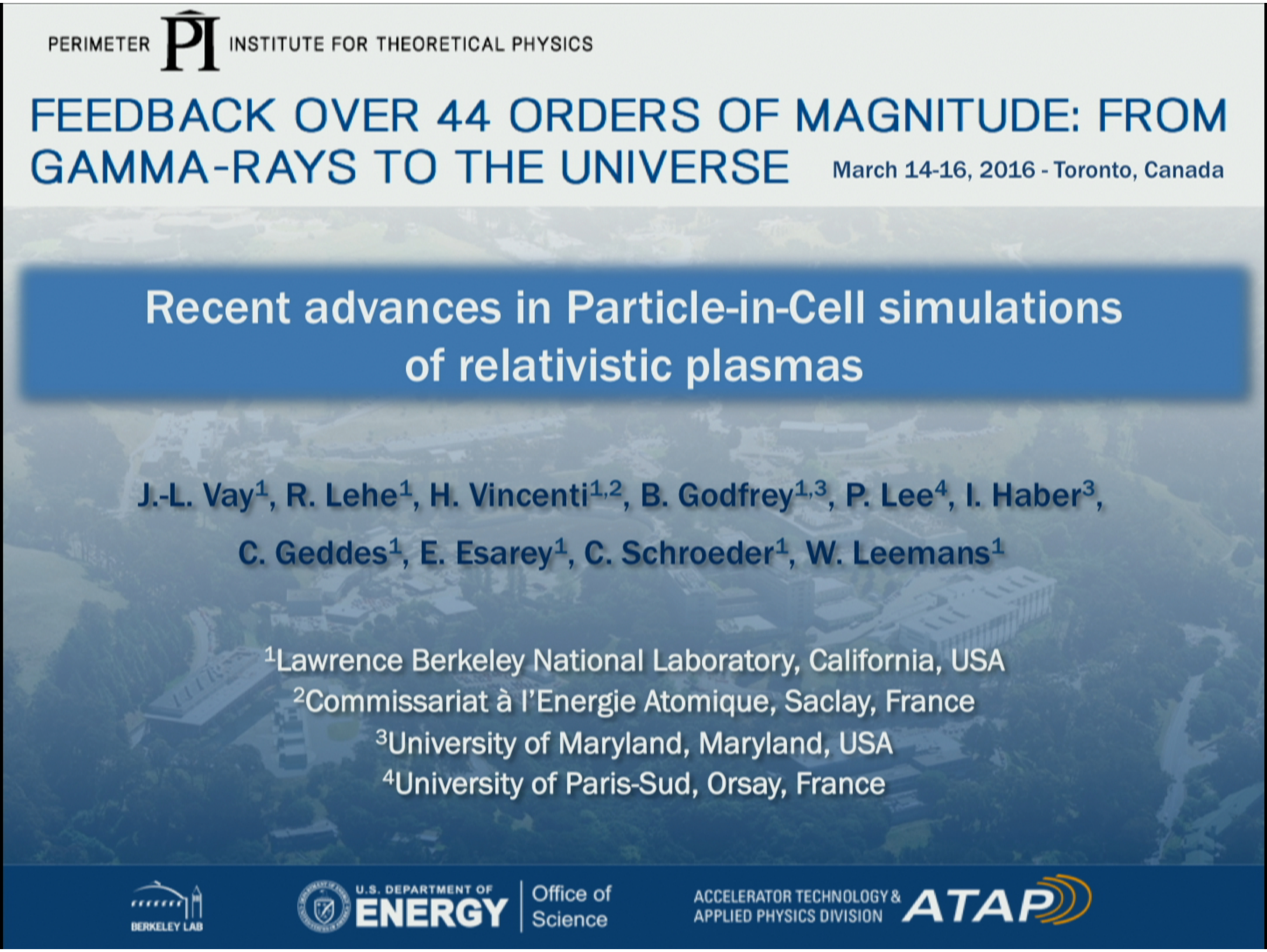
Title: recent advances in Particle-In-Cell simulations of relativistic plasmas

