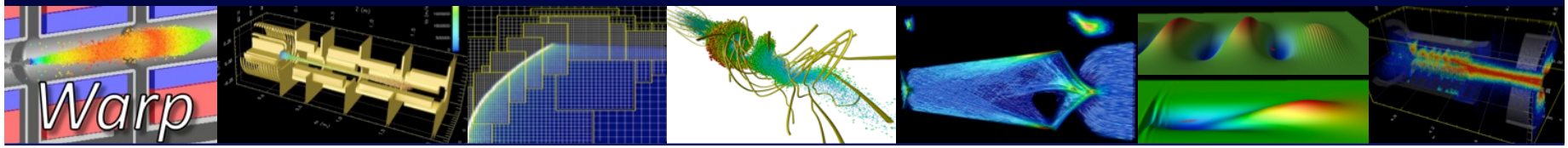
Novel Simulation Methods in the Particle-In-Cell Framework Warp



J.-L. Vay*

Lawrence Berkeley National Laboratory, CA, USA

D.P. Grote, R.H. Cohen, A. Friedman

Lawrence Livermore National Laboratory, CA, USA

I. Haber

U. Maryland, MD, USA

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*jlvay@lbl.gov

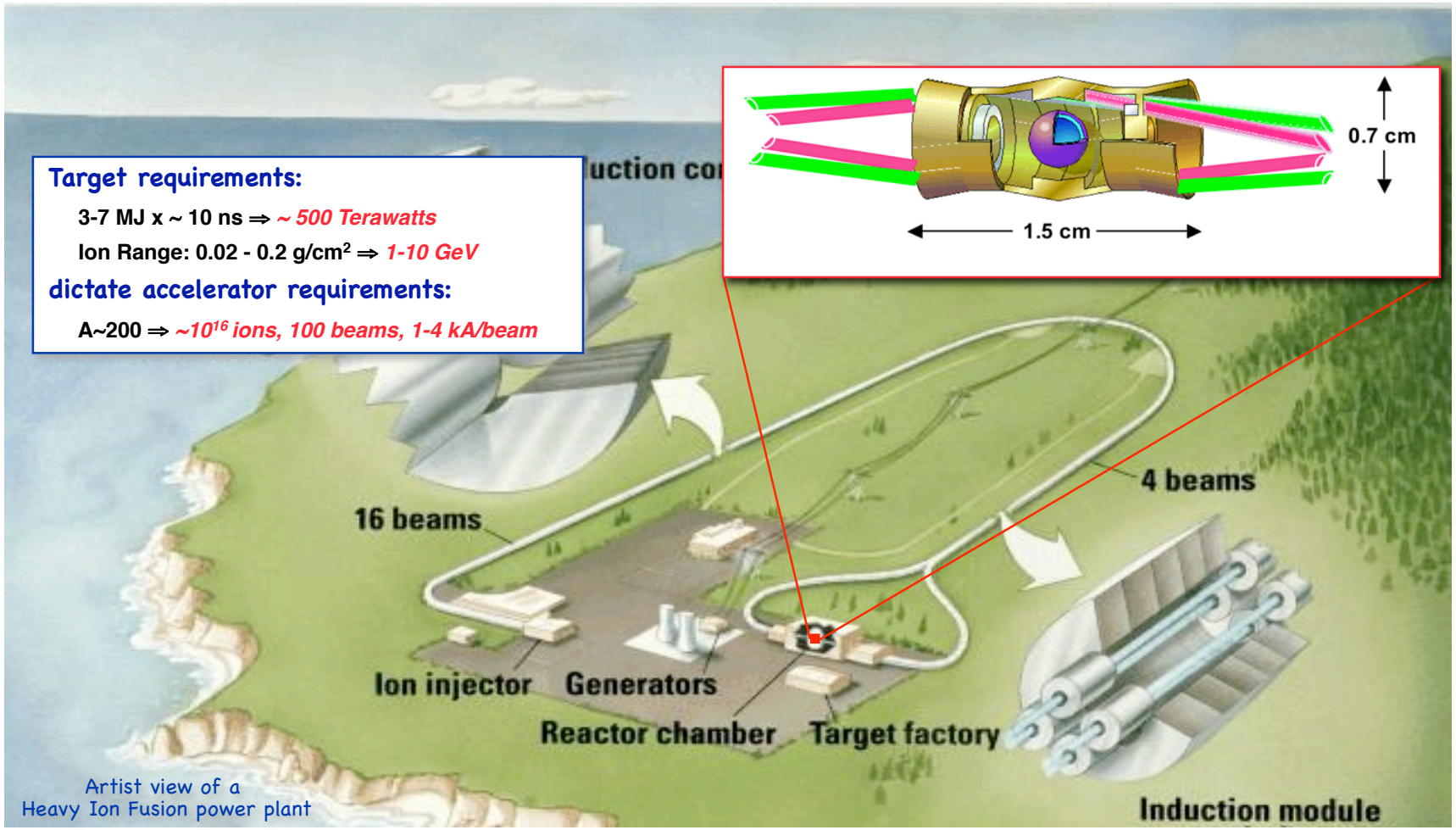
The Heavy Ion Fusion Science Virtual National Laboratory

SciDAC-II Compass

Outline

- Warp overview
  - origins (Heavy Ion Inertial Fusion)
  - geometry, particle pushers, field solvers, etc
- Novel algorithms
  - tunable EM field solver & "strided" filtering
    - application to boosted frame modeling of laser plasma accelerators
  - Mesh Refinement
  - ultra-relativistic particle pusher
  - "Drift-Lorentz" mover for large time-step in magnetic fields
- Summary

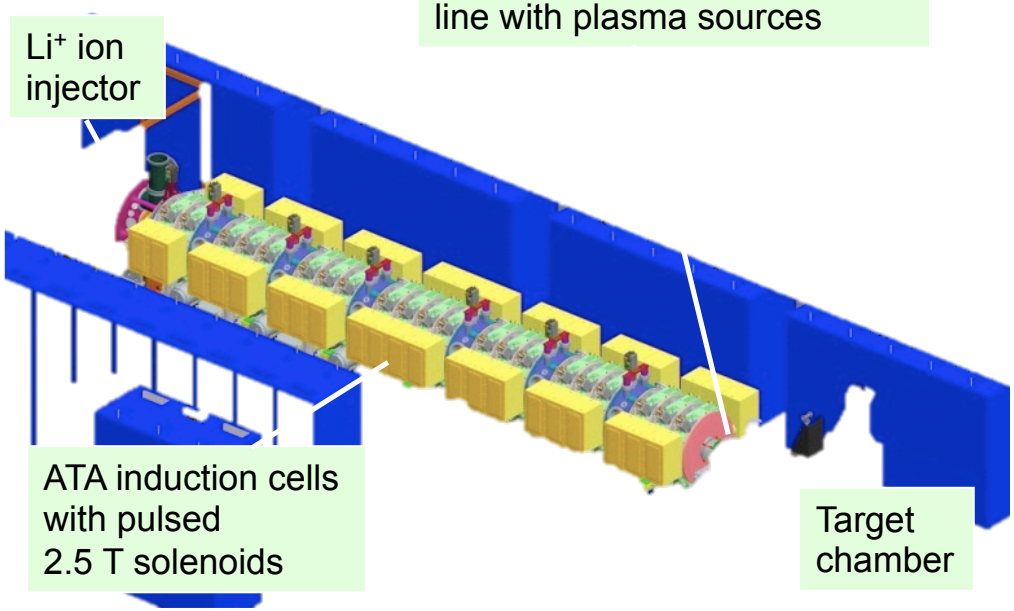
Goal of Heavy Ion Inertial Fusion (HIF) program is to develop an accelerator that can deliver beams to ignite a D+T target

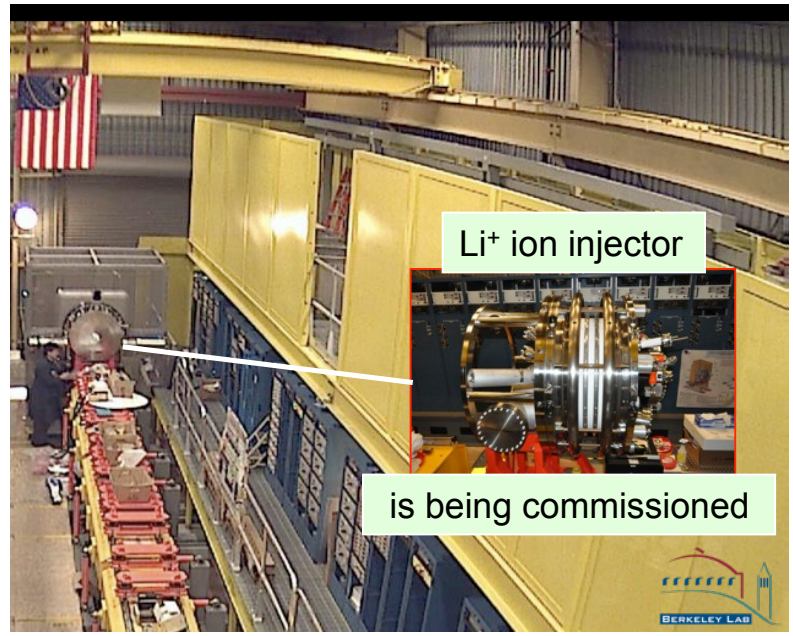


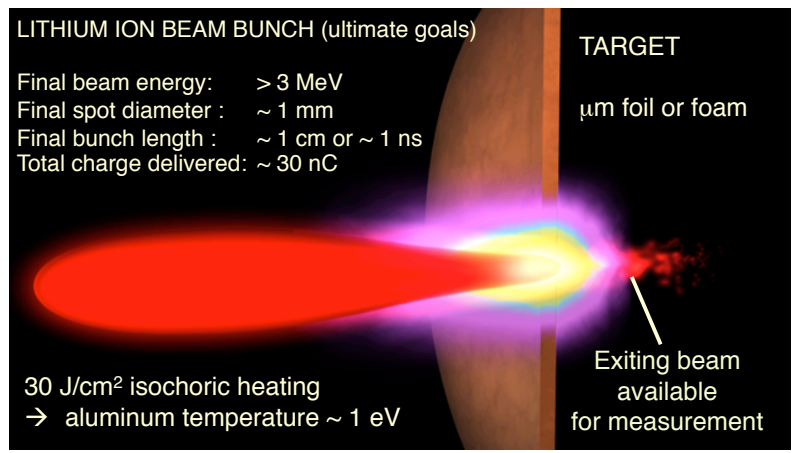
Artist view of a
Heavy Ion Fusion power plant

Near term: perform High-Energy Density Physics (HEDP) studies.

NDCX-II, a short-pulse Ion Beam Driver for WDM and Target Physics Studies is under construction at Berkeley Lab



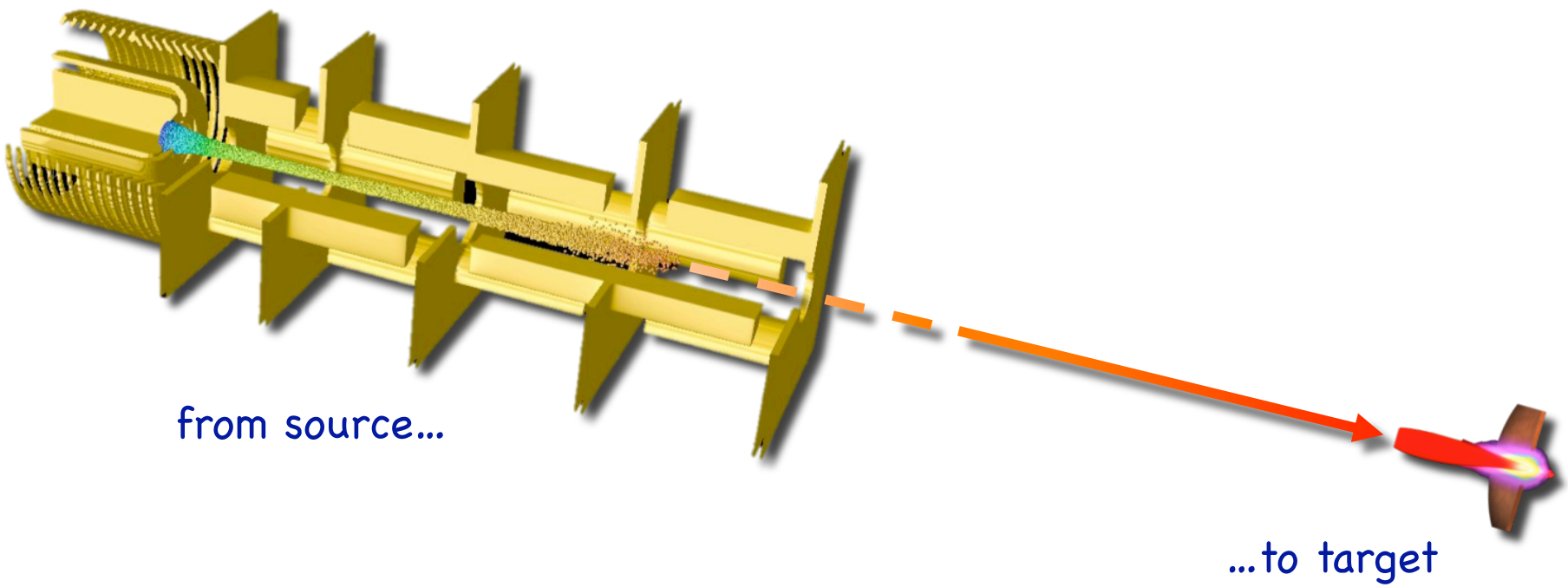




NDCX-II will enable studies of warm dense matter…

…and key physics for ion direct drive.

