Innovative use of High Performance Computing through the Modeling of Particle Accelerators.

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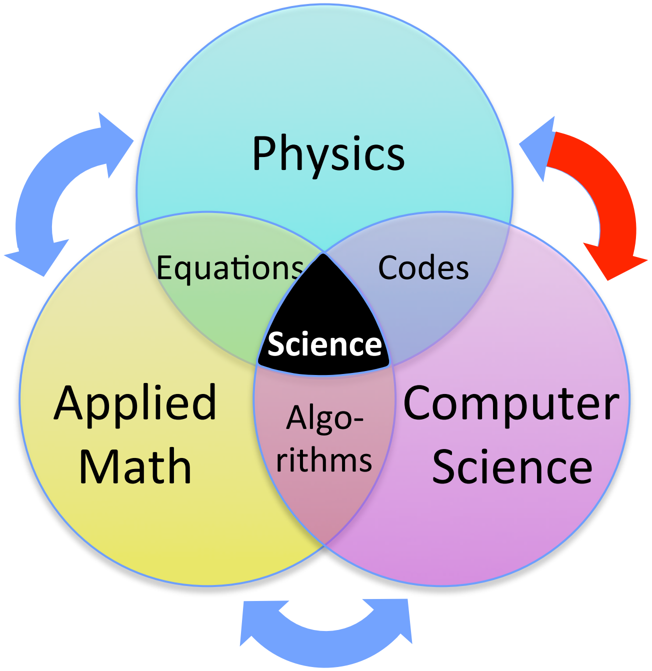
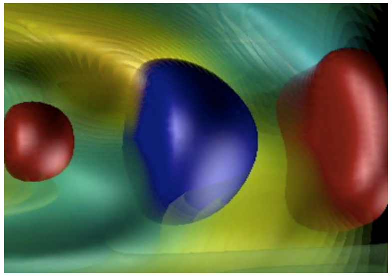
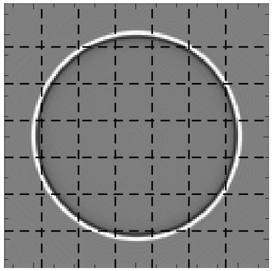
Using physics to influence HPC accelerator modeling

Conventional wisdom assumes serial process for building codes:



but reality is much more complex, w/ physics even being used to alter algorithms & codes.

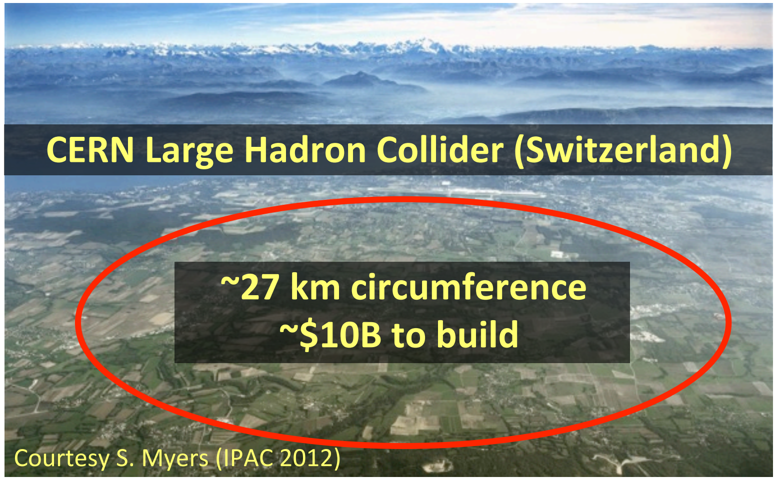
Examples

Lorentz boosted frame	***Parallel spectral solver***
	
Uses special relativity to speedup simulations by orders of magnitude.	Uses finite speed of light to enable direct scaling to many cores.
J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)	J.-L. Vay, I. Haber & B. B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