Date: Mar 16, 2016 04:00 PM

URL: http://pirsa.org/16030108

Abstract:



PERIMETER PI INSTITUTE FOR THEORETICAL PHYSICS

FEEDBACK OVER 44 ORDERS OF MAGNITUDE: FROM GAMMA-RAYS TO THE UNIVERSE

March 14-16, 2016 - Toronto, Canada

Recent advances in Particle-in-Cell simulations of relativistic plasmas

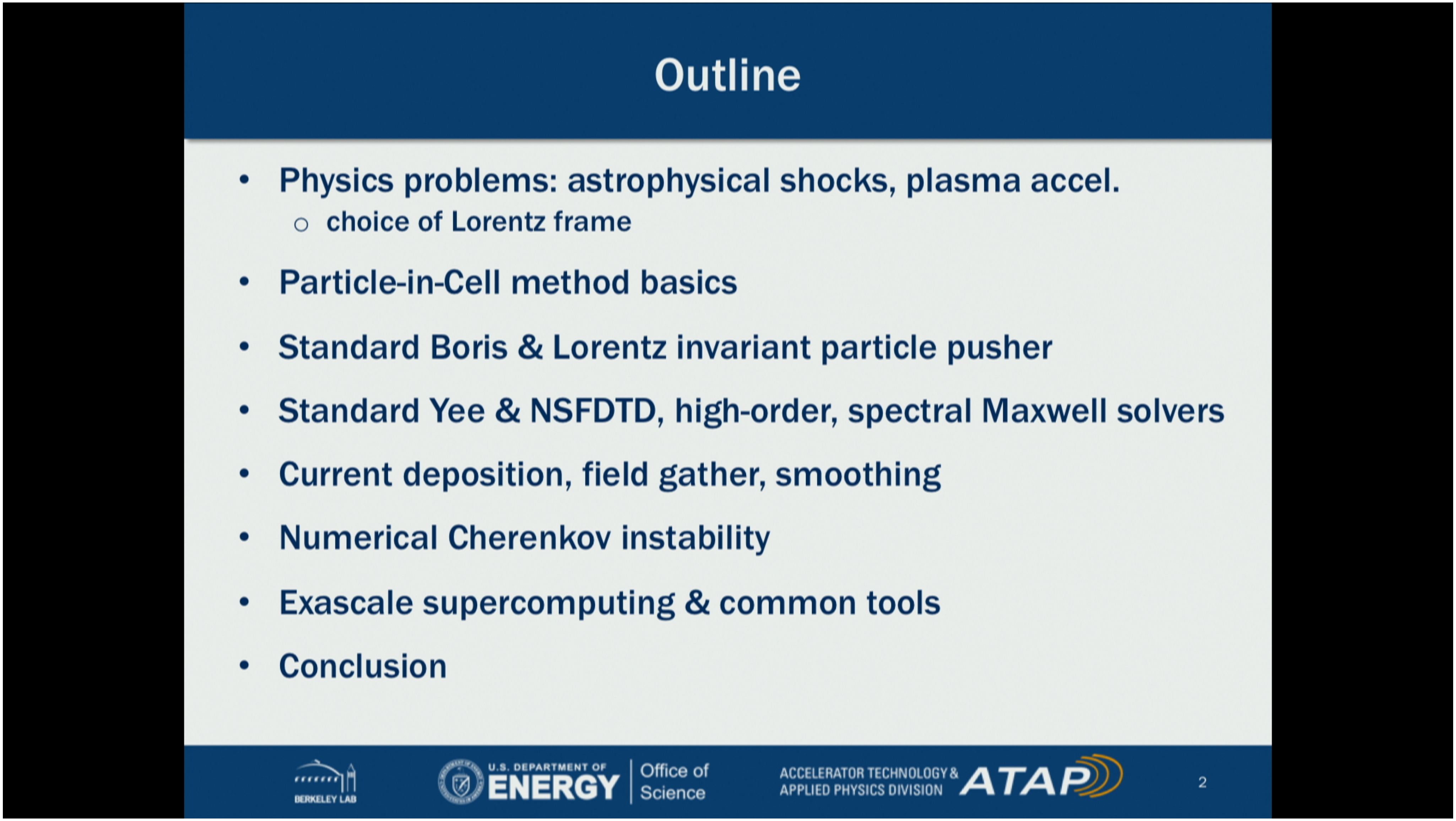
J.-L. Vay[1], R. Lehe[1], H. Vincenti[1,2], B. Godfrey[1,3], P. Lee[4], I. Haber[3],
C. Geddes[1], E. Esarey[1], C. Schroeder[1], W. Leemans[1]