Simulation goal – end-to-end self-consistent predictive capability

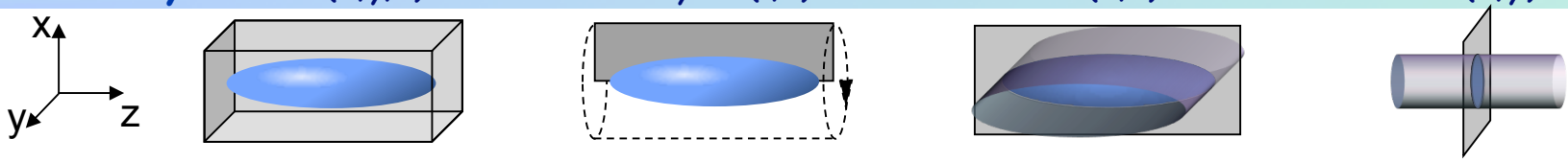


including:

- 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.

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)



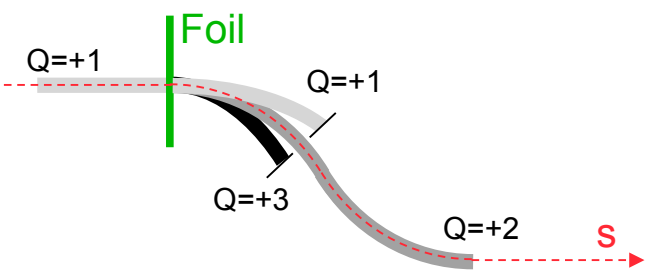
- **Reference frame:**

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

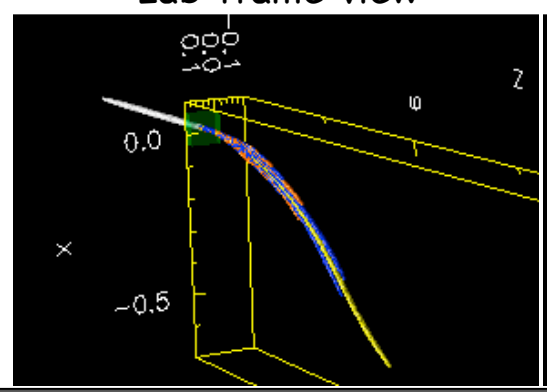
- **Bends:** "warped" coordinates (no "reference orbit")

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

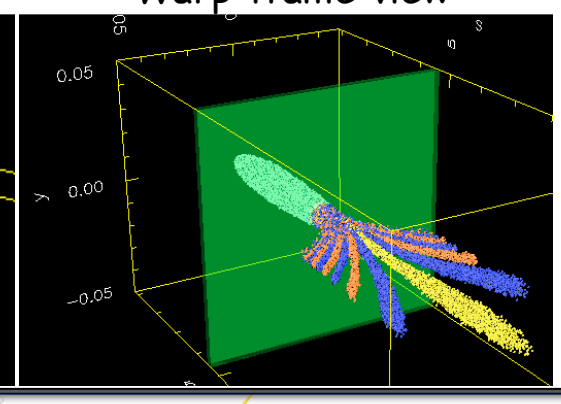
Example: beam stripping through a foil & charge selection in a chicane.



Lab frame view

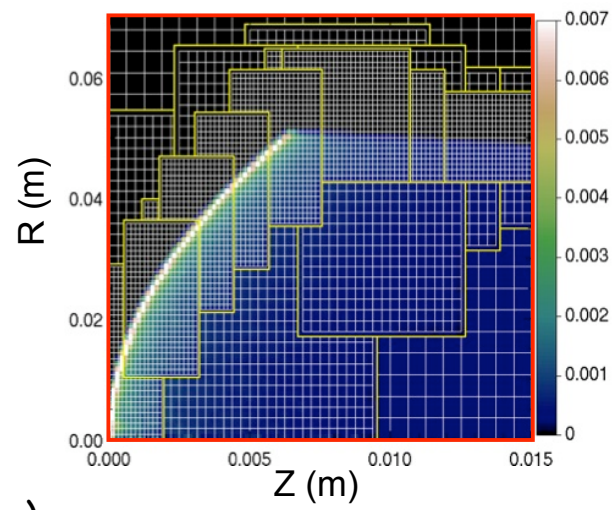


Warp frame view



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* ($v_z >> v_x, v_y$)

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

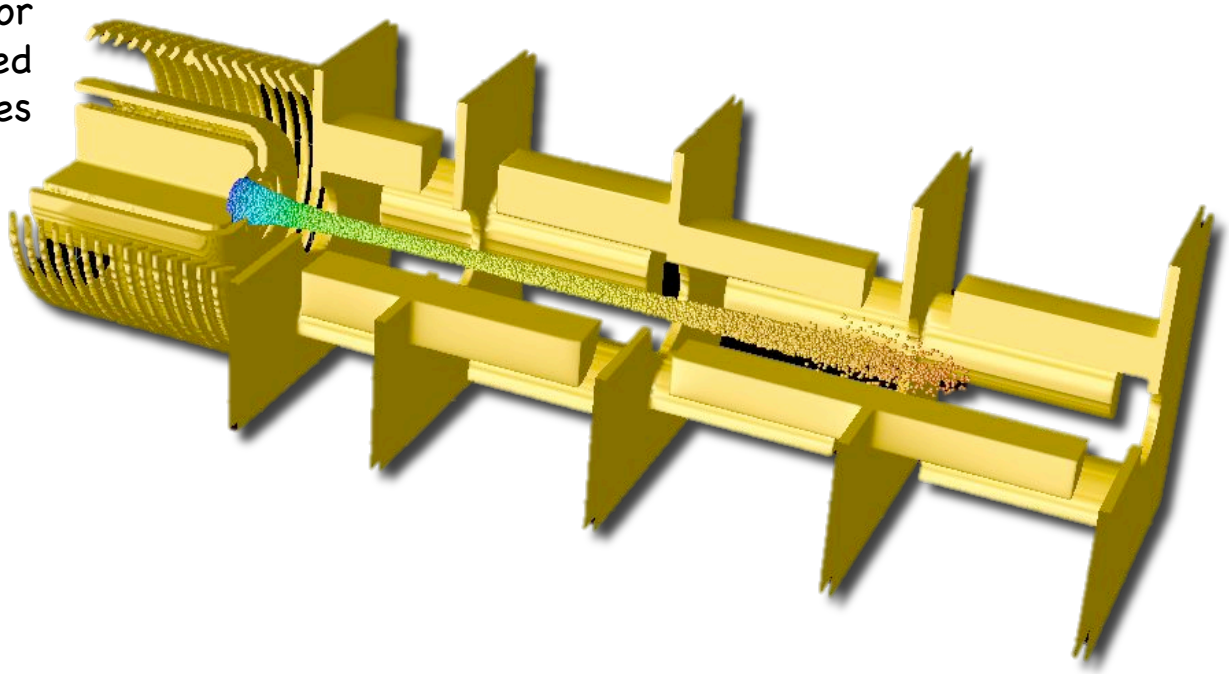
Only one Poisson solve with stretched z coordinate gives all E and B field components.

*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 (massless momentum 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

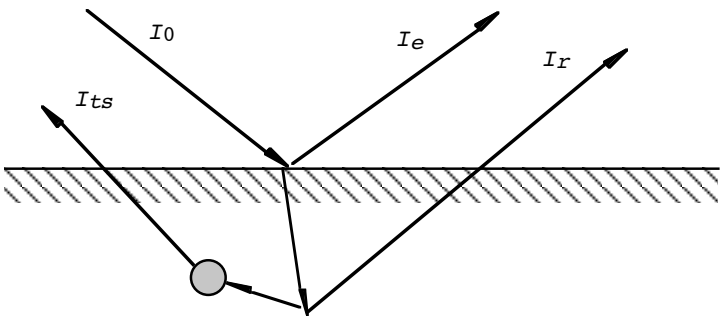
- standard Boris,
- Boris with "tan(α)/α" rotation angle correction,
- "drift-Lorentz"[1] (for taking large time steps > cyclotron period),
- ultra-relativistic[2] (provides proper treatment of self **E**+**v**×**B**).

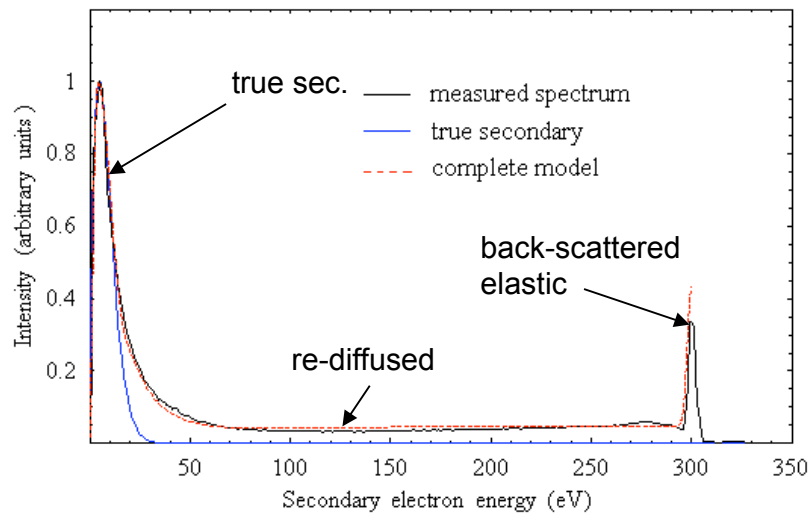
[1]R. Cohen et. al., *Phys. Plasmas* **12,** 056708 (2005)
[2]J.-L. Vay, *Phys. Plasmas* **15**, 056701 (2008)

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**

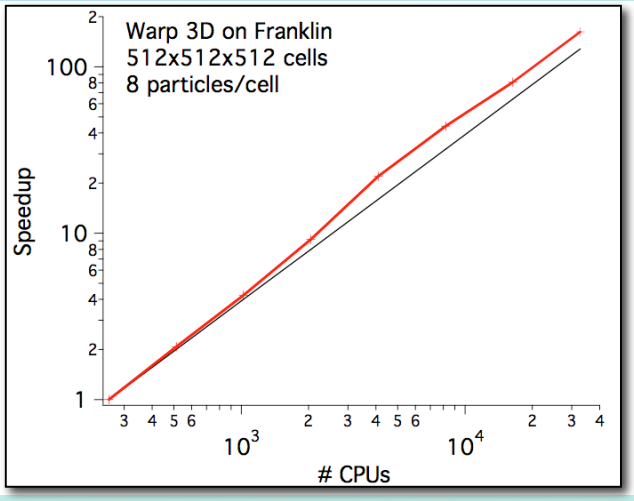
- **Ion impact-induced gas emission, tracking**

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

Parallel, combining modern and efficient programming languages

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

Parallel 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
…	

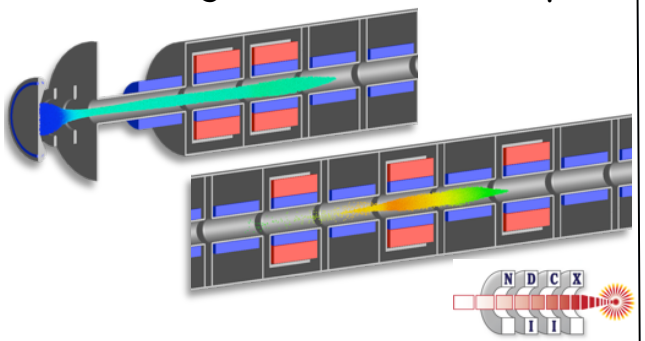
*http://hifweb.lbl.gov/Forthon (wrapper supports FORTRAN90 derived types)

