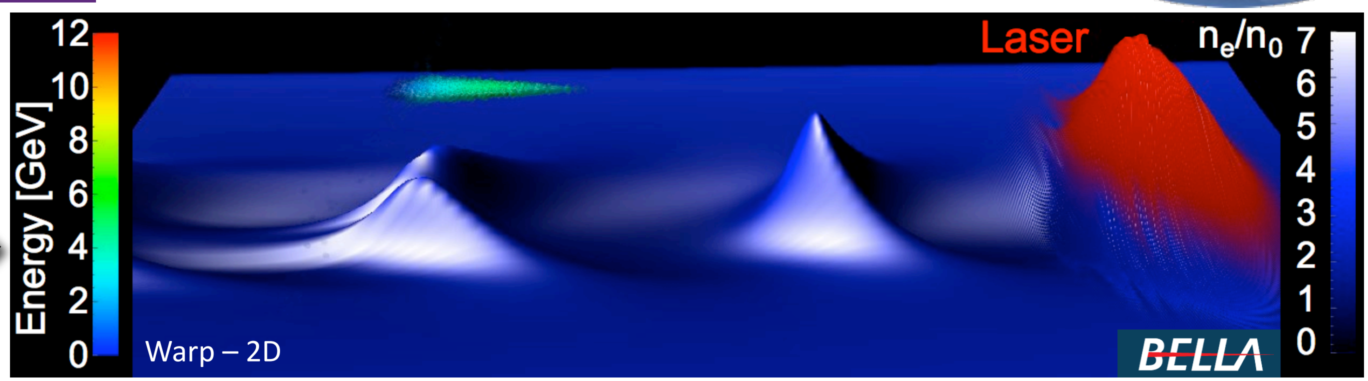
Positron acceleration + PWFA expt.'s



Radiation sources



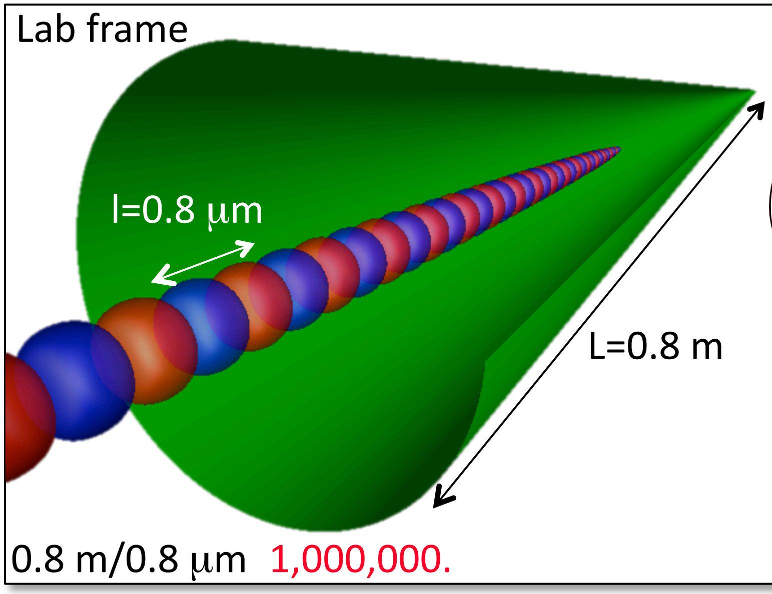
Warp simulation of
10 GeV stage



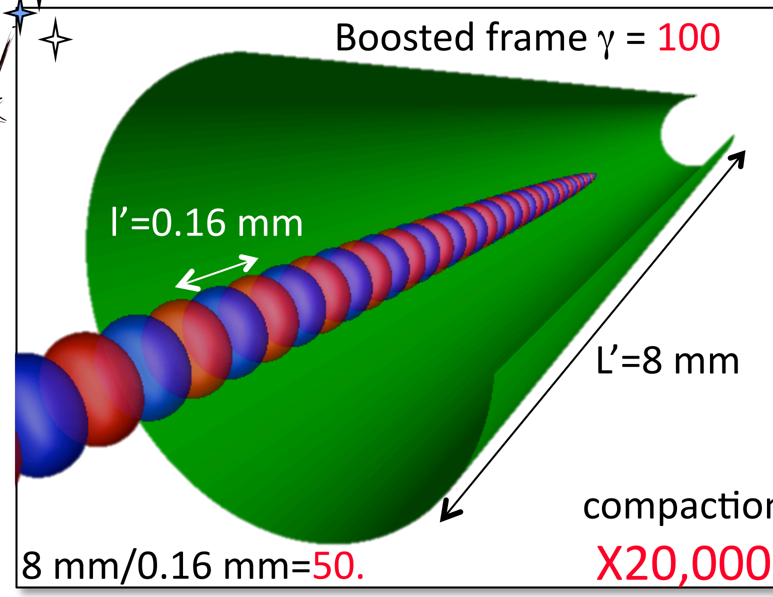
Collaboration with C. Geddes/LOASIS Group - LBNL

LPAs difficult to model because of large separation of scales

Simulations in a Lorentz "boosted frame" reduces numerical difficulty by orders of magnitude*