Accelerator modeling at the crossroad of 2 mutations

Supercomputers

Accelerators

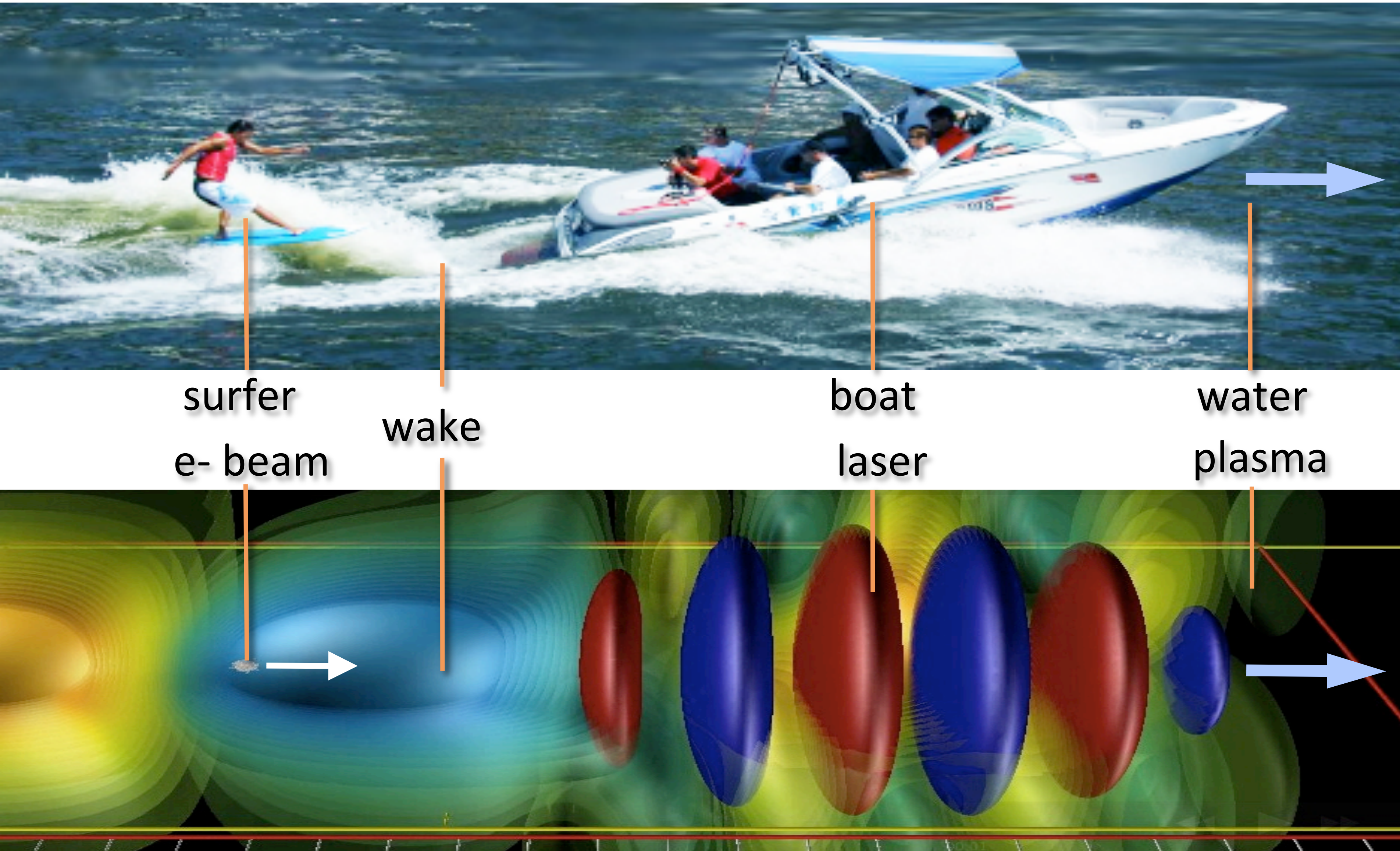


In each case, scaling w/ current technologies is not sustainable:
➔ need for change in paradigm.

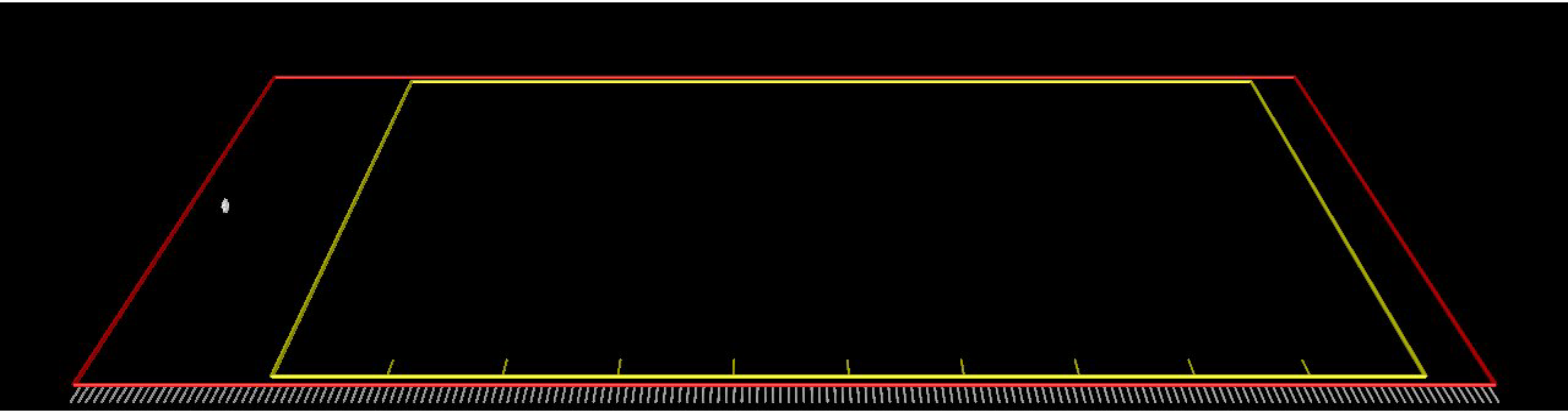
One limiting factor of accelerators based on standard technologies:
metallic electrical breakdown limit of ~50-100 MV/m.

Plasma based accelerators - i.e. Berkeley Lab Laser Accelerator (BELLA):
electric fields >50 GV/m ➔ shorter, cheaper accelerators!

Laser plasma acceleration (LPA)