Warp's versatile programmable framework allows great adaptability

Standard PIC

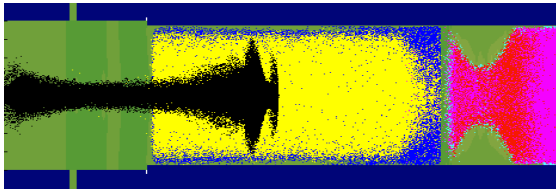
Moving window

Example:
Beam generation & transport



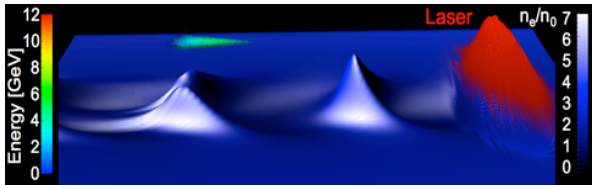
Laboratory frame

Example: Beam neutralization in plasma



Boosted frame

Example:
Laser plasma acceleration

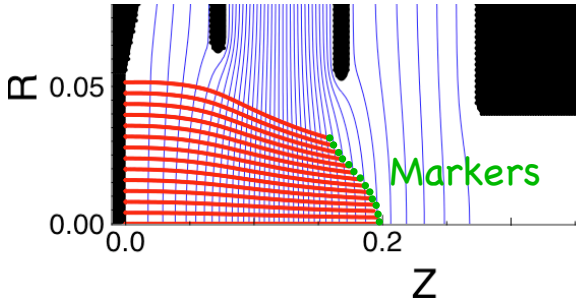


BELLA

Non-standard PIC

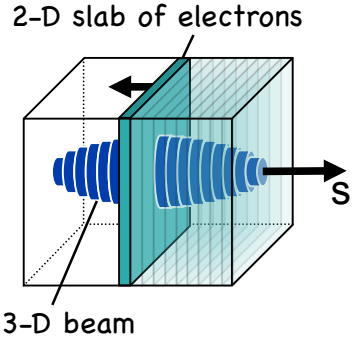
Steady flow

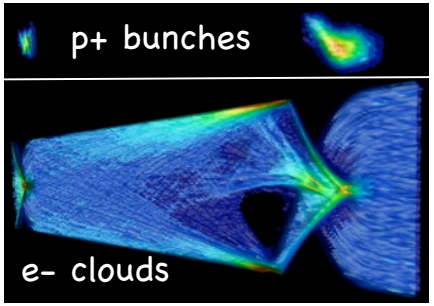
Example: Injector design



Quasi-static

Example: electron cloud studies





SPS - CERN

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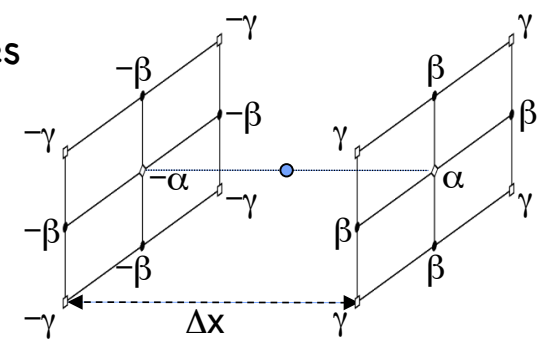
Warp electromagnetic solver is based on Non-Standard Finite-Difference (NSFD) stencil

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

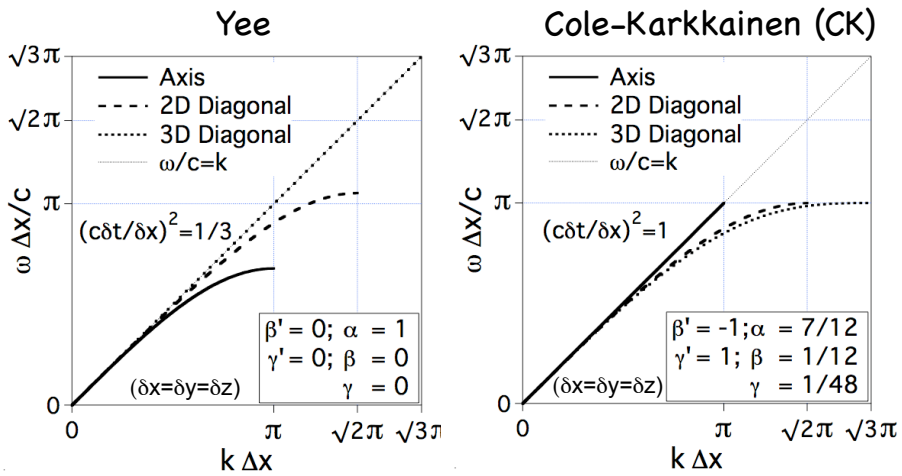
NSFD=FD if
$\alpha=1$
$\beta=\gamma=0$



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

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

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



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

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

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

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

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

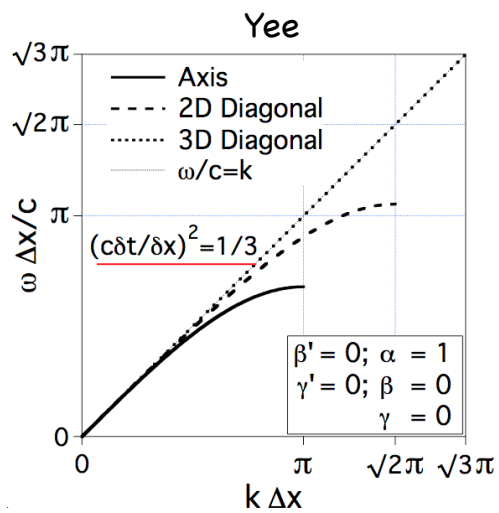
$$\nabla^* \cdot \mathbf{B} = 0 \qquad \text{NSFD}$$

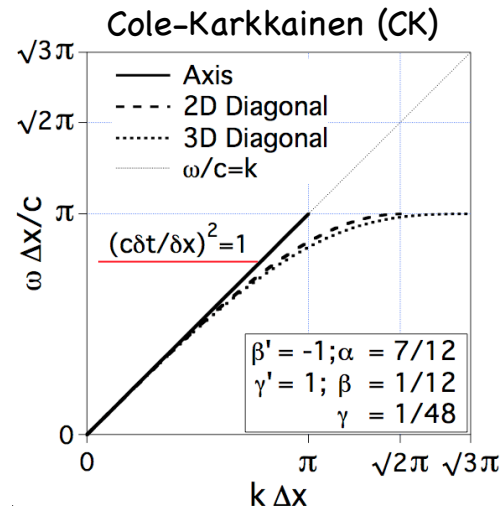
=> FD on source terms, i.e. standard exact current deposition schemes still valid.

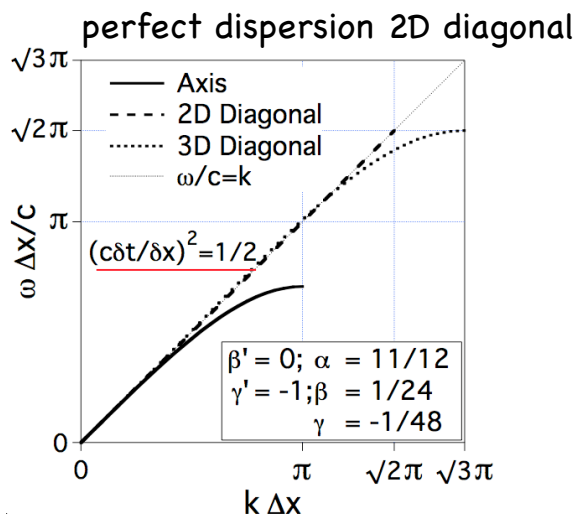
[1]J. B. Cole, IEEE Trans. Microw. Theory Tech. **45** (1997).
J. B. Cole, IEEE Trans. Antennas Prop. **50** (2002).
[2]M. Karkkainen et al., Proc. ICAP, Chamonix, France (2006).

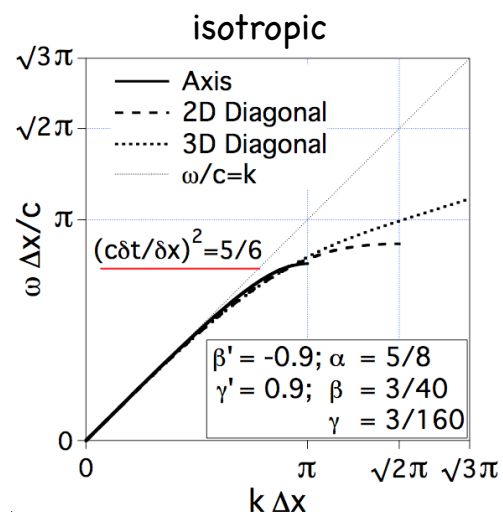
[3]J.-L. Vay, et al., J. Comput. Phys. **230** (2011) 5908

NSFD-based solver offers tunability of numerical dispersion









Solver can be tuned to better fit particular needs.

Perfectly Matched Layer[1,2] (PML) implemented with NSFD solver

- for absorption of outgoing waves -

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

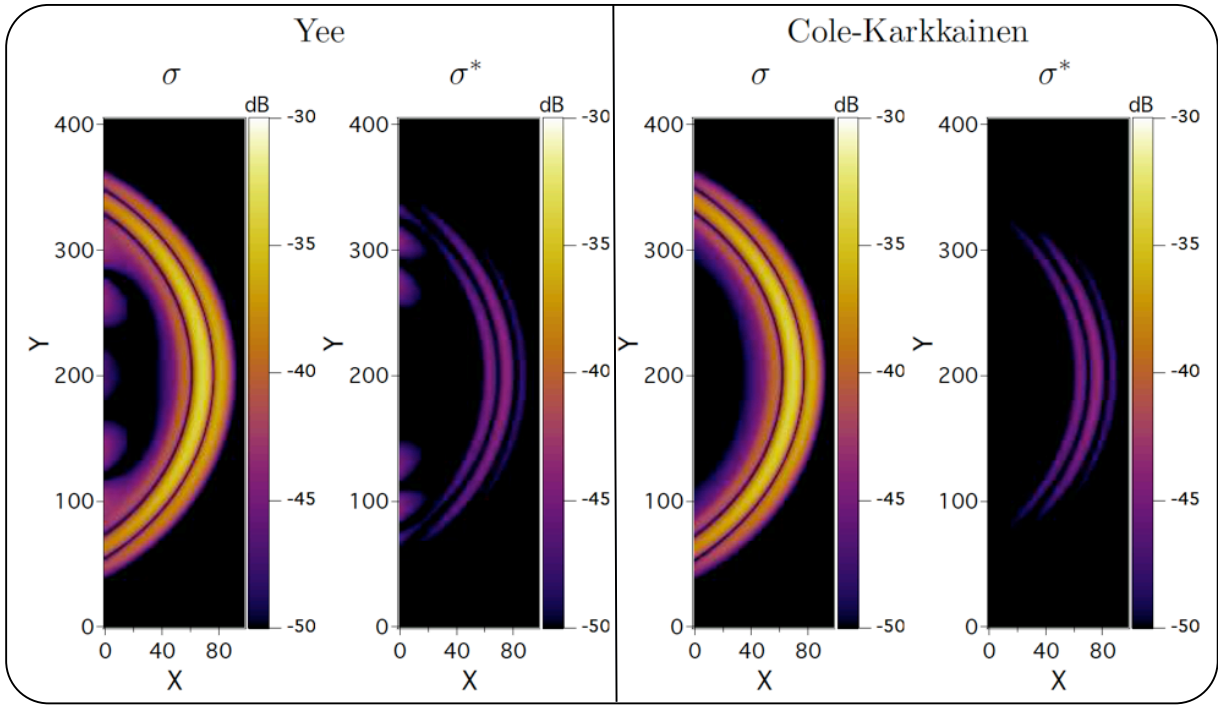
Example:

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^*

$$\sigma_i = \sigma_m \left(i\Delta x / \Delta\right)^2$$

$$\sigma_m = 4 / \Delta x$$

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



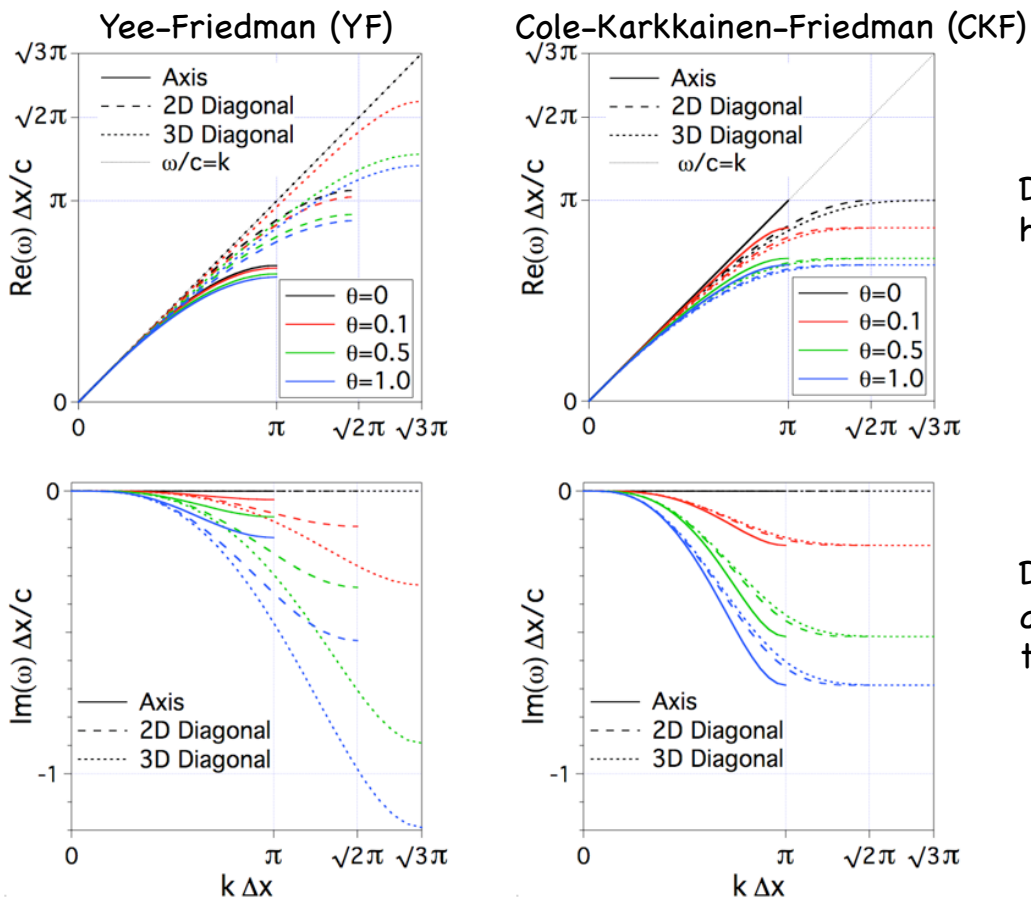
[1]JP Berenger, J. Comput. Phys. **127** (1996) 363
[2]J.-L. Vay, J. Comput. Phys. **183** (2002) 367

Same high efficiency as with Yee.

as well as Friedman damping algorithm
- for noise control -

B push modified to $$\mathbf{B}^{n+3/2} = \mathbf{B}^{n+1/2} - \delta t \nabla^* \times \left[\left(1 + \frac{\theta}{4}\right) \mathbf{E}^{n+1} - \frac{1}{2}\mathbf{E}^n + \left(\frac{1}{2} - \frac{\theta}{4}\right) \bar{\mathbf{E}}^{n-1} \right]$$

with $$\bar{\mathbf{E}}^{n-1} = \left(1 - \frac{\theta}{2}\right) \mathbf{E}^n + \frac{\theta}{2} \bar{\mathbf{E}}^{n-2}$$ where θ is damping parameter.



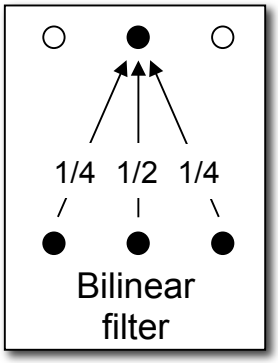
Dispersion degrades with higher values of θ.

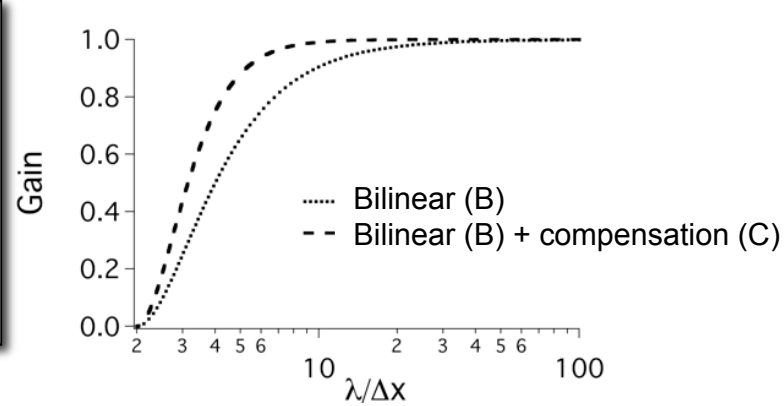
Damping more potent on axis and more isotropic for CKF than YF.

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

Multiple pass of bilinear filter
+ compensation routinely used

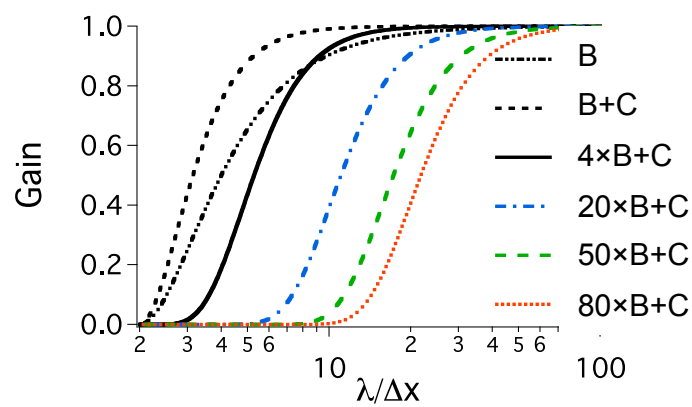
100% absorption at Nyquist freq.





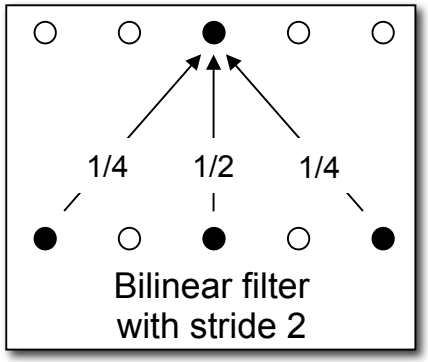
Wideband filtering difficult in parallel (footprint limited by size of local domains) or expensive

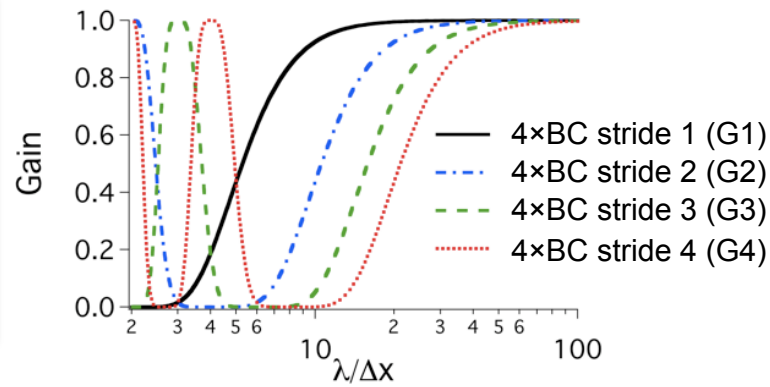
Example: wideband filters using
N repetitions of bilinear filter



"Strided" bilinear filters enable efficient and versatile filtering

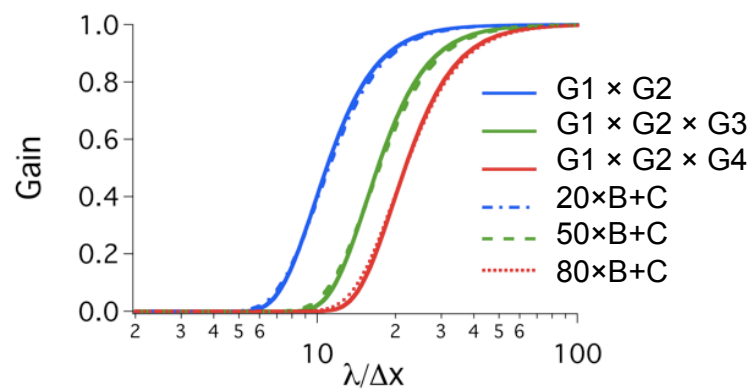
Using a stride N shifts the 100% absorption frequency to $F_{nyquist}/N$





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



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Berkeley Lab Laser Accelerator (BELLA) under construction