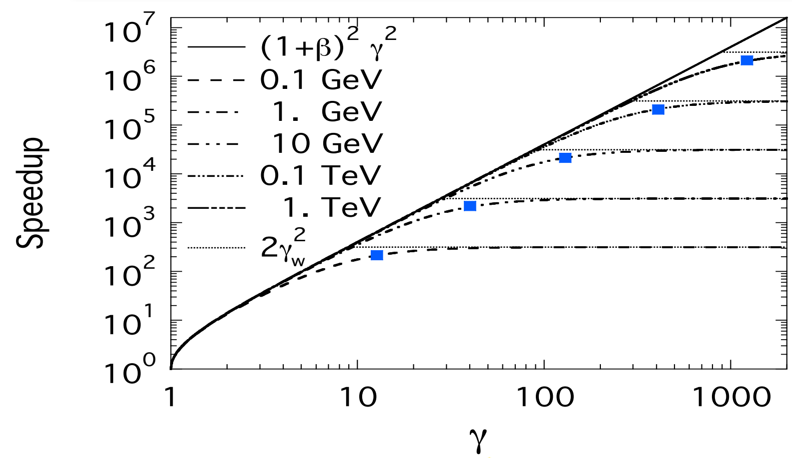


Hendrik Lorentz



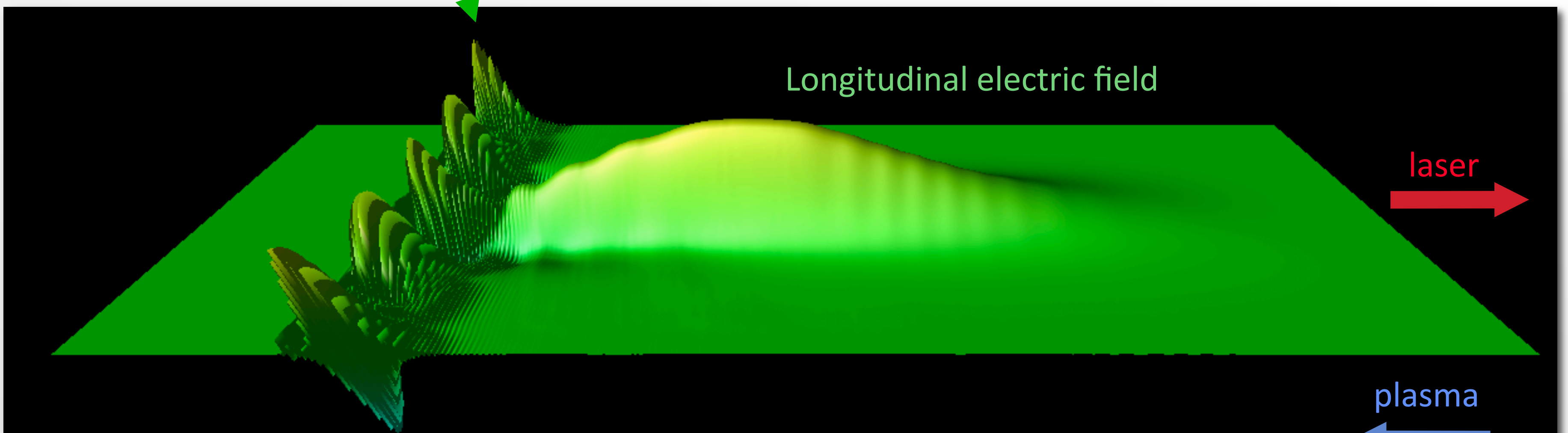
Predicted speedup:

- > 10,000 for a 10 GeV (Bella) stage,
- > 1,000,000 for a 1 TeV stage.



*J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)

But short wavelength instability observed at front of plasma for large γ (≥100)



Warp 2D simulation 10 GeV LPA ($n_e=10^{17}$cc, $\gamma=130$)

Conjectured that instability related to numerical dispersion, i.e. a kind of numerical Cerenkov:
=> can it be cured with lower numerical dispersion/wideband smoothing?

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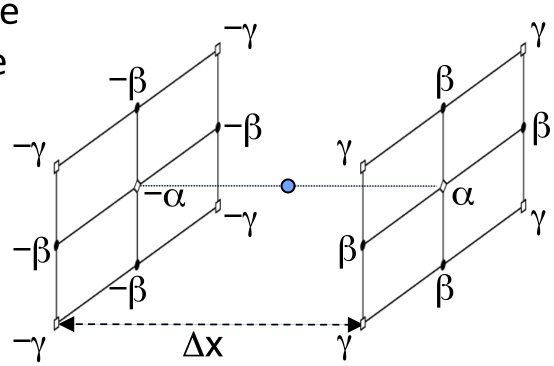
Warp electromagnetic solver is based on Non-Standard Finite-Difference (NSFD) stencil

NSFD: weighted average of quantities transverse to FD ($\alpha+4\beta+4\gamma=1$).

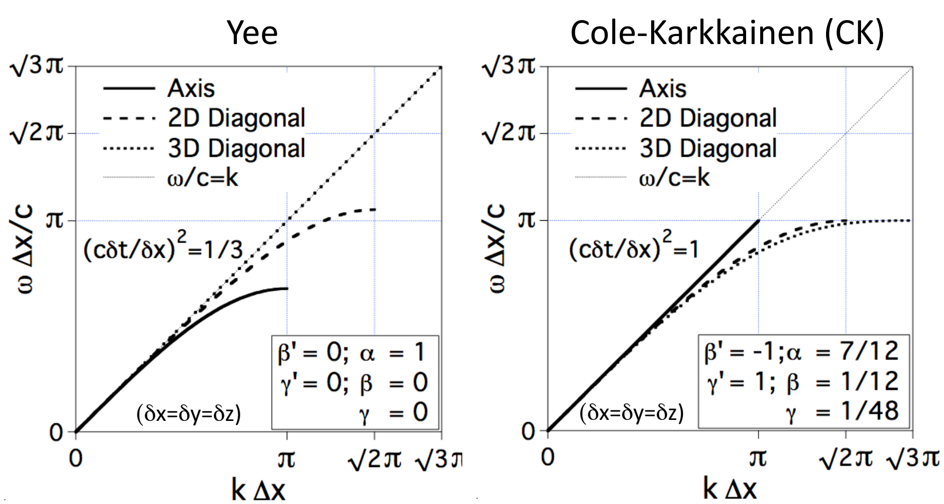
NSFD=FD if
$\alpha=1$
$\beta=\gamma=0$



Cole[1] and Karkkainen[2] have applied NSFD to source free Maxwell equations

$$\Delta_t \mathbf{B} = -\nabla \times \mathbf{E} \quad \text{FD}$$

$$\Delta_t \mathbf{E} = c^2 \nabla^* \times \mathbf{B} \quad \text{NSFD}$$



Yee/CK allows for perfect dispersion along 3D/principal axes.