Modeling from first principle is very challenging

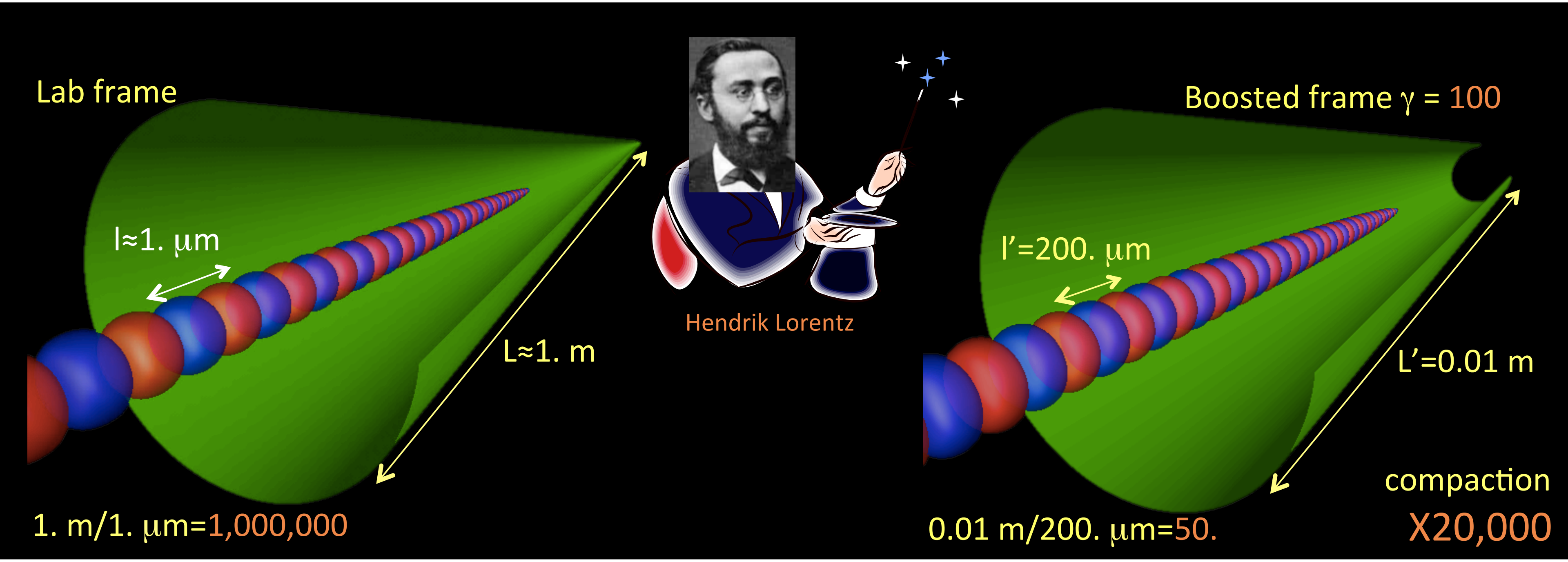


For a 10 GeV scale stage (e.g. BELLA):

~1μm wavelength laser propagates into ~1m plasma

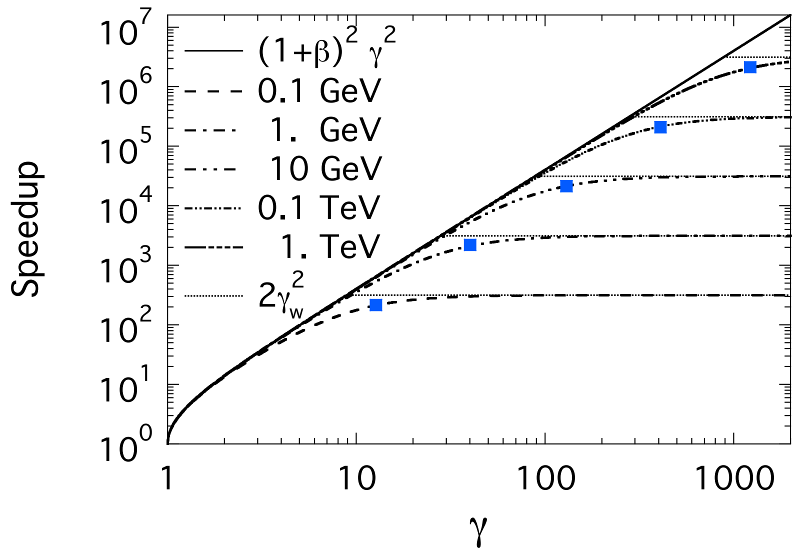
➔ tens of millions of time steps needed!

Solution: model in frame moving near the speed of light*



Predicted speedup:

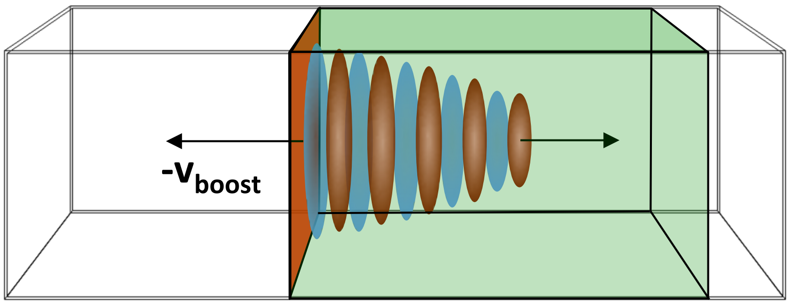
- > 10,000 for single 10 GeV (BELLA) stage,
- > 1,000,000 for single 1 TeV stage.



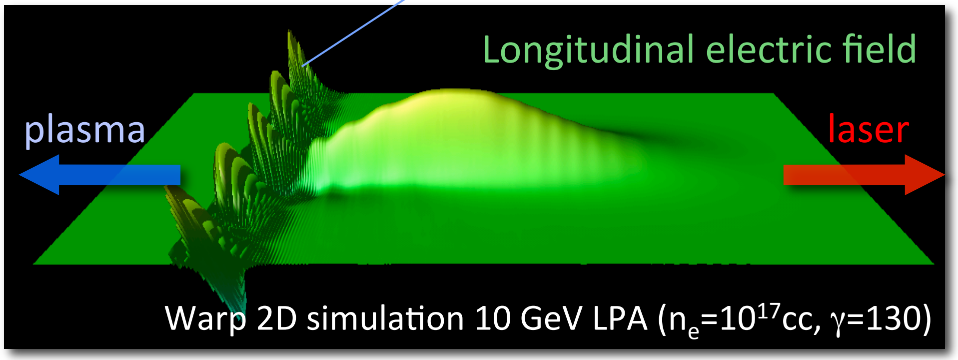
*J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)