Laser Plasma Accelerators (LPAs) promise acceleration over short distances

10 GeV stages

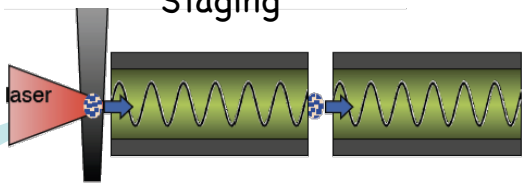
Energy spread &
Emittance preservation

BERKELEY LAB

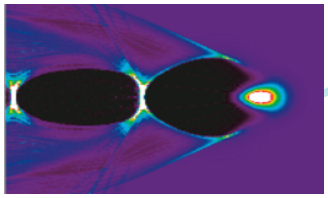
BELLA

PW laser
40 J / 40 fs

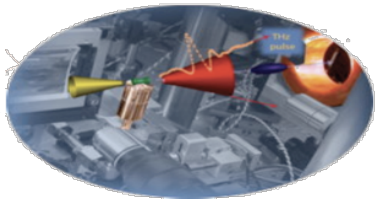
Staging



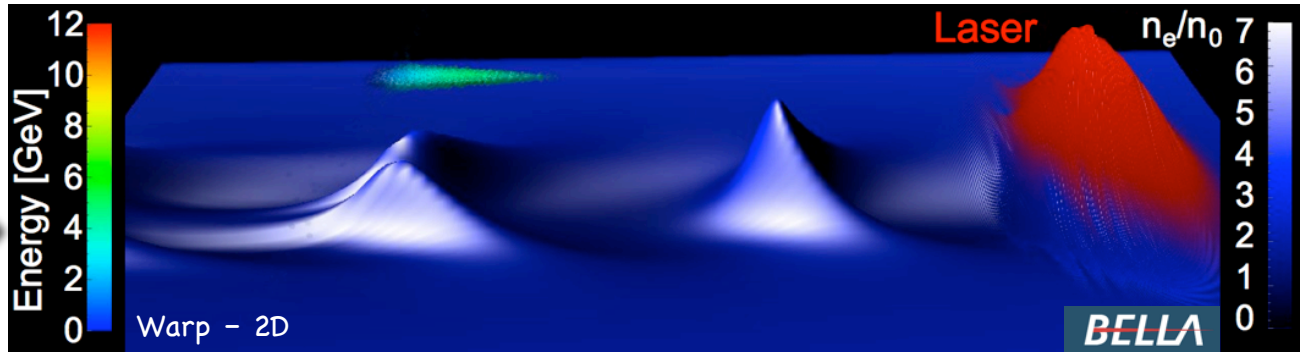
Positron acceleration + PWFA
expt.'s



Radiation sources



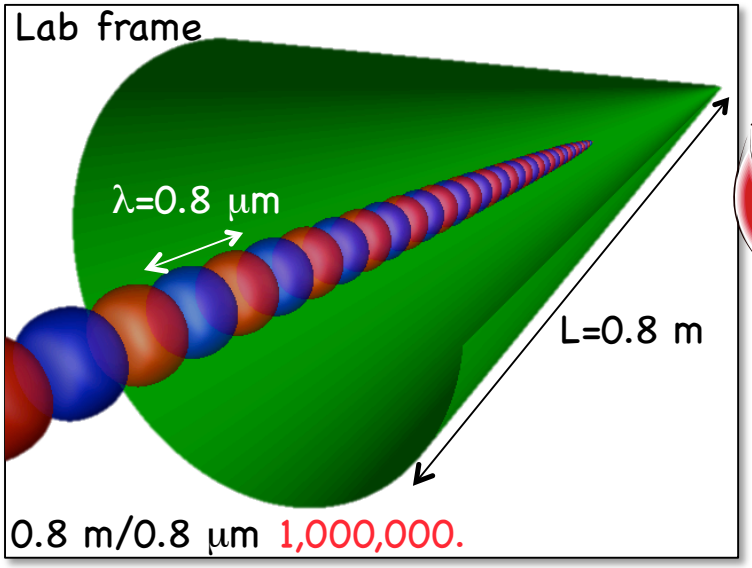
Warp simulation
of 10 GeV stage

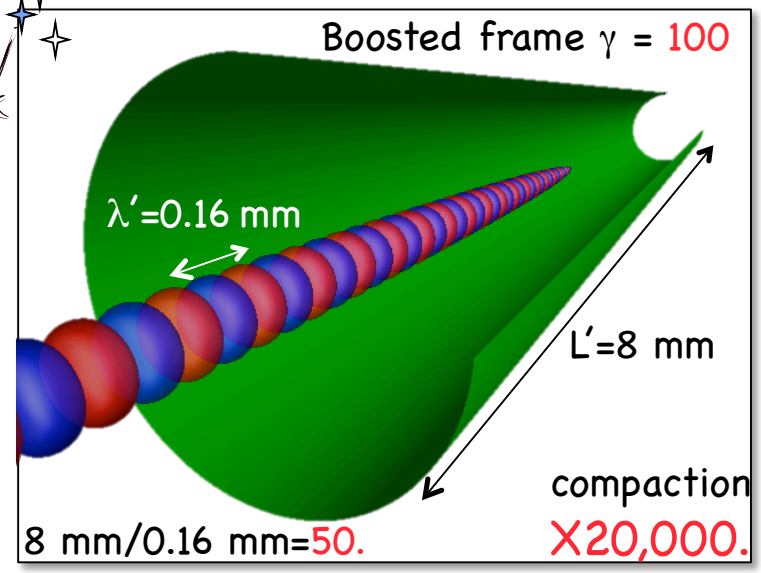


Collaboration with C. Geddes/LOASIS Group - LBNL

LPAs difficult to model because of large separation of scales

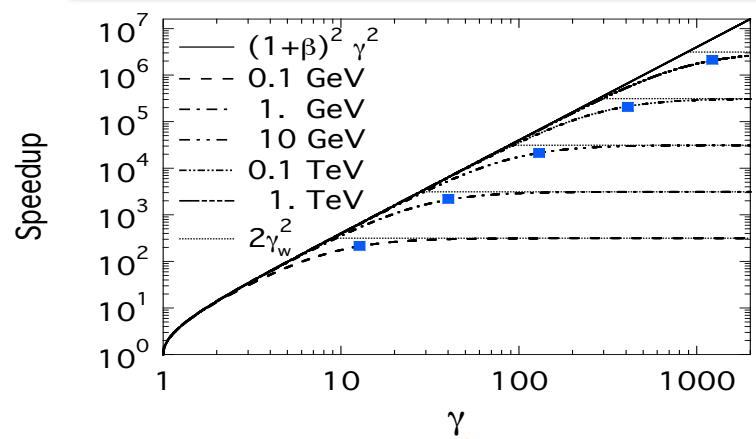
Simulations in a Lorentz "boosted frame" reduces numerical difficulty by orders of magnitude*





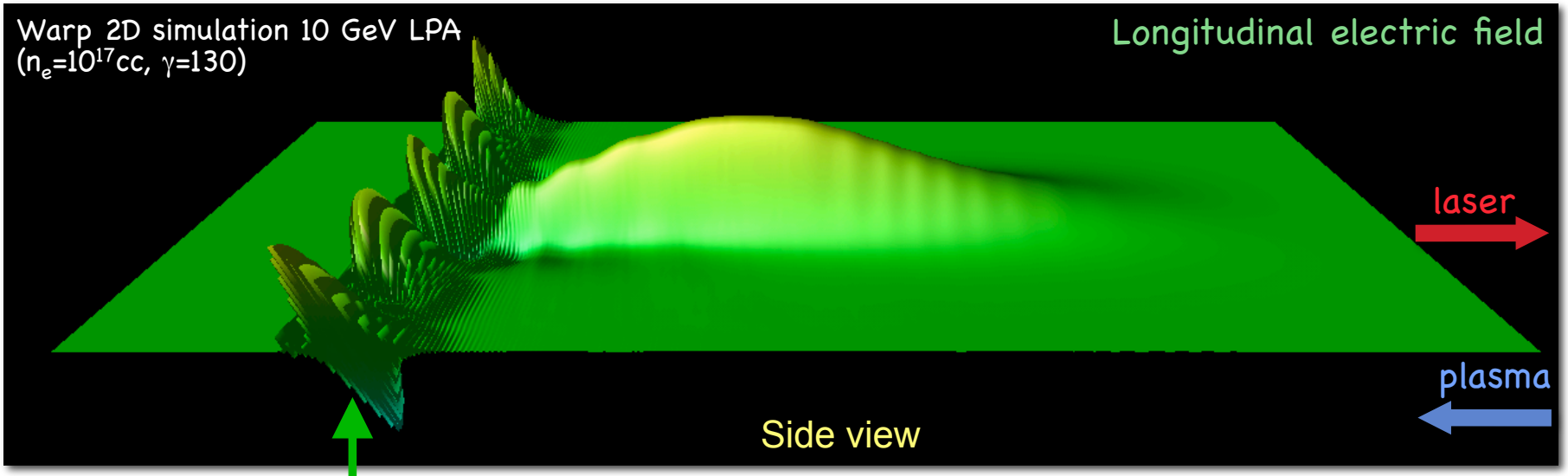
Predicted speedup:

- > 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)

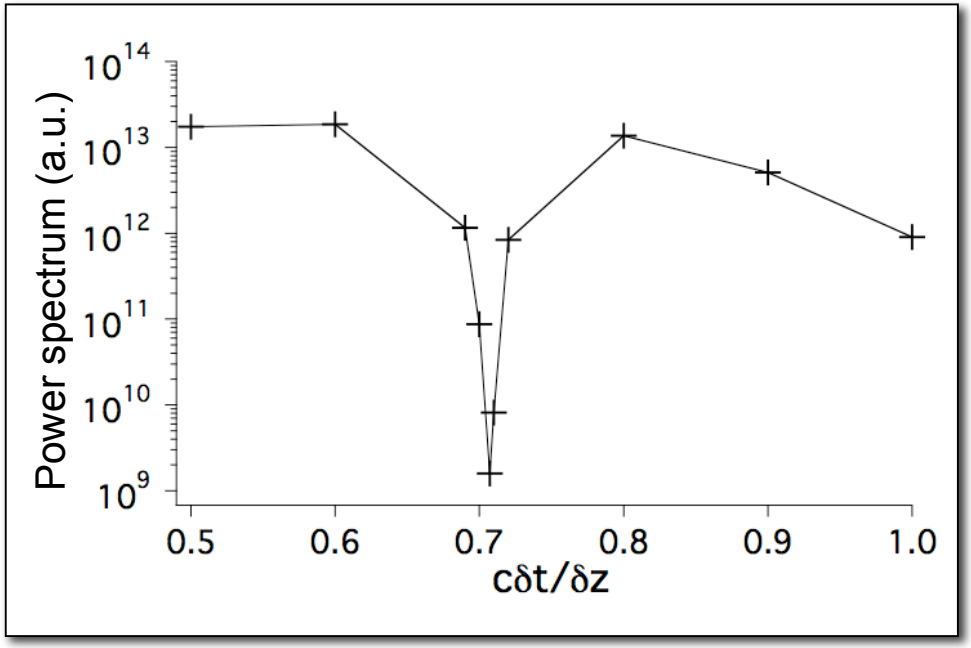
But instability reported for large γ boost using standard PIC



Short wavelength instability at front of plasma

Numerical "curiosity" alleviates problem

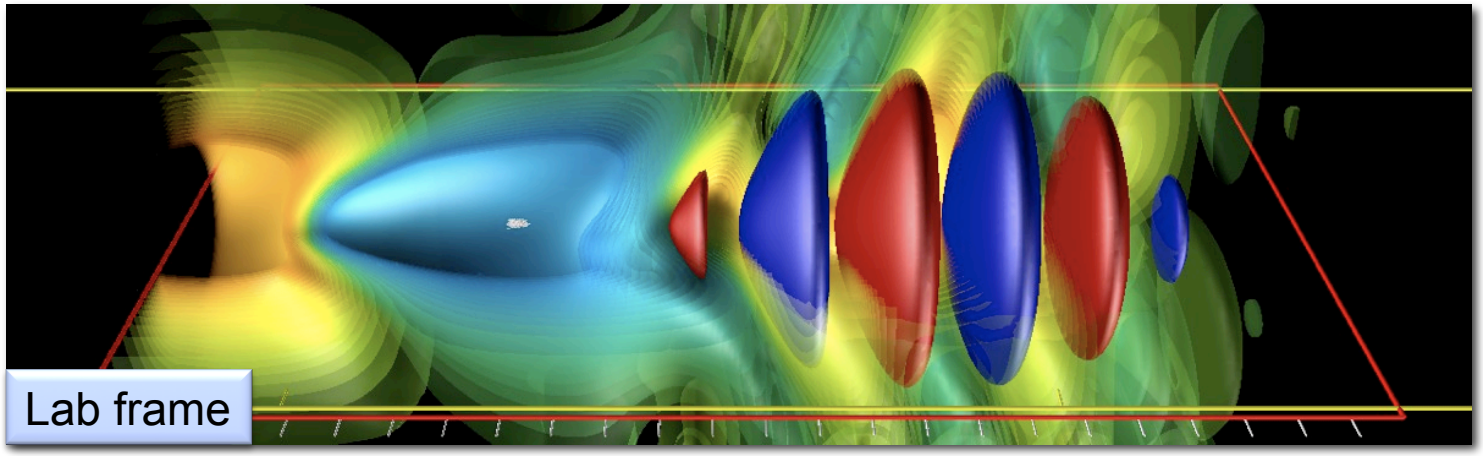
Sharp decrease of instability level at $c\delta t=\delta z/\sqrt{2}$!

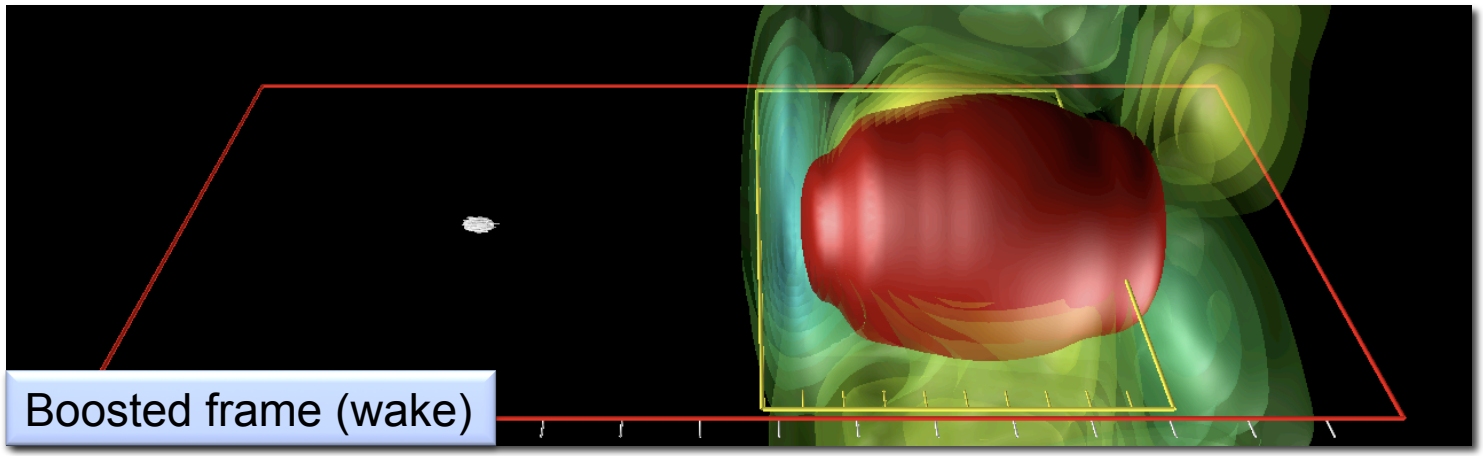


- Tunable NSFD solver allows $c\delta t=\delta z/\sqrt{2}$ time step for (near) cubic cells
  - $c\delta t=\delta z/\sqrt{2}$ time step restricted to "pancake" cells in 3D using Yee FDTD solver
- Origin of "magical" time step is unknown
  - Numerical Cerenkov? Does not seem to be dependent on numerical dispersion…