Warp[3]: switched FD/NSFD to B/E.

$$\Delta_t \mathbf{B} = -\nabla^* \times \mathbf{E} \quad \text{NSFD}$$

$$\Delta_t \mathbf{E} = c^2 \nabla \times \mathbf{B} - \frac{\mathbf{J}}{\epsilon_0} \quad \text{FD}$$

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad \text{FD}$$

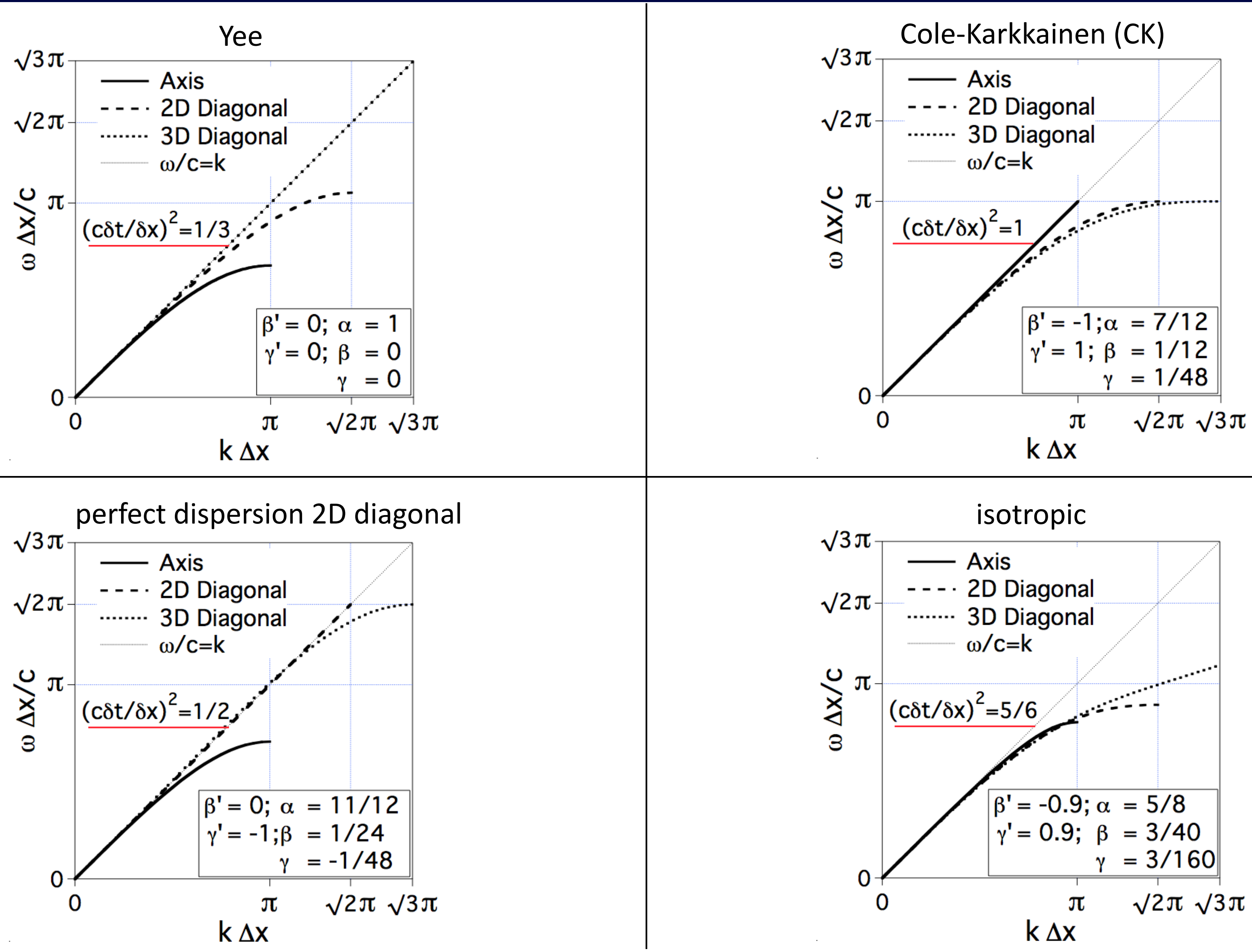
$$\nabla^* \cdot \mathbf{B} = 0 \quad \text{NSFD}$$

=> FD on source terms, i.e. standard exact current deposition schemes still valid.

[1] J. B. Cole, IEEE Trans. Microw. Theory Tech. **45** (1997).
J. B. Cole, IEEE Trans. Antennas Prop. **50** (2002).
[2] M. Karkkainen et al., Proc. ICAP, Chamonix, France (2006).

[3] J.-L. Vay, et al., J. Comput. Phys. **230** (2011) 5908

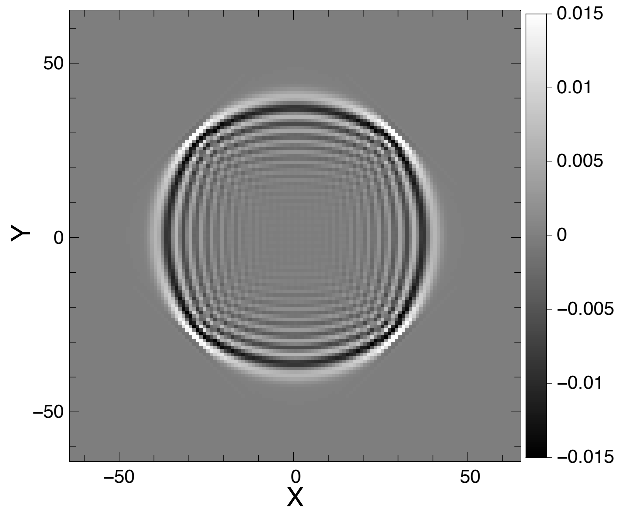
NSFD-based solver offers tunability of numerical dispersion