[1]Lawrence Berkeley National Laboratory, California, USA
[2]Commissariat à l'Energie Atomique, Saclay, France
[3]University of Maryland, Maryland, USA
[4]University of Paris-Sud, Orsay, France

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP

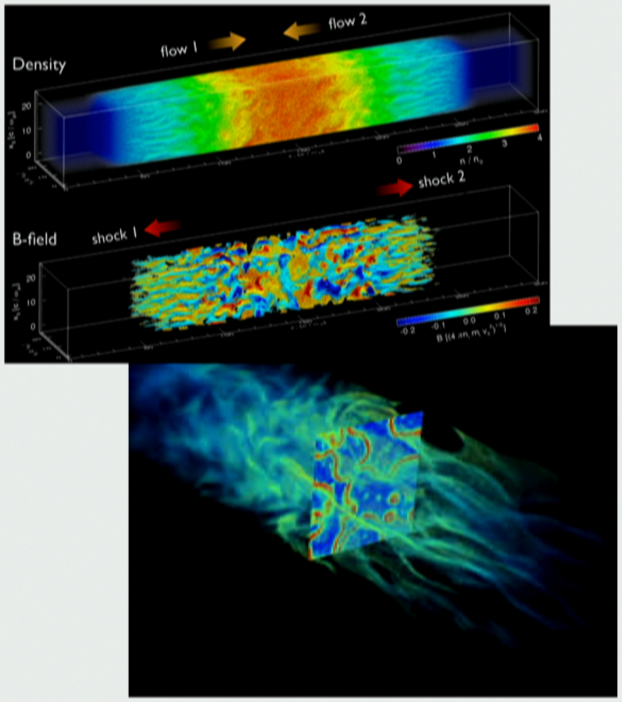


Outline

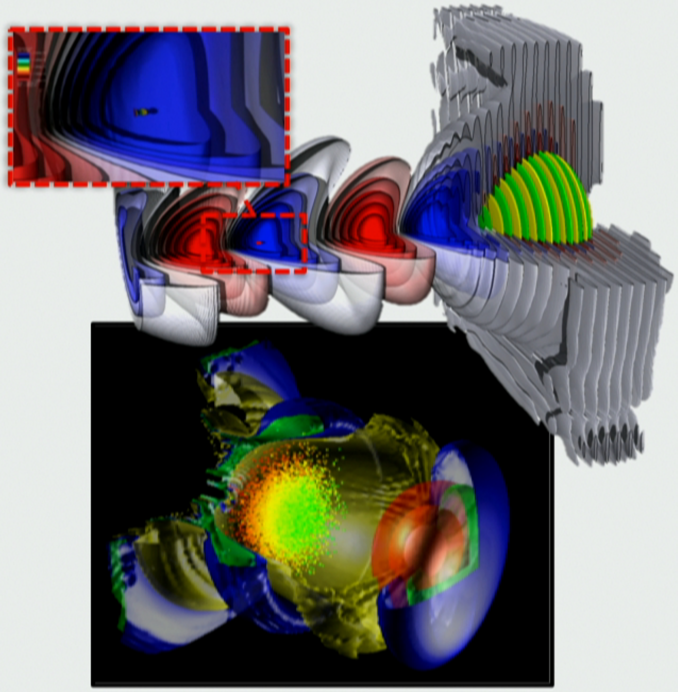
- Physics problems: astrophysical shocks, plasma accel.
    - choice of Lorentz frame
- Particle-in-Cell method basics
- Standard Boris & Lorentz invariant particle pusher
- Standard Yee & NSFDTD, high-order, spectral Maxwell solvers
- Current deposition, field gather, smoothing
- Numerical Cherenkov instability
- Exascale supercomputing & common tools
- Conclusion