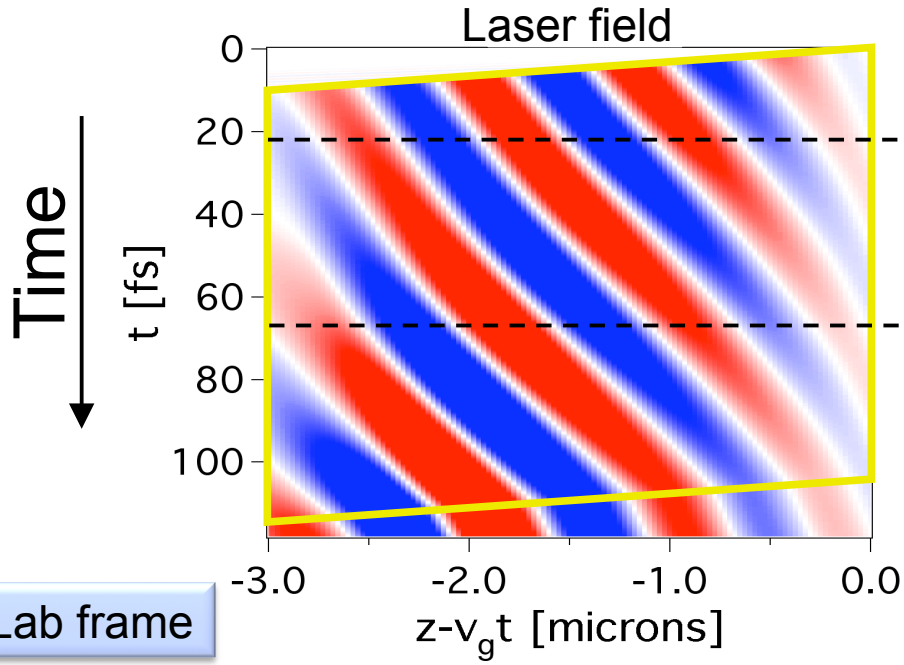
Specific boost frame helps further, thanks to space-time rotation

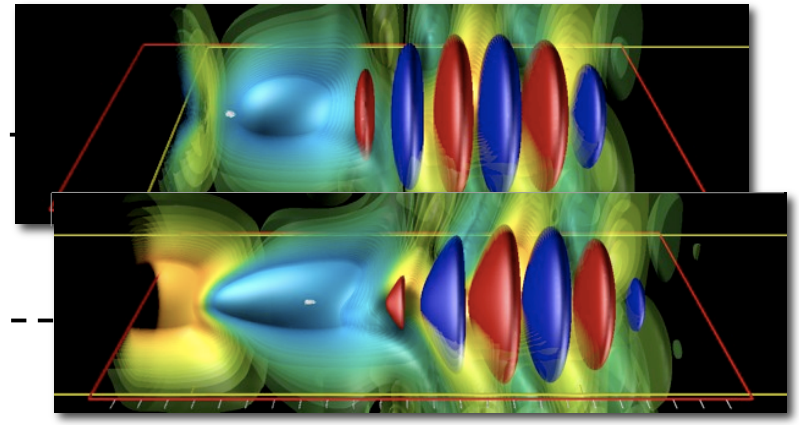
Snapshots look very different in lab and wake frame



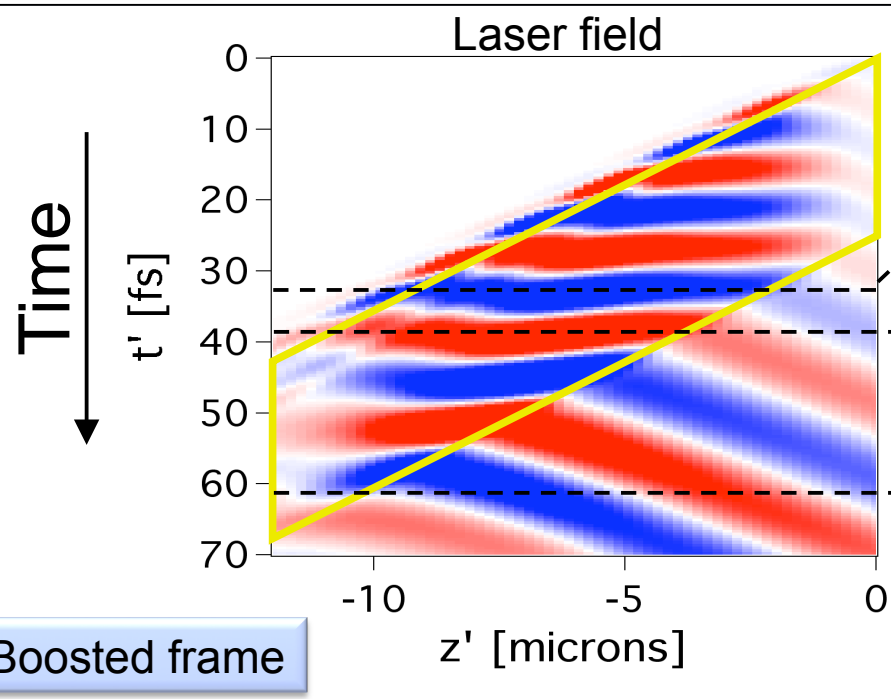


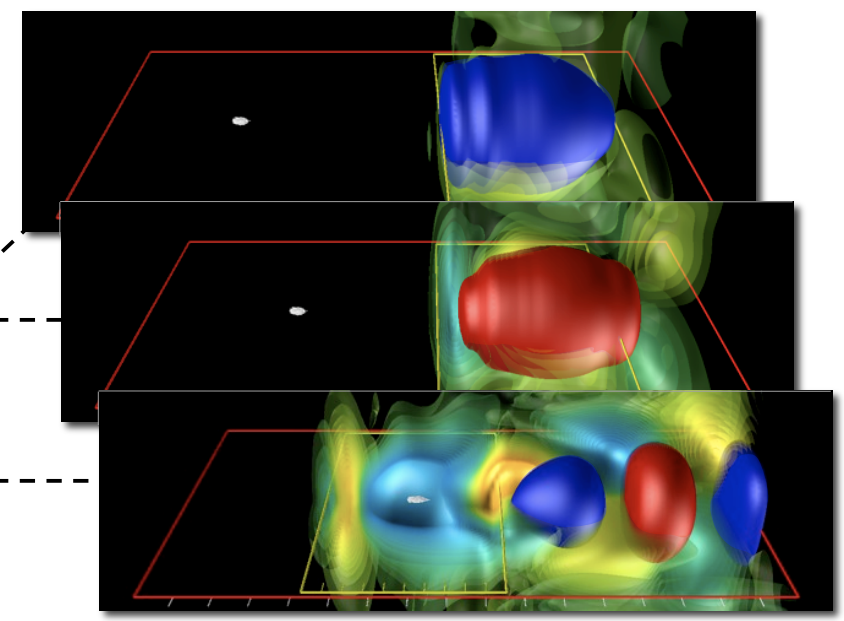
(snapshot from scaled run for clarity; actual Bella runs at full scale exhibit many more laser oscillations per pulse)





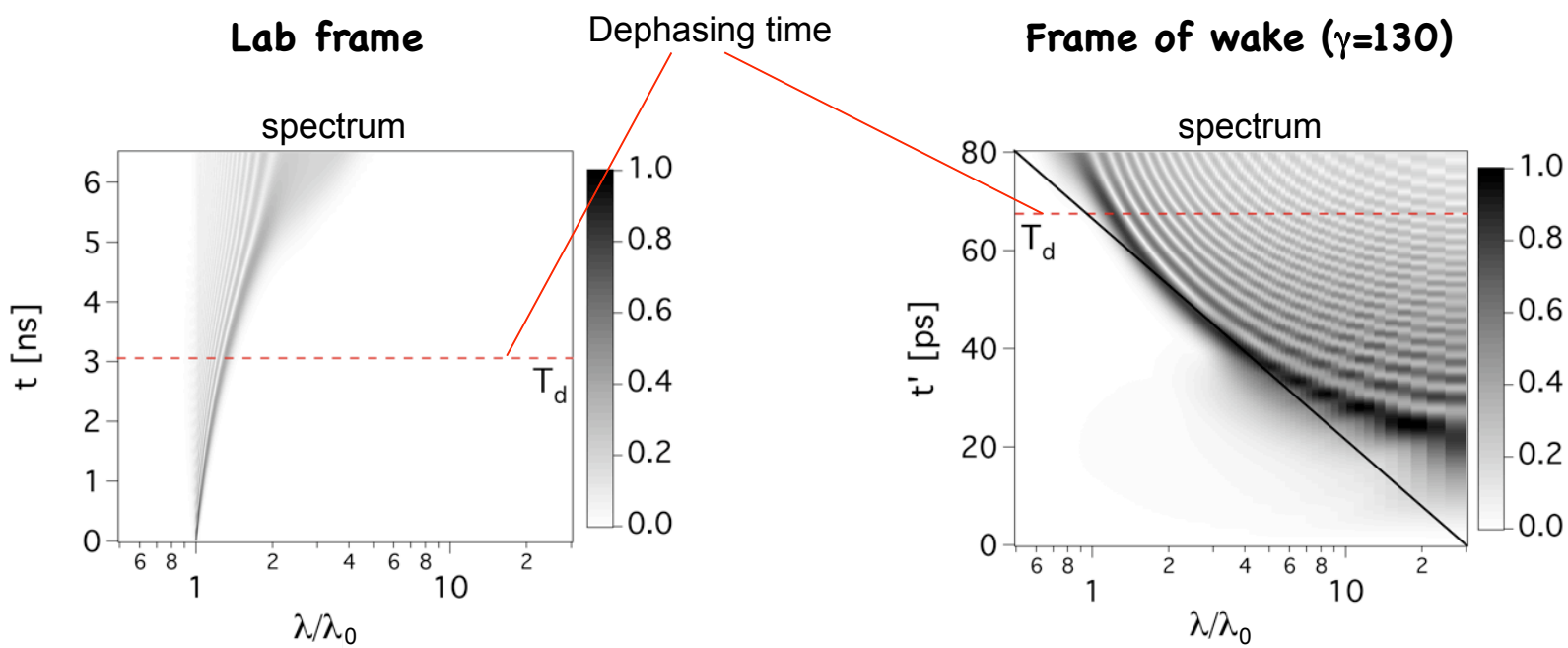
Hyperbolic rotation from Lorentz Transformation converts laser spatial oscillations into time beating.





Spectrum very different in boosted and lab frames

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



Content concentrated around λ_0

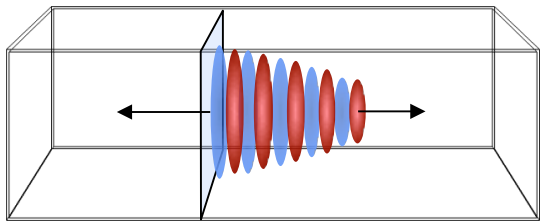
Content concentrated at much larger λ

More filtering possible without altering physics.

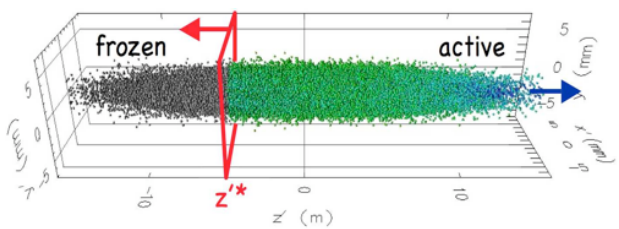
Controlling the numerical instability with tunable EM solver & filtering

+ new laser/particle injection and diagnostics through planes:

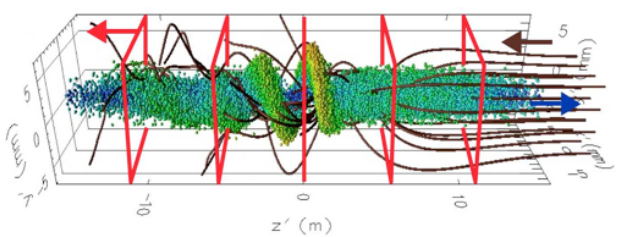
Laser injection



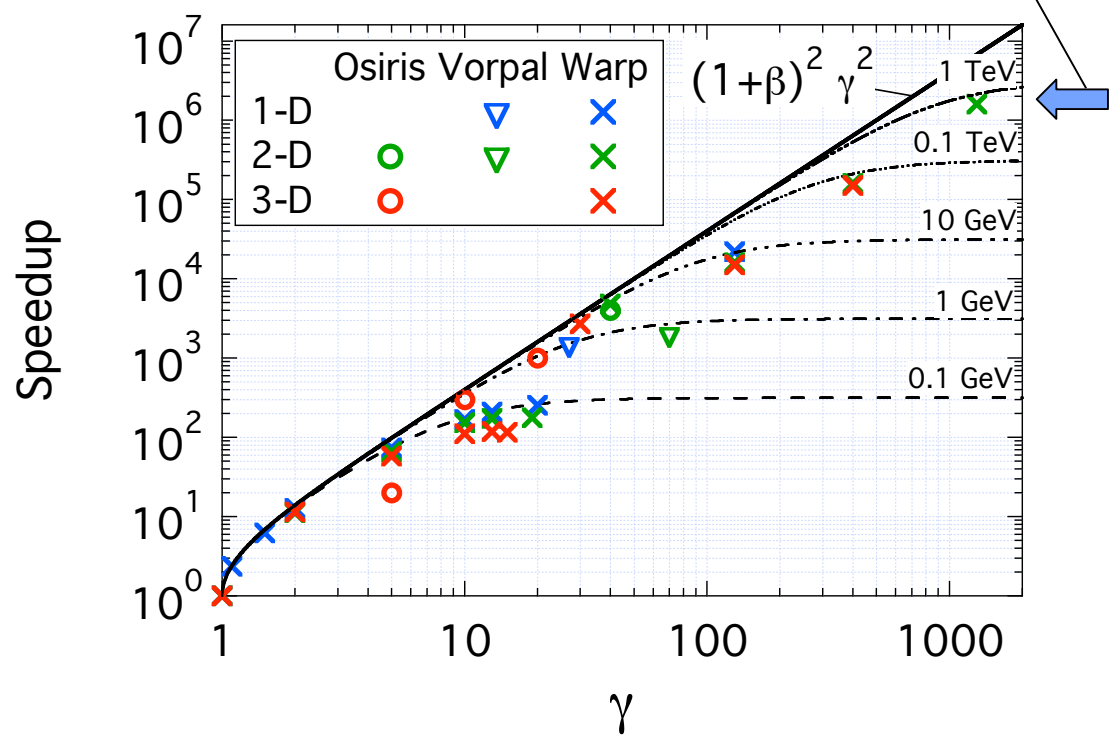
Particle injection



Diagnostics



led to over 1 million x speedup



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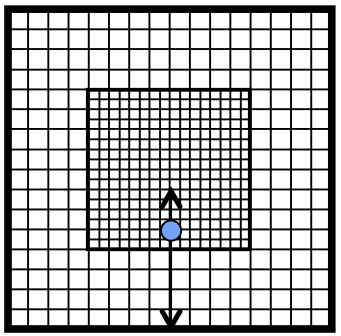
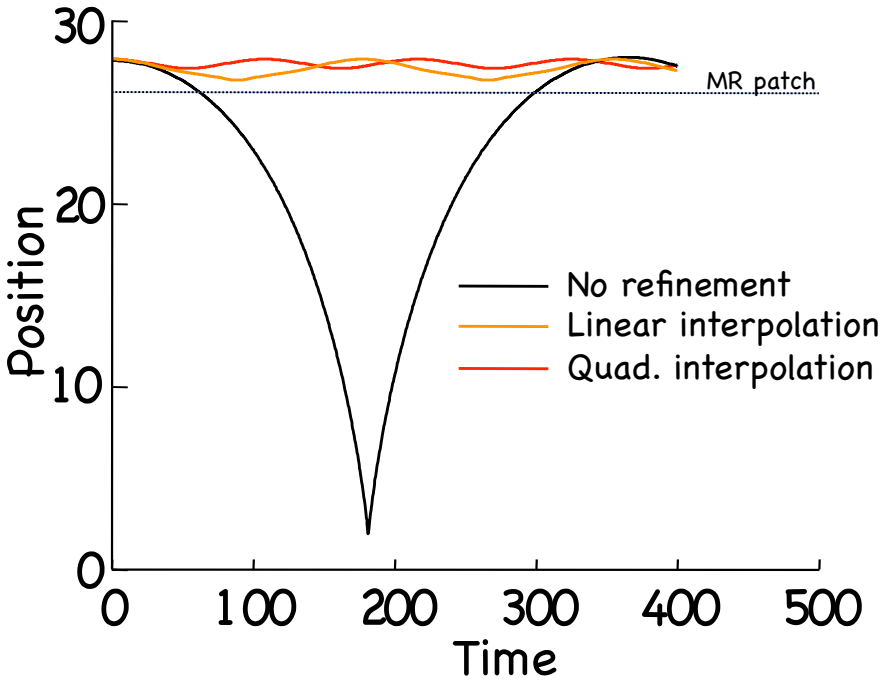
Warp mesh refinement method: electrostatic

MR introduces spurious force[1]

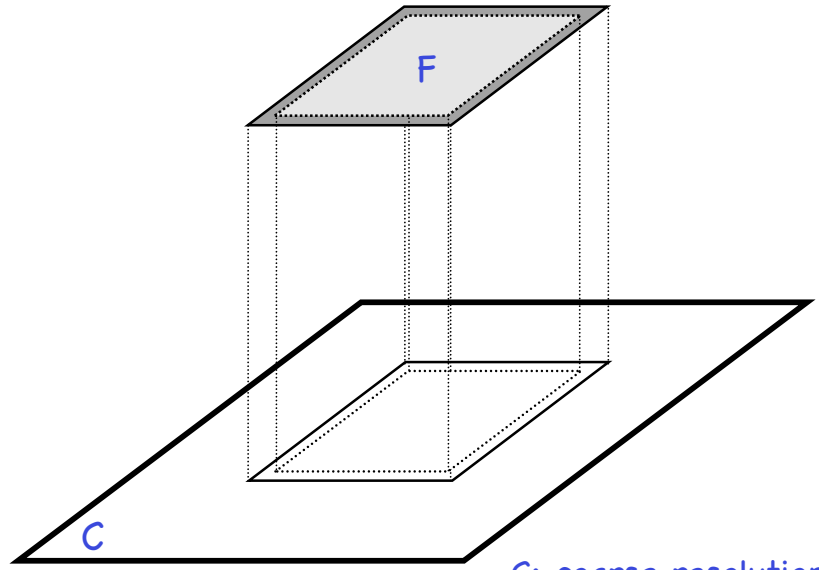


particle feels its own field and can by trapped in patch



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

Warp's MR solver[1,2]



C: coarse resolution
F: fine resolution

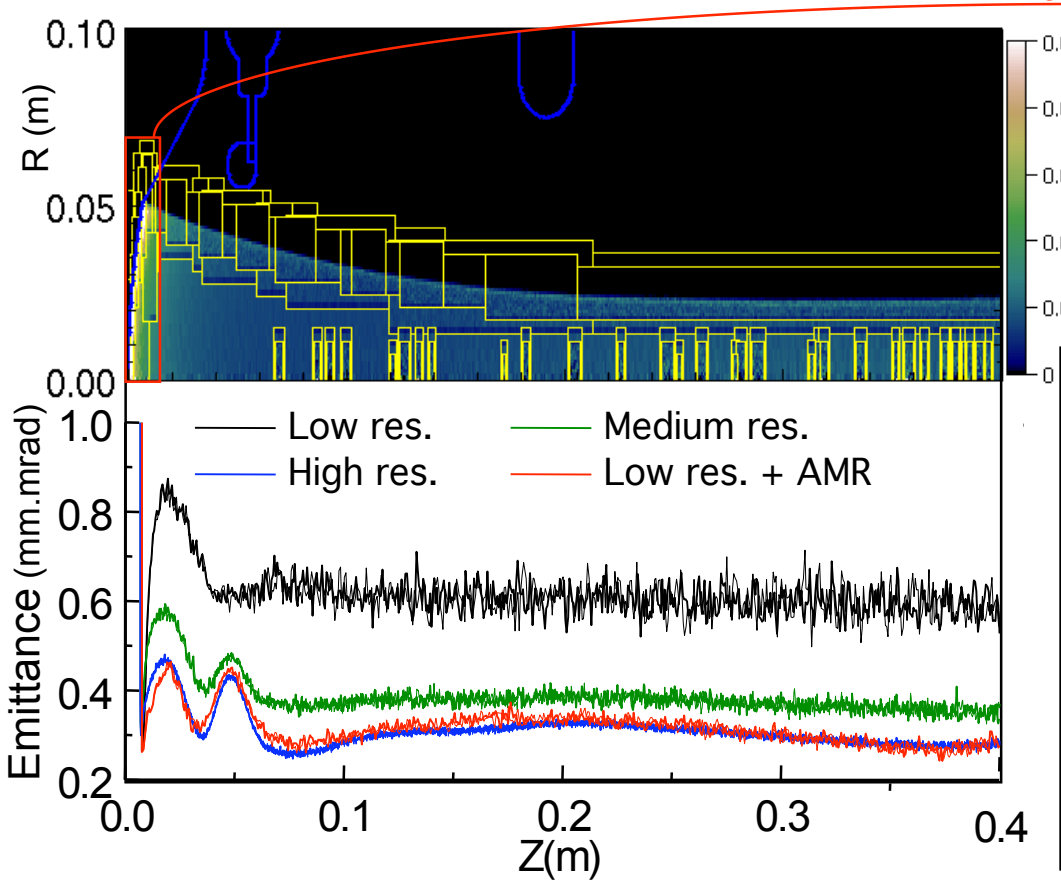
1 – solve on coarse grid,
2 – interpolate on fine grid boundaries,
3 – solve on fine grid,
4 – disregard fine grid solution close to edge.

Step 4 provides user control of relative magnitude of spurious force[(2)].

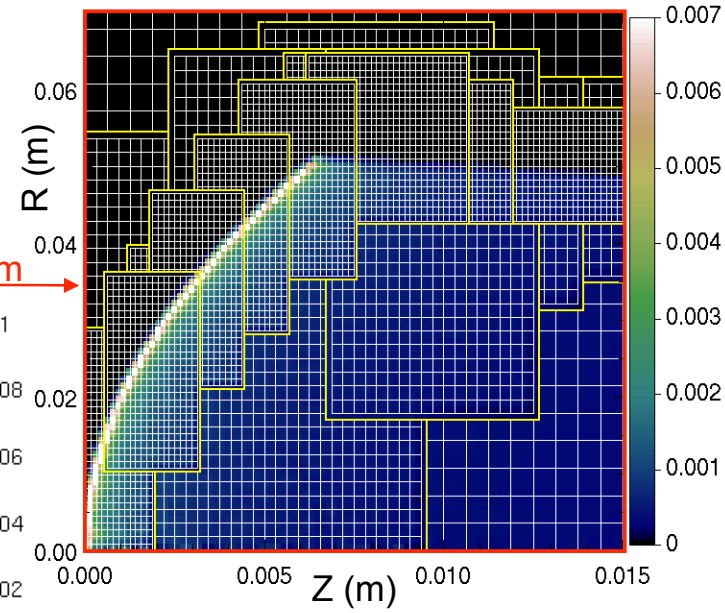
(2) Vay et al., *Phys. Plasmas* **11** (2004)

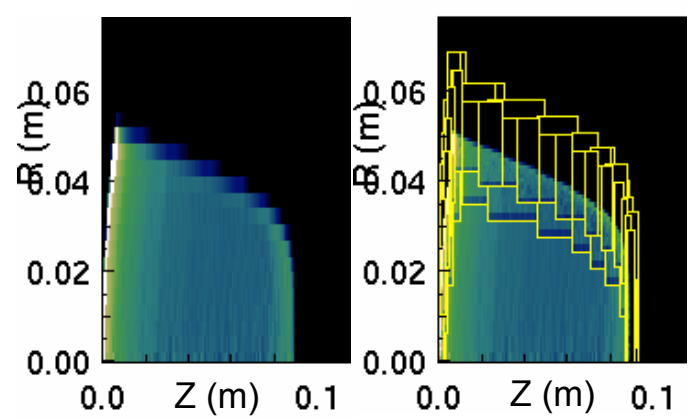
Electrostatic AMR simulation of ion source: speedup x10

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



zoom



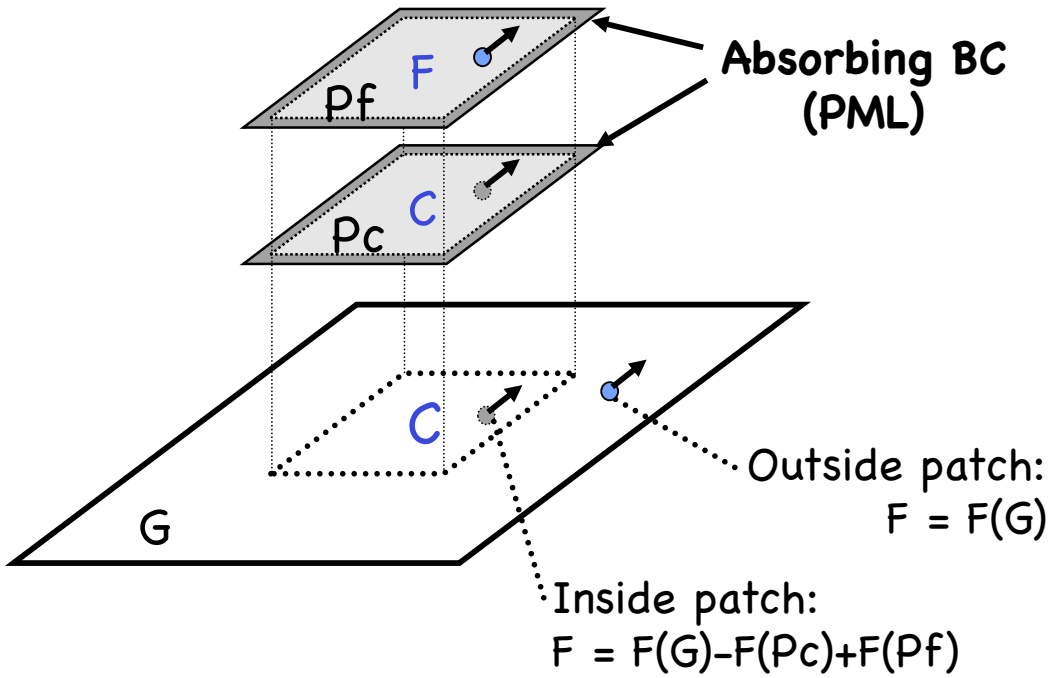


Automatic mesh refinement follows gradients: emitting area, beam edge and front.