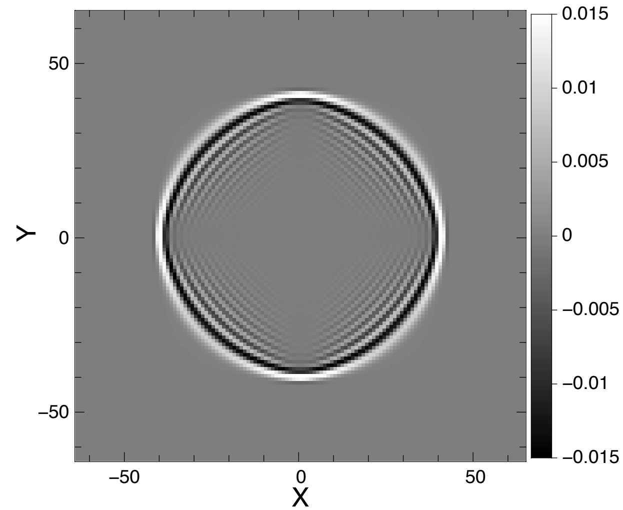
Solver can be tuned to better fit particular needs.

Examples of tuning of numerical dispersion on unit pulse in 2D

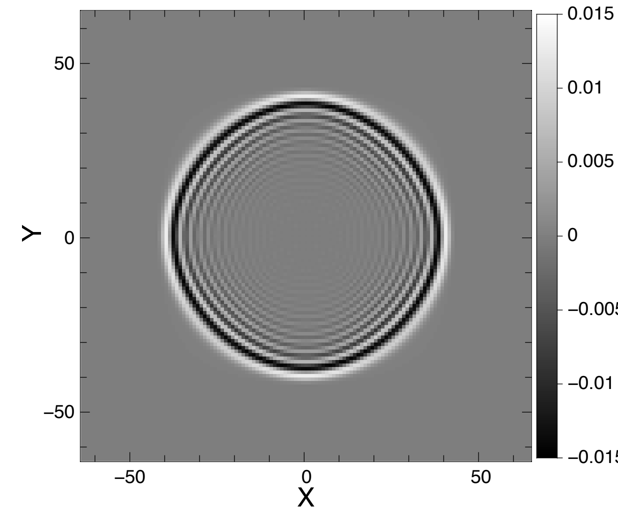
Yee



Cole-Karkkainen (CK)



“isotropic”



Note: Cole-Karkkainen (CK) is sometimes improperly referred to as “dispersionless solver”.

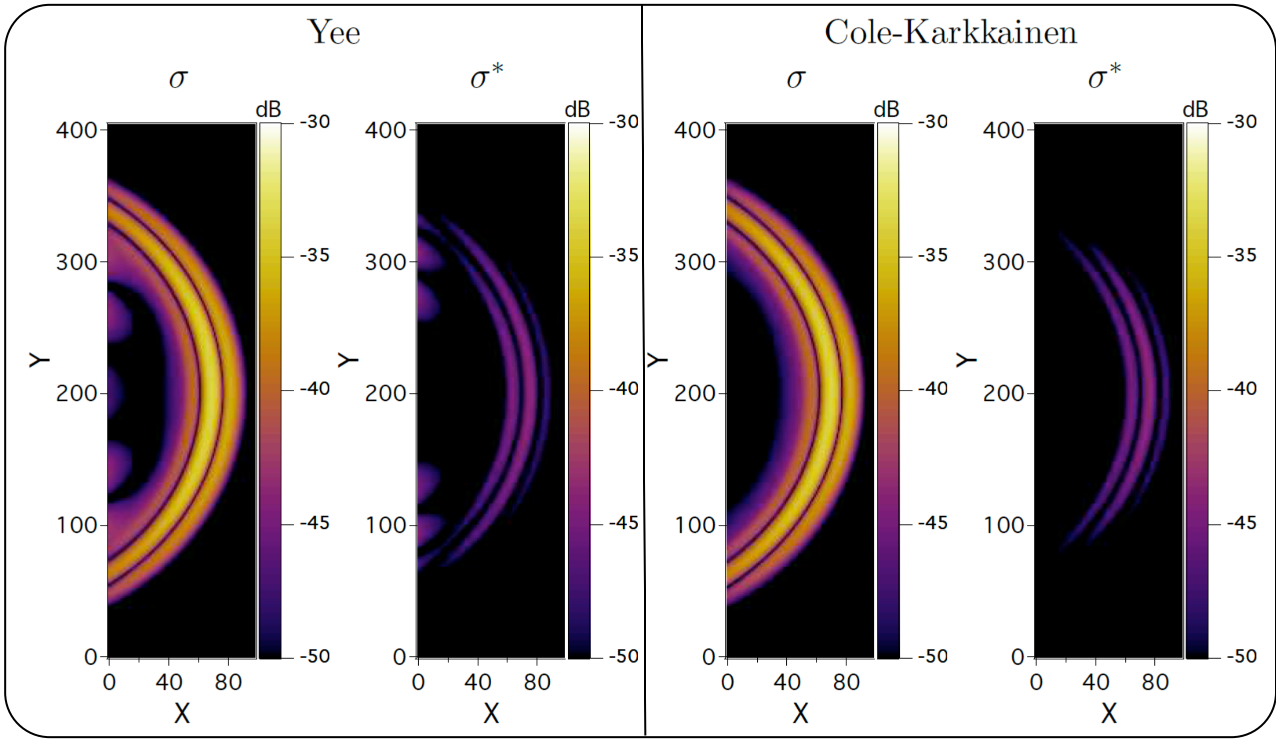
Perfectly Matched Layer[1,2] (PML) implemented with NSFD solver
- for absorption of outgoing waves -

$$\left(\Delta_t + \sigma_x\right) B_{zx} = -\Delta_x^* E_y \quad \text{NSFD}$$
$$\left(\Delta_t + \sigma_y\right) B_{zy} = \Delta_y^* E_x \quad \text{NSFD}$$
$$\left(\Delta_t + \sigma_x\right) E_y = -c^2 \Delta_x \left(B_{zx} + B_{zy}\right) \quad \text{FD}$$
$$\left(\Delta_t + \sigma_y\right) E_x = c^2 \Delta_y \left(B_{zx} + B_{zy}\right) \quad \text{FD}$$