Concept simple but application not straightforward

- New algorithm for laser injection using moving antenna[1]



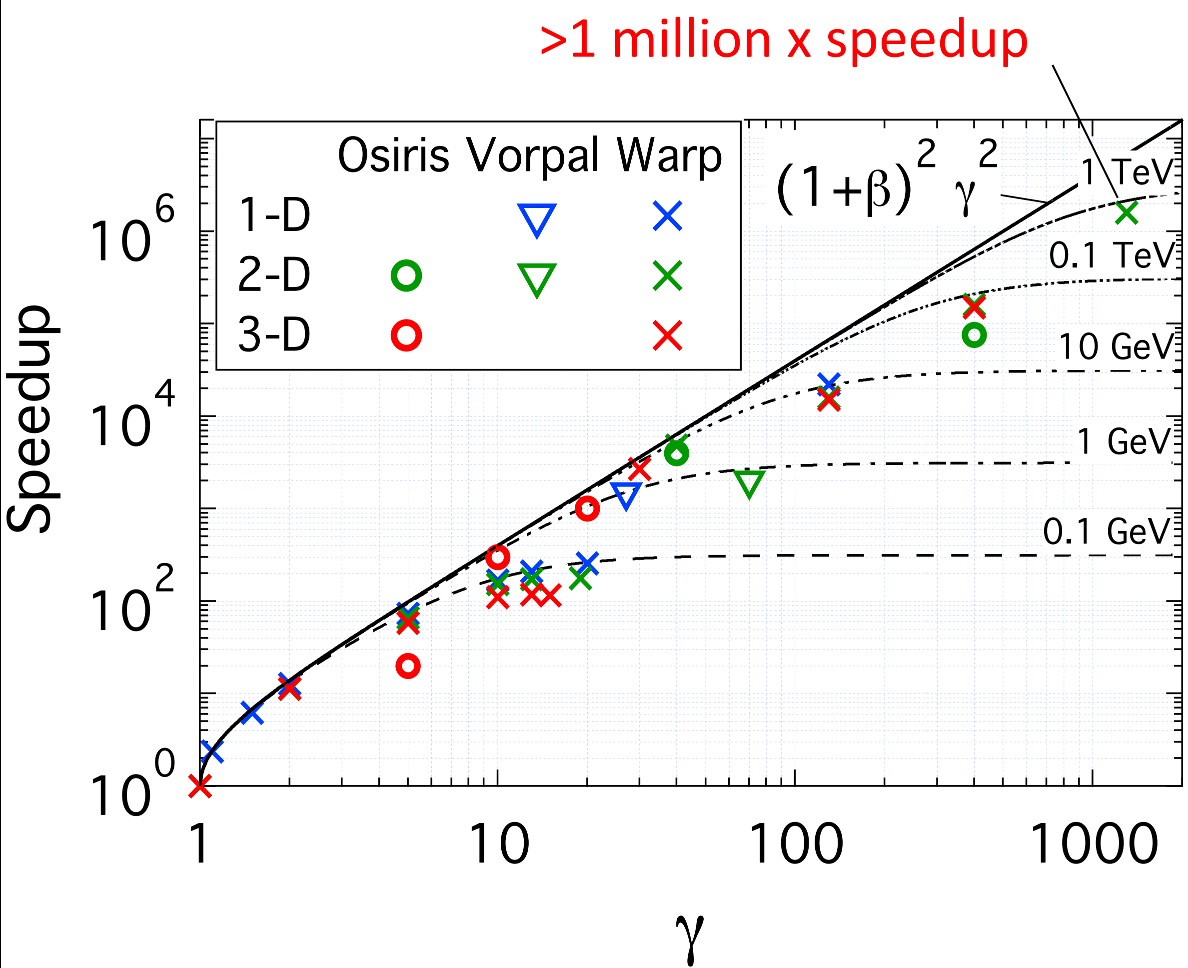
- Short wavelength instability at large γ (≥100)[2]



- Various solutions developed to mitigate instability
  - discovered a "magical time step" with ultra low instability growth rate[2]
  - developed efficient wideband parallel filtering using strides[2]
  - determined that hyperbolic rotation of laser from Lorentz tr. enabled wideband filters[3]
  - understood instability and developed better solutions[4,5]

[1]J.-L. Vay, C. Geddes, E. Cormier-Michel, D. Grote, *Phys. Plasmas* **18**, 123103 (2011)
[2]J.-L. Vay, C. Geddes, E. Cormier-Michel, D. Grote, *J. Comput. Phys.* **230**, 5908 (2011).
[3]J.-L. Vay, C. Geddes, E. Cormier-Michel, D. Grote, *PoP Lett.* **18** (2011).
[4]B. Godfrey, J.-L. Vay, *J. Comput. Phys.* **248**, 33 (2013).
[5]B. Godfrey, J.-L. Vay, *submitted*.