Electromagnetic MR solver also controls spurious waves reflections*

To avoid wave reflections at MR patches edges:

- no interpolation between coarse and fine grids,
- patches terminated with absorbing BC (PML).



User controls relative magnitude of spurious force & wave reflections.

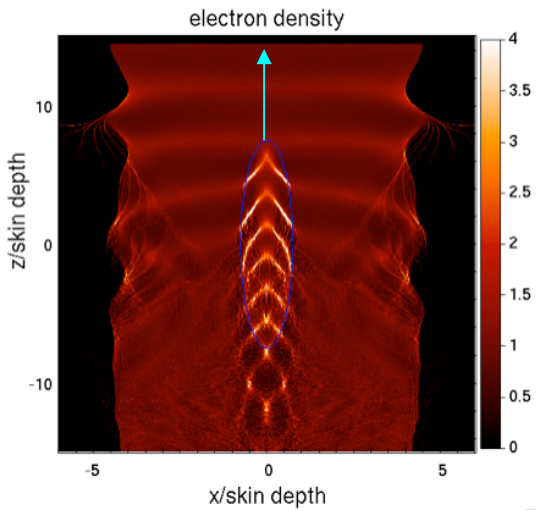
*Vay, Adam, Heron, *Comp. Phys. Comm.* 164 (2004)

Electromagnetic MR simulation of beam-induced plasma wake

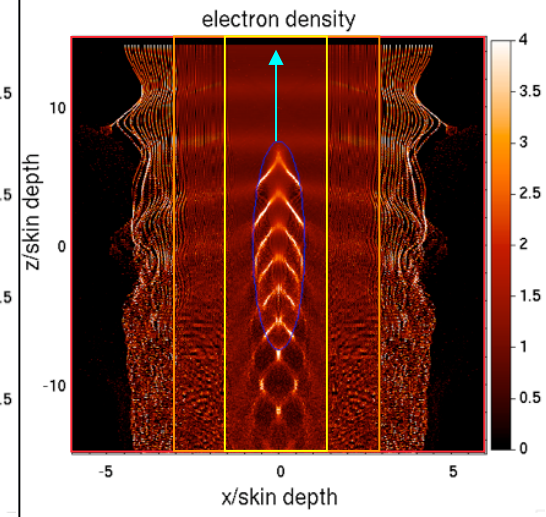
no refinement

2 levels of mesh refinement (MR)

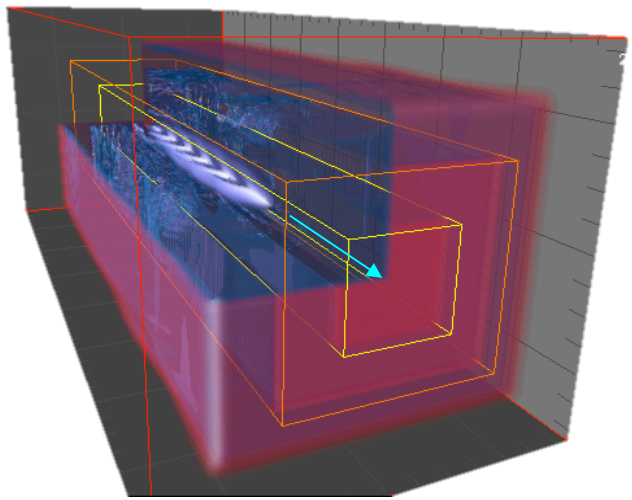
2-D high resolution



2-D low resolution + MR



3-D



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

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Leapfrog pusher for ultra-relativistic charged particle beam

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

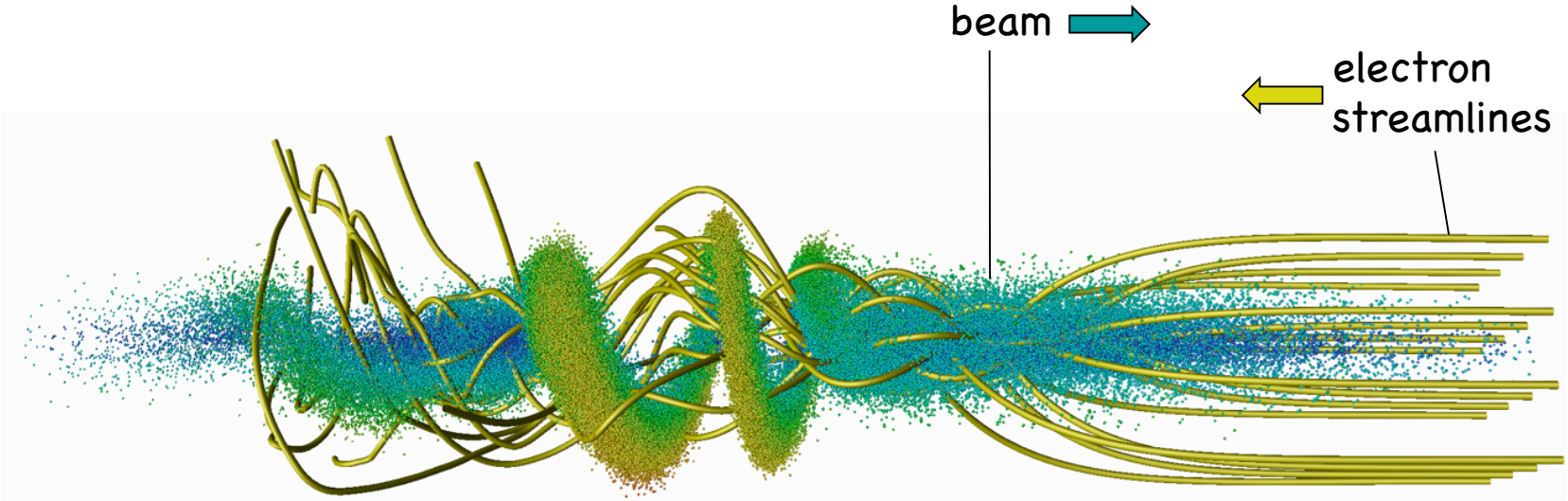
$u^* = \mathbf{u}' \cdot \boldsymbol{\tau}/c$, $\sigma = \gamma'^2 - \tau^2$, $\gamma' = \sqrt{1 + u'^2/c^2}$, $\mathbf{t} = \boldsymbol{\tau}/\gamma^{i+1}$).

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

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

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

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



Beam was lost after a few betatron oscillations with Boris pusher.

Successful with new pusher.

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

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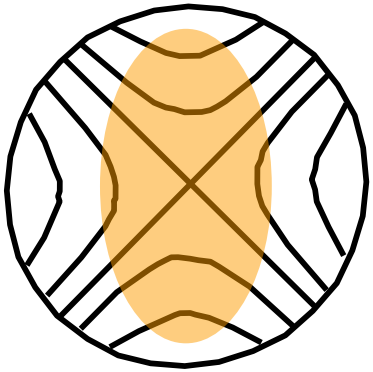
"Drift-Lorentz" mover* relaxes the problem of short electron timescales in magnetic field*

Magnetic quadrupole



Problem: Electron gyro timescale

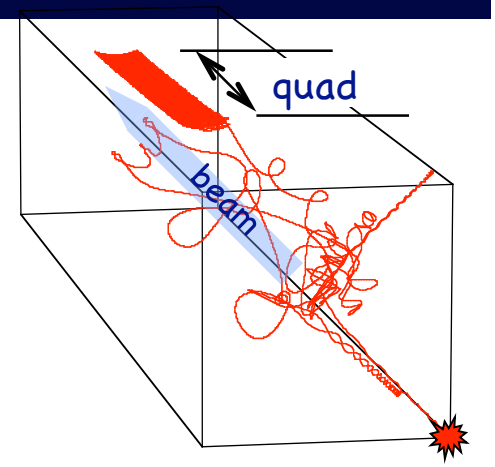
<< other timescales of interest

⇒ brute-force integration very slow due to small Δt

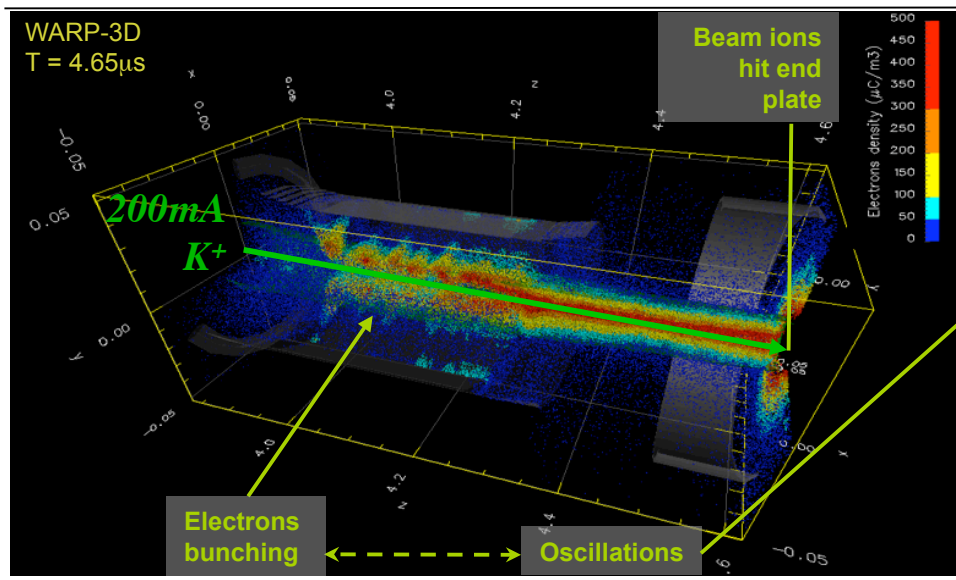
Solution*: Interpolation between full-particle dynamics ("Boris mover") and drift kinetics (motion along B plus drifts)

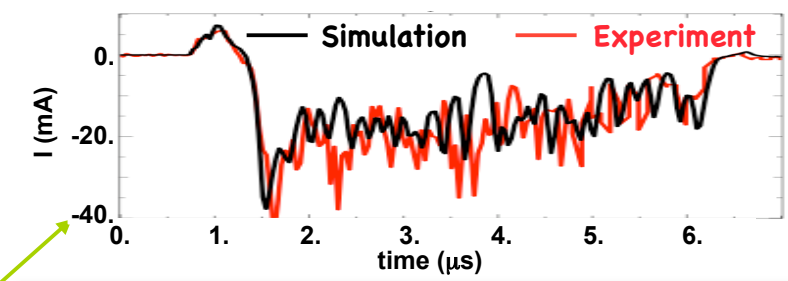
$$\vec{v}_{eff} = \vec{B}\left(\vec{B}.\vec{v}_L\right) + \alpha\vec{v}_{L,\perp} + \left(1-\alpha\right)\vec{v}_d$$

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



Sample electron motion in a quad





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

Summary

Warp is a parallel Particle-In-Cell simulation framework for the modeling of accelerators, beams, plasmas and laser-plasma interaction.

Novel algorithms include

- tunable electromagnetic field solver,
- strided filtering,
- boosted frame input/output,
- mesh refinement,
- ultra-relativistic particle pusher,
- a "Drift-Lorentz" particle pusher for large time steps of magnetized particles.