Example:

Reflection of circular pulse using 5 cells PML $\Delta = 5\Delta x$ with quadratic progression and standard coefficients σ_i or improved coefficients[2] σ_i^*

$$\sigma_i = \sigma_m \left(i\Delta x / \Delta\right)^2$$
$$\sigma_m = 4 / \Delta x$$
$$\sigma_i^* = \left(e^{-\sigma_{i+1/2}\Delta t} - e^{\sigma_i \Delta t}\right)$$

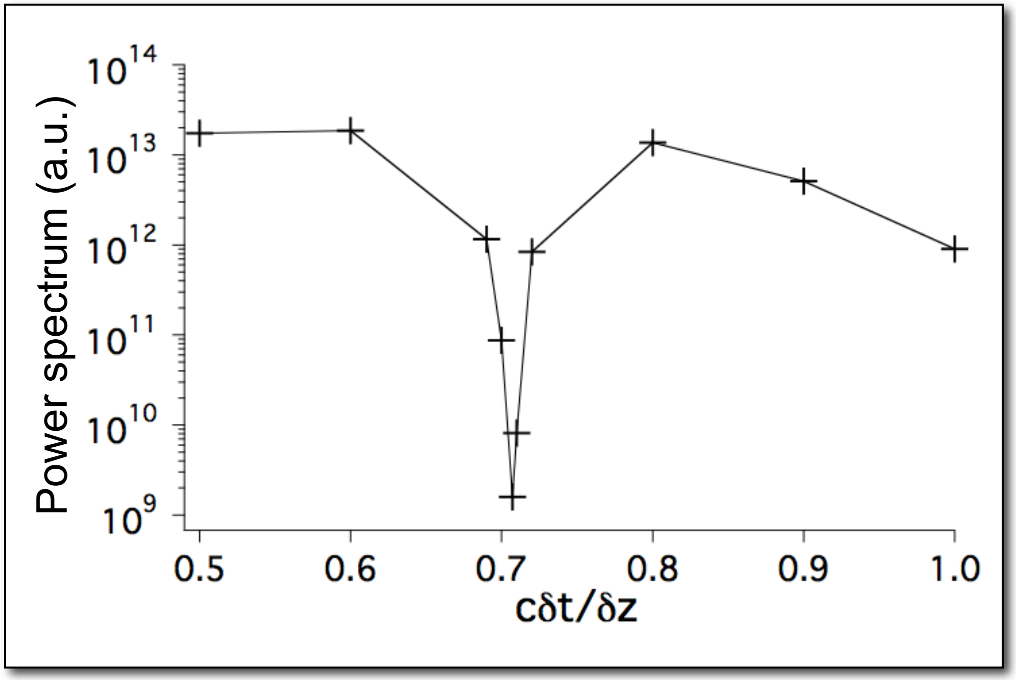


[1]JP Berenger, J. Comput. Phys. **127** (1996) 363
[2]J.-L. Vay, J. Comput. Phys. **183** (2002) 367

Same high efficiency as with Yee.

Instability mostly insensitive to tuning of numerical dispersion… …but very sensitive to time step!

Sharp decrease of instability level at $c\delta t=\delta z/\sqrt{2}$



- Tunable NSFD solver allows $c\delta t=\delta z/\sqrt{2}$ time step for (near) cubic cells
  - $c\delta t=\delta z/\sqrt{2}$ time step restricted to "pancake" cells in 3D using Yee FDTD solver

- Use of special time step was helpful but not sufficient for large γ boost

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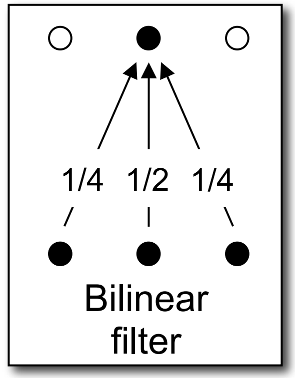
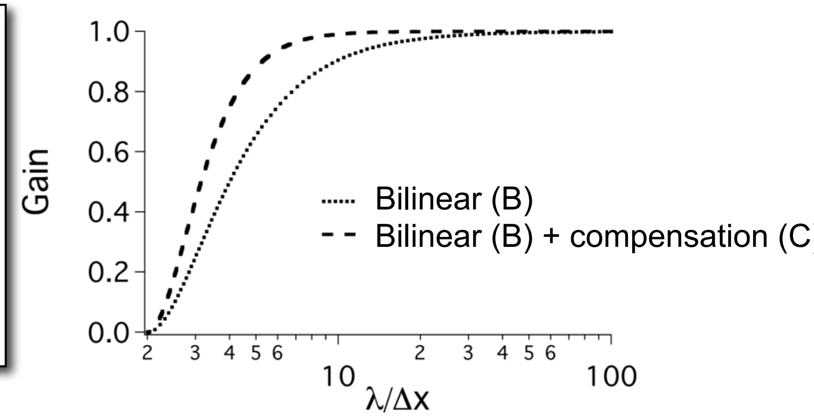
- Summary

Digital filtering of current density and/or fields
-- commonly used for improving stability and accuracy

Multiple pass of bilinear filter
+ compensation routinely used

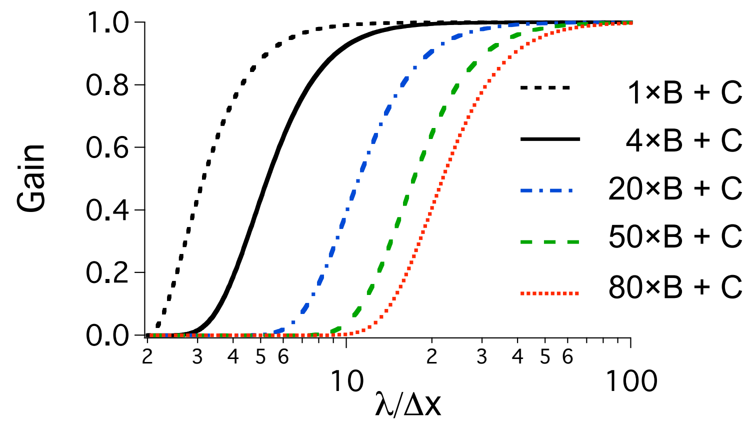
100% absorption at Nyquist freq.