Speedup verified by us and others to over a million



Warp:

1. J.-L. Vay, et al., *Phys. Plasmas* **18** 123103 (2011)
2. J.-L. Vay, et al., *Phys. Plasmas (letter)* **18** 030701 (2011)
3. J.-L. Vay, et al., *J. Comput. Phys.* **230** 5908 (2011)
4. J.-L. Vay et al, PAC Proc. (2009)

Osiris:

1. S. Martins, et al., *Nat. Phys.* **6** 311 (2010)
2. S. Martins, et al., *Comput. Phys. Comm.* **181** 869 (2010)
3. S. Martins, et al., *Phys. Plasmas* **17** 056705 (2010)
4. S. Martins et al, PAC Proc. (2009)

Vorpal:

1. D. Bruhwiler, et al., *AIP Conf. Proc* **1086** 29 (2009)

Enabled simulations previously untractable (e.g. 10 GeV BELLA stage):

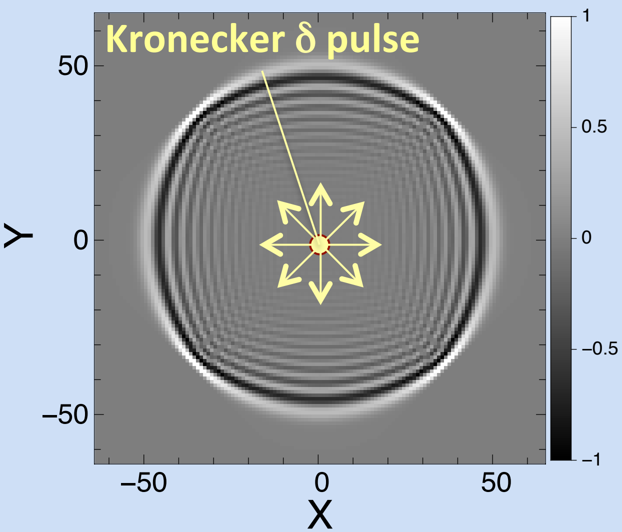
2006 (lab) in 1D: ~ 5k CPU-hours ➔ 2011 (boost) in 3D: ~ 1k CPU-hours

Speed & accuracy required for ultra high quality beams

Electromagnetic solvers

Finite-Difference Time Domain

Warp (LBNL/LLNL/U. Maryland), Osiris (UCLA), V-sim (Tech-X), etc.

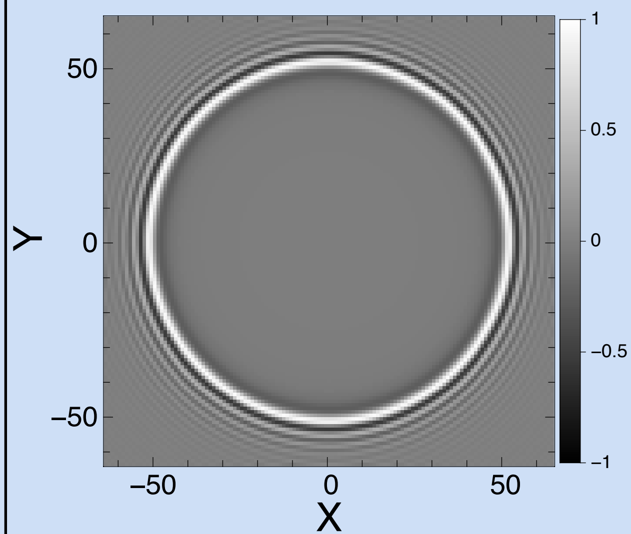


- Numerical dispersion,
- anisotropy,
- Courant condition:

$$c\Delta t \leqslant 1/\sqrt{\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta x^2}}$$

Pseudo-Spectral Time Domain

UPIC-EMMA (UCLA)

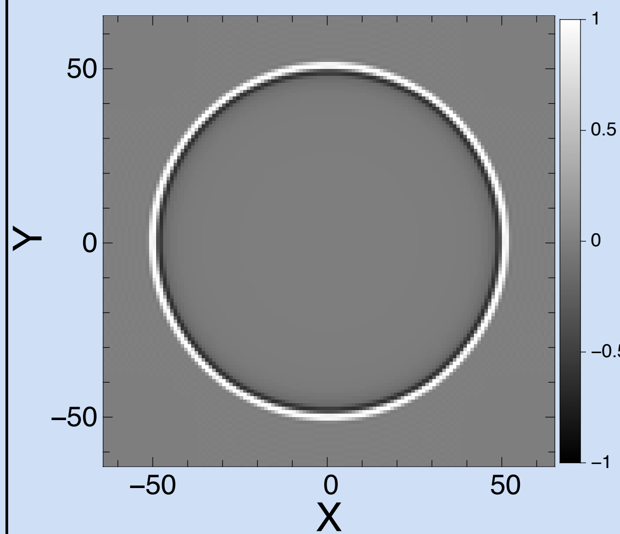


- Numerical dispersion,
- isotropy,
- Courant condition:

$$c\Delta t \leqslant 2/\pi\sqrt{\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta x^2}}$$

Pseudo-Spectral Analytic Time Domain[1,2]

Warp (LBNL/LLNL/U. Maryland)



- Exact dispersion,
- isotropy,
- Courant condition:

None

[1]I. Haber, R. Lee, H. Klein & J. Boris, *Proc. Sixth Conf. on Num. Sim. Plasma,* Berkeley, CA, 46-48 (1973)

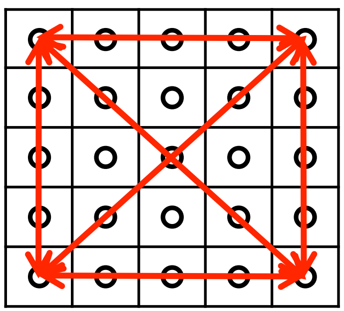
[2]J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

But spectral solvers hard to scale to large # of cores

Spectral

global

communications



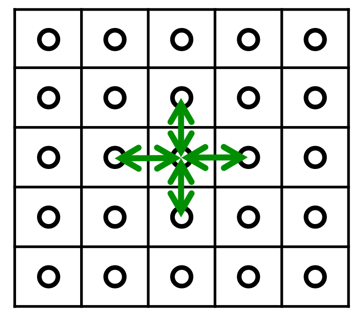
Hard/costly to scale

vs

Finite Difference

local

communications

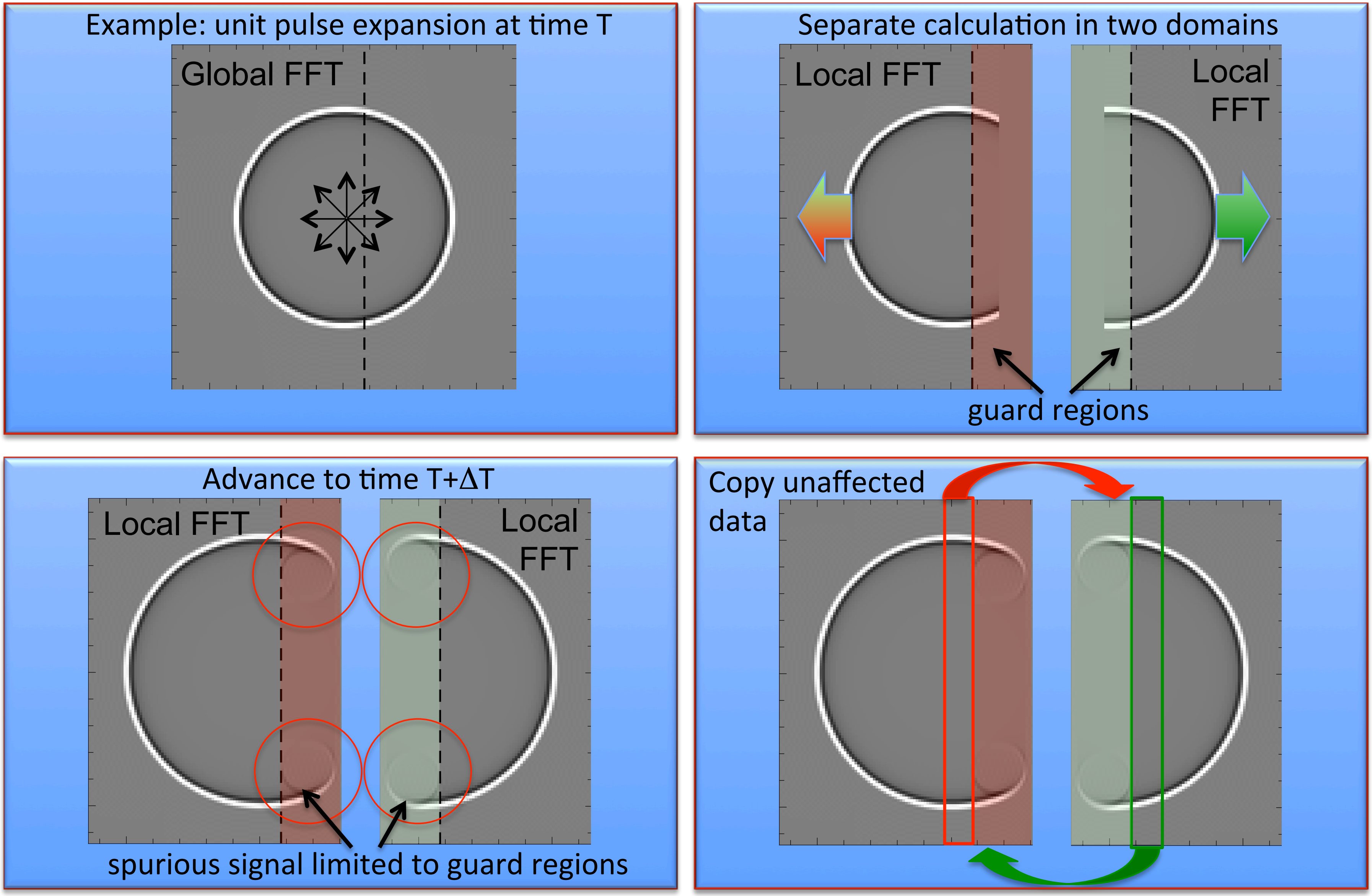


Easy/cheap to scale

But thanks to finite speed of light,
Maxwell update is local during finite time interval ΔT.

➔ local communications may be used with spectral Maxwell.

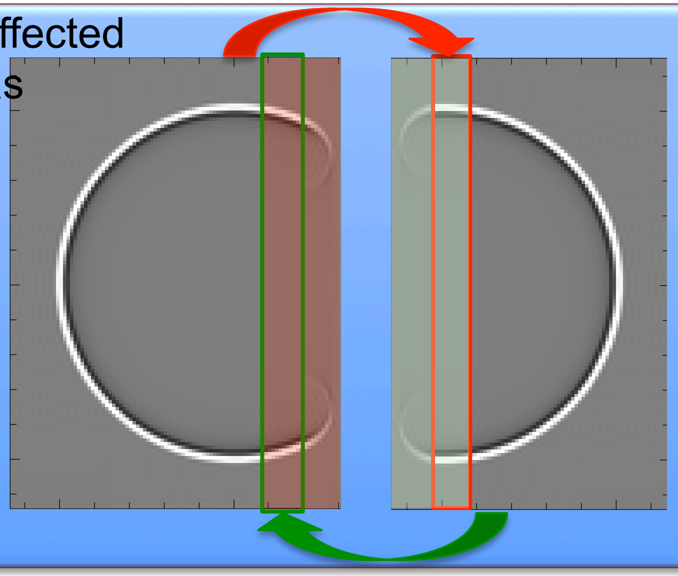
New concept on single pulse – part 1



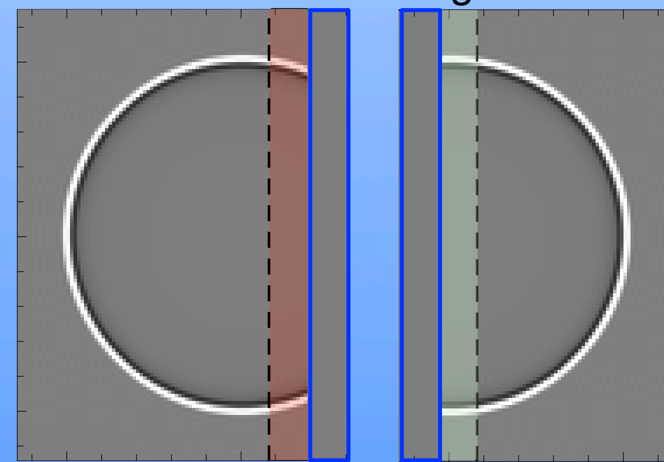
*J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

New concept on single pulse – part 2

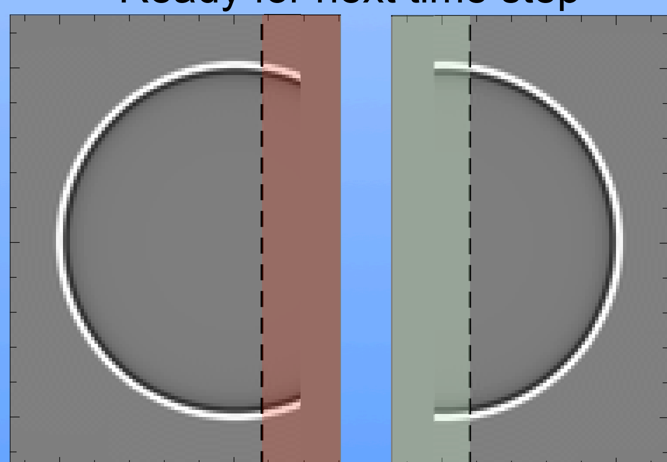
To affected areas



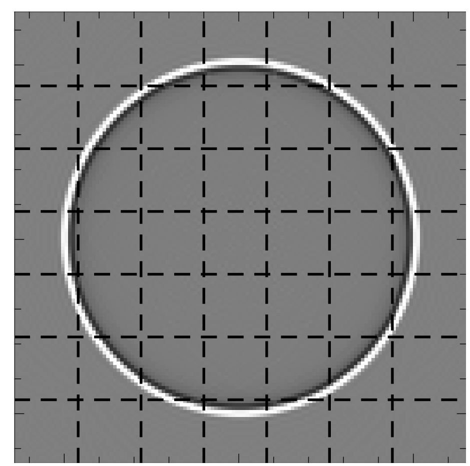
zero out remaining areas



Ready for next time step



Successfully tested on 7x7 domain



Local FFTs in each subdomain!

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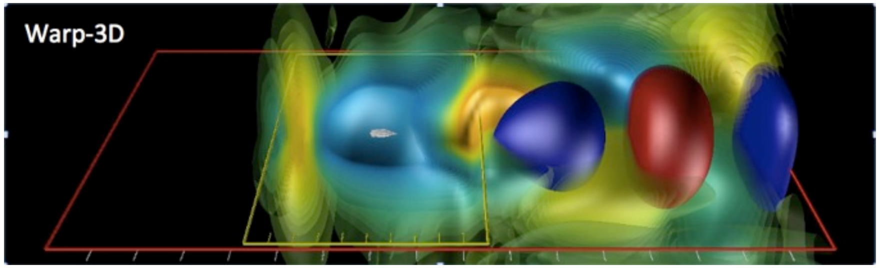
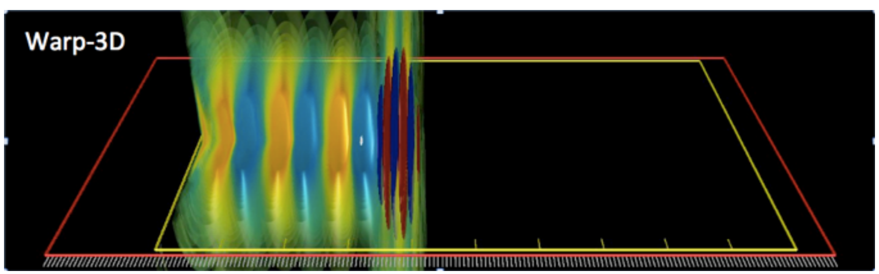
Successfully tested on 2-D modeling of short LPA stages

Lorentz boosted frame (wake)

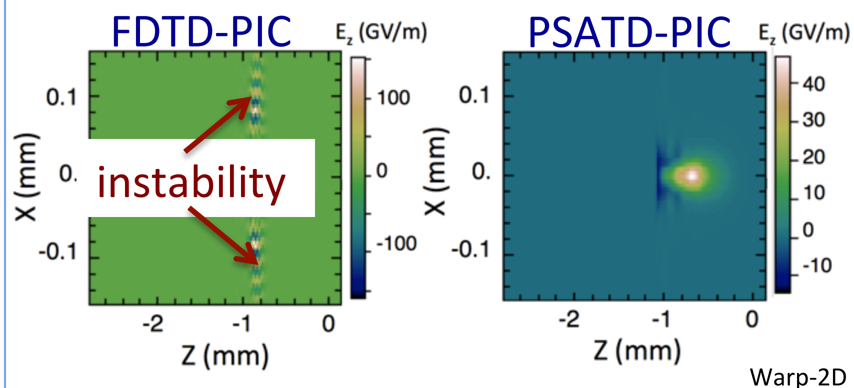


Small proof-of-principle simulations using 8 cores.

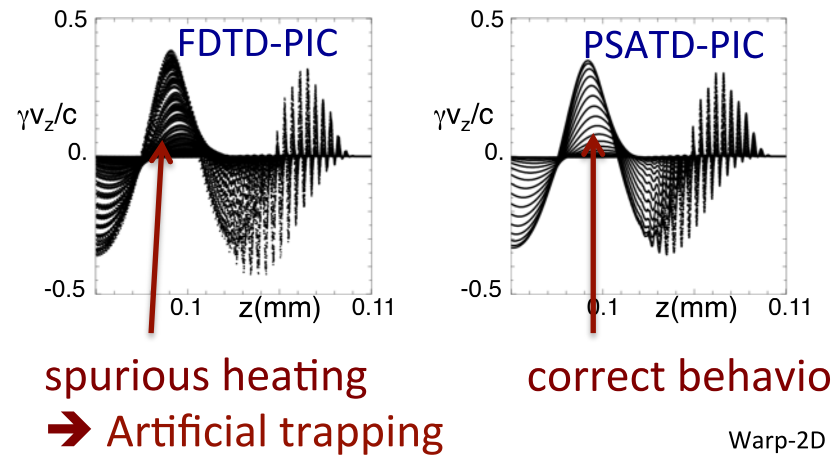
Lab frame



Improved stability



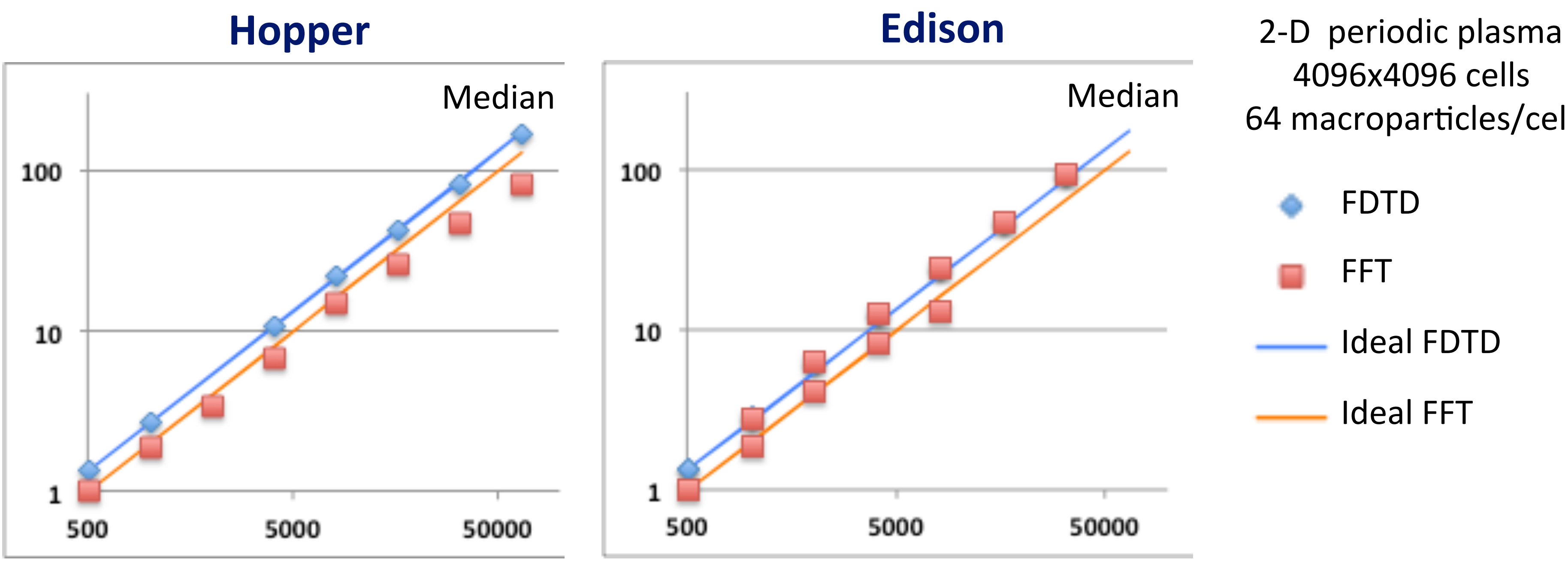
Improved phase space accuracy



*J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

Warp strong scaling on Hopper and Edison

Joint AFRD/CRD/NERSC LDRD on new spectral solver decomposition



Courtesy: A. Koniges, NERSC

- Near linear scaling up-to 65,636 cores on Hopper, 32,768 on Edison.
- Prototype FFT Maxwell solver implemented with numpy & pyMPI.
- Optimized C implementation underway; 3-D to follow (T. Drummond, CRD).

Thanks!

- NERSC for this prize, supercomputer time & support.
- Department of Energy OS: HEP (incl. SciDAC ComPASS), FES.
- LBNL (AFRD/CRD): critical LDRD seed support.
- A. Friedman/D. Grote (LLNL):
  - originator & main developer of Warp,
  - Warp's Python+FORTRAN/C fosters creativity at full speed.
- Colleagues from:
  - AFRD: C. Geddes, W. Fawley, M. Furman, M. Venturini, E. Cormier,
  - CRD/NERSC: A. Koniges, T. Drummond,
  - U. Maryland: B. Godfrey, I. Haber.