Examples of relativistic plasmas

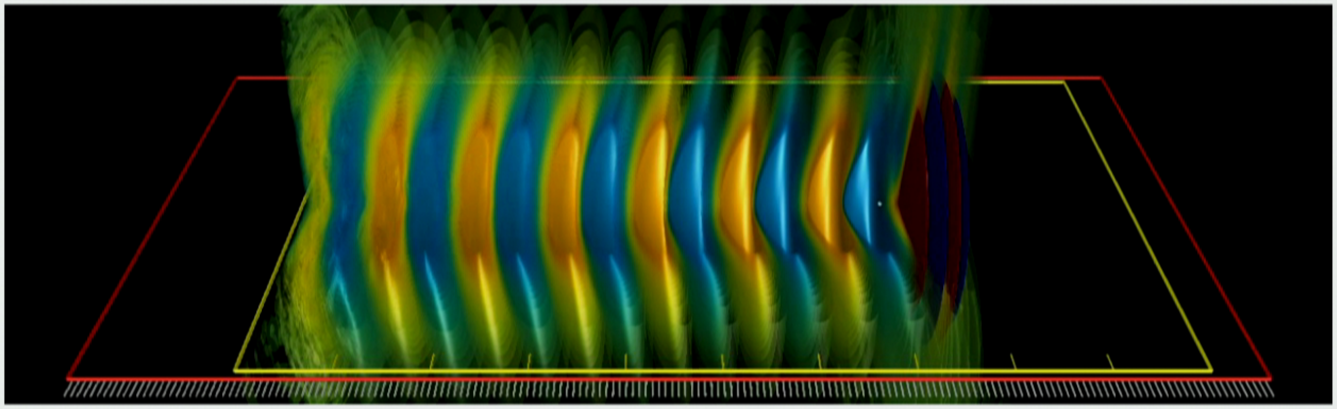
Astro shocks



Plasma-based accelerators



Modeling from first principle is very challenging

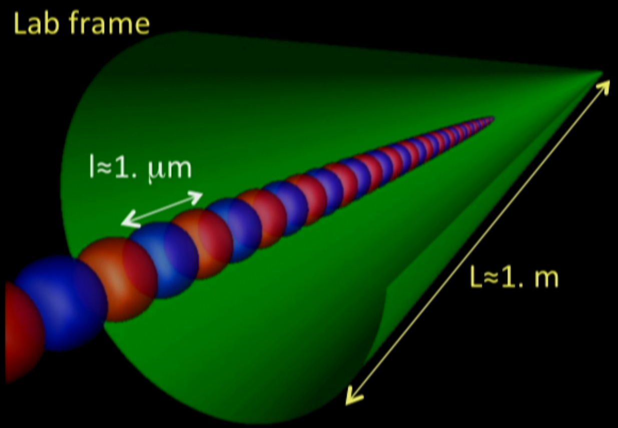


For a 10 GeV scale stage:

~1μm wavelength laser propagates into **~1m** plasma

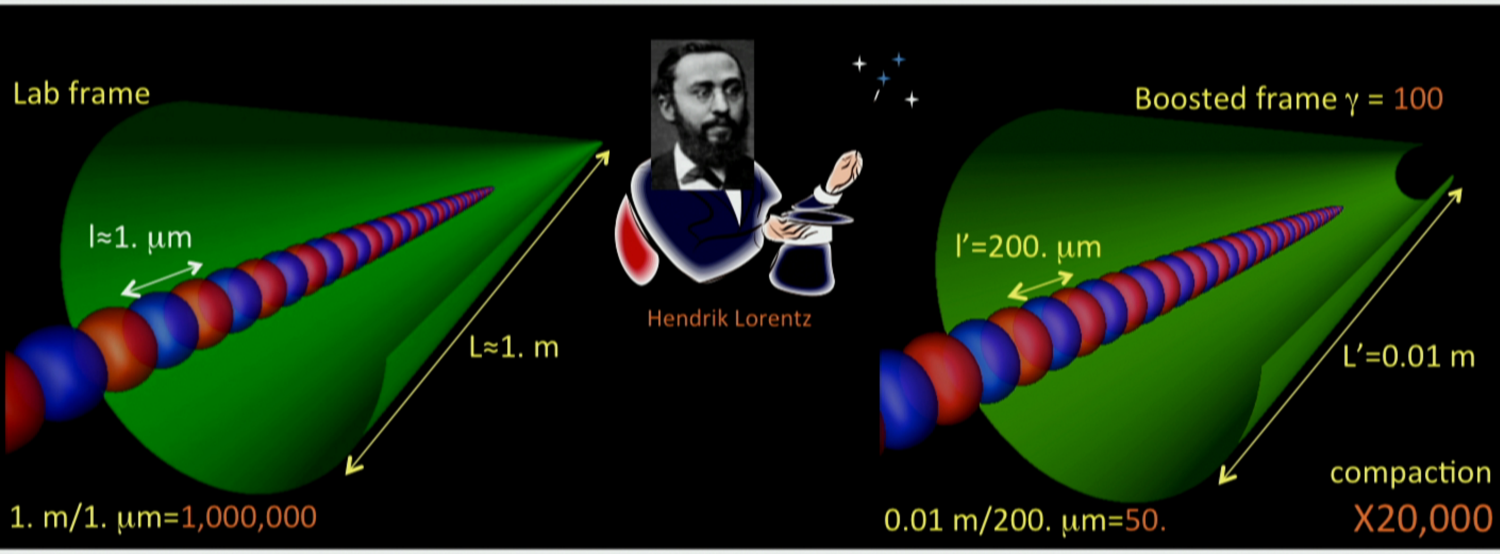
➔ millions of time steps needed

Solution: use frame moving close to speed of light*



1. m/1. µm=1,000,000

Solution: use frame moving close to speed of light*

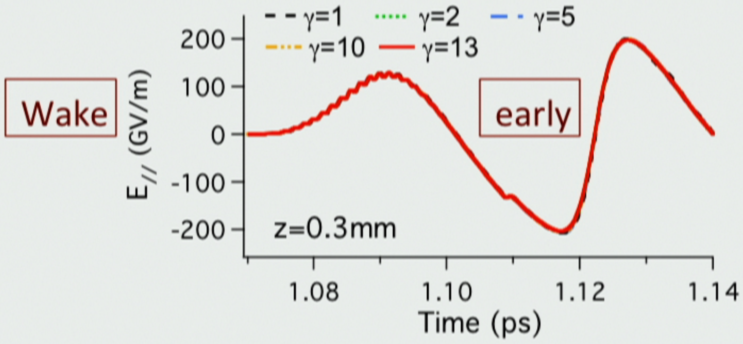


*J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)

LBF method carefully validated in deeply depleted beam loaded stages

-- Excellent agreement between runs at various γ boost

Warp-3D – a_0=1, n_0=10^{19}cm^{-3} (~100 MeV) scaled to 10^{17}cm^{-3} (~10 GeV)