Wideband filtering difficult in parallel (footprint limited by size of local domains) or expensive

Example: wideband filters using
N repetitions of bilinear filter



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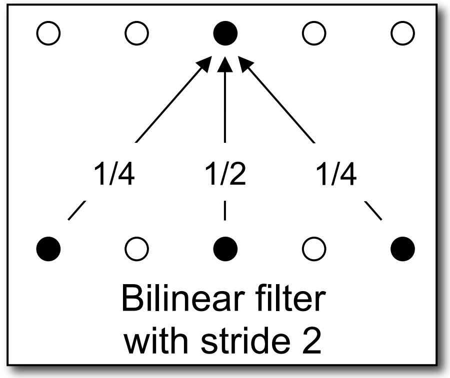
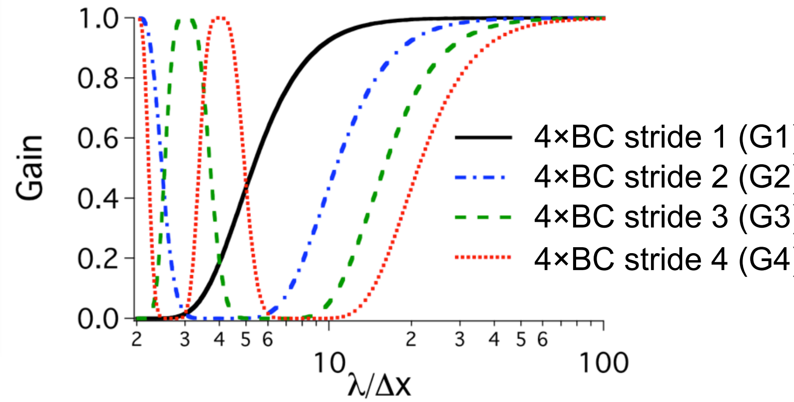
"Strided" bilinear filters enable efficient and versatile filtering[1]

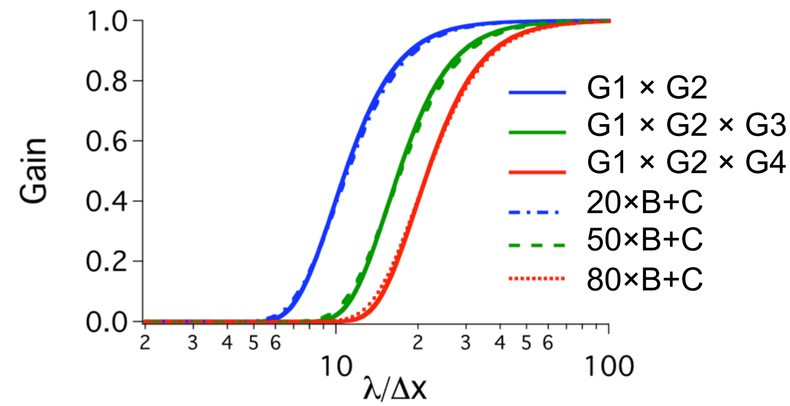
Using a stride N shifts the 100% absorption frequency to $F_{nyquist}/N$





Combination of filters with strides allows for more efficient filtering:

- $G_1G_2 \equiv 20*B+C$; speedup ×2
- $G_1G_2G_3 \equiv 50*B+C$; speedup ×3.5
- $G_1G_2G_4 \equiv 80*B+C$; speedup ×5.5



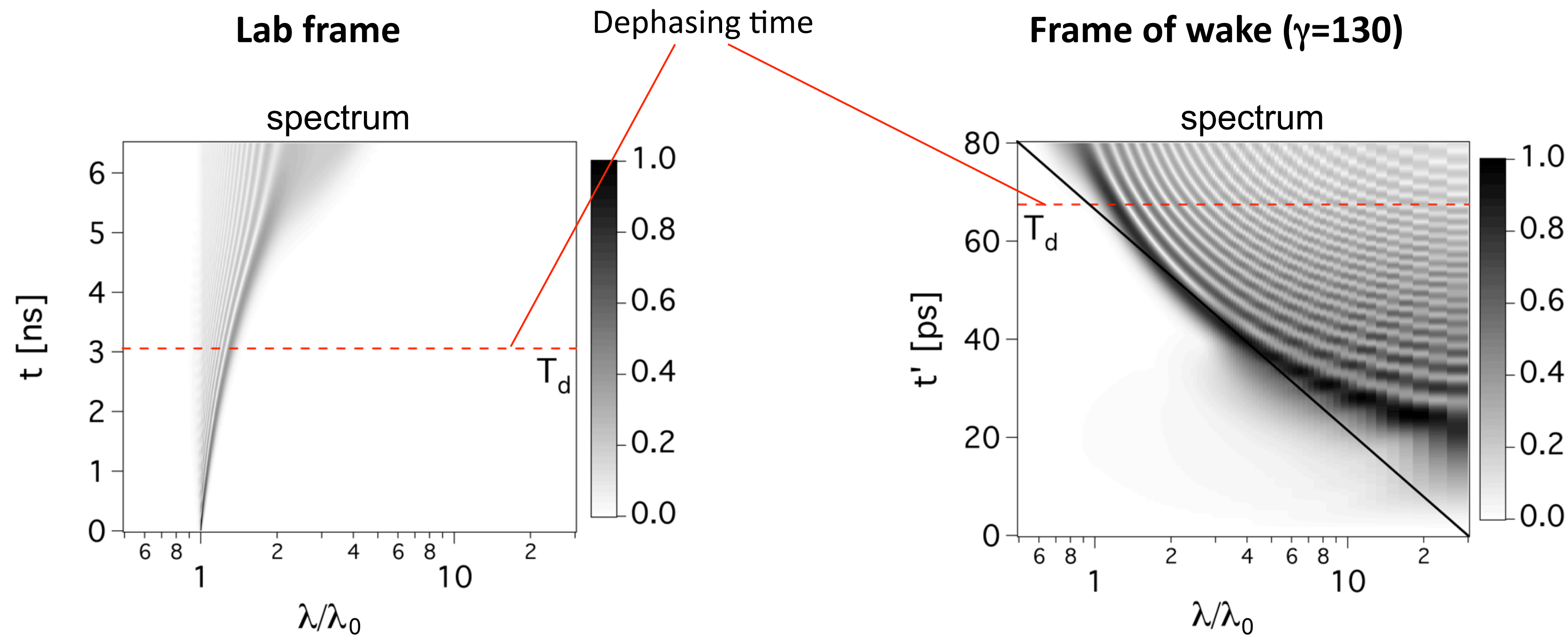
[1] J.-L. Vay, et al., *J. Comput. Phys.* **230** (2011) 5908.

Does physics allow to use wideband filtering?

Time history of laser spectrum (relative to laser λ_0 in vacuum)

Spectrum very different in lab and boosted frames

Lab frame **Frame of wake (γ=130)**

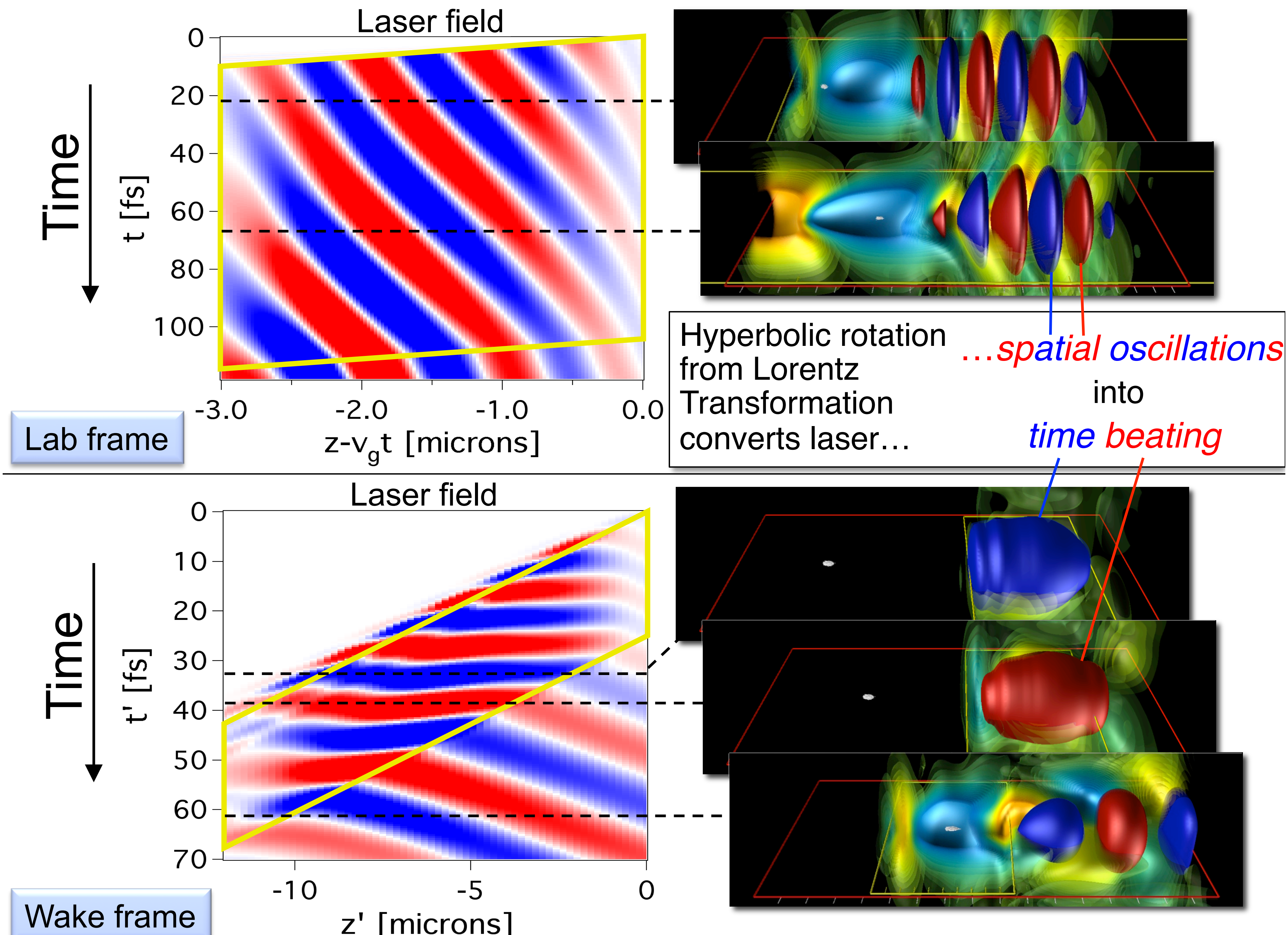


Content concentrated around λ_0

Content concentrated at much larger λ

➡ More filtering possible without altering physics*.

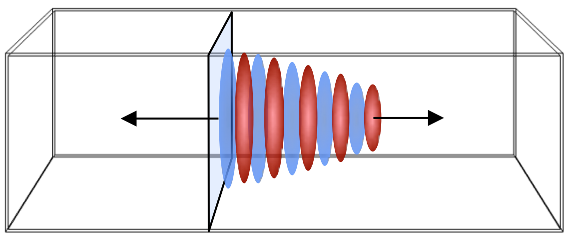
*J.-L. Vay, et al., *PoP Lett.* **18** (2011).


Laser field
Time
t [fs]
0
20
40
60
80
100
-3.0
-2.0
-1.0
0.0
z-v$_g$t [microns]
Lab frame
Hyperbolic rotation from Lorentz Transformation converts laser…
…spatial oscillations
into
time beating
Laser field
Time
t' [fs]
0
10
20
30
40
50
60
70
-10
-5
0
z' [microns]
Wake frame

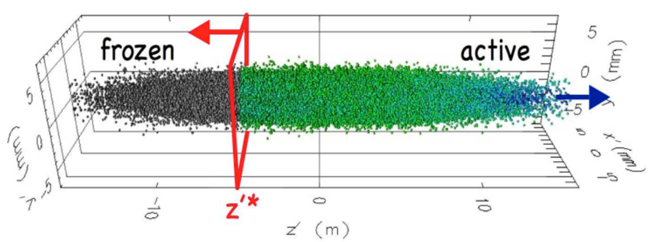
Numerical instability under control with tunable EM solver & filtering

+ new laser/particle injection and diagnostics through planes[1]:

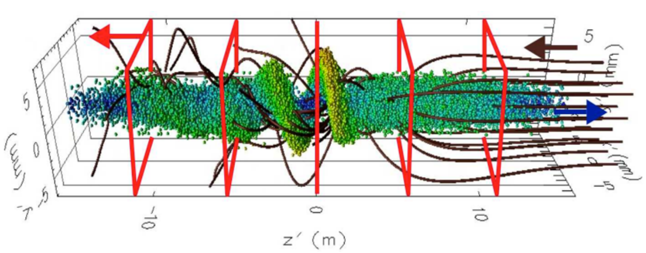
Laser injection[2]



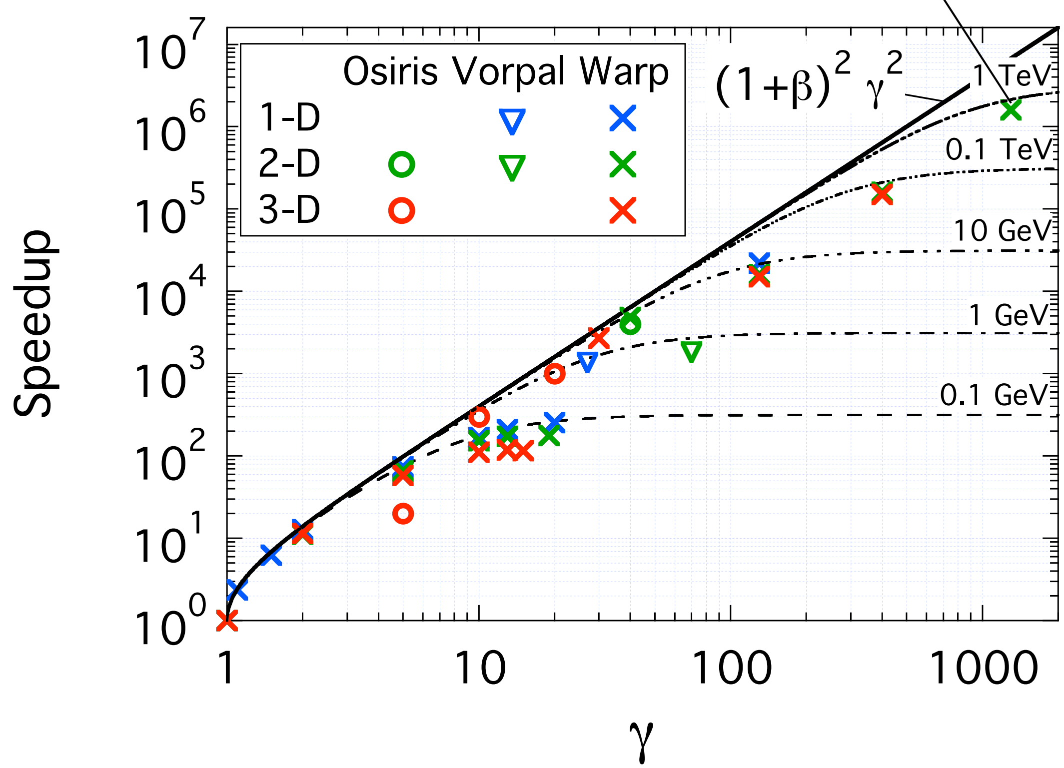
Particle injection



Diagnostics



led to over 1 million x speedup



[1]J.-L. Vay, et al., *J. Comput. Phys.* **230** (2011).

[2]J.-L. Vay, et al., *PoP* **18** (2011).

The Heavy Ion Fusion Science Virtual National Laboratory

SciDAC-II Compass

Summary

- Warp is a parallel Particle-In-Cell simulation framework for the modeling of accelerators, beams, plasmas and laser-plasma interaction.
- Challenges such as space and time scale disparities, discretization errors, numerical dispersion, have pushed toward the development of new methods:
  - "Drift-Lorentz" particle pusher for large time steps of magnetized particles,
  - Lorentz invariant particle pusher,
  - mesh refinement for PIC,
  - boosted frame methods (including laser injection through moving plane),
  - tunable electromagnetic field solver,
  - strided filtering.
- The novel algorithms are quite general and have broad applicability, including to the modeling of high energy density plasmas.
- For questions regarding Warp, email to
  - DPGrote@lbl.gov
  - AFriedman@lbl.gov
  - JLVay@lbl.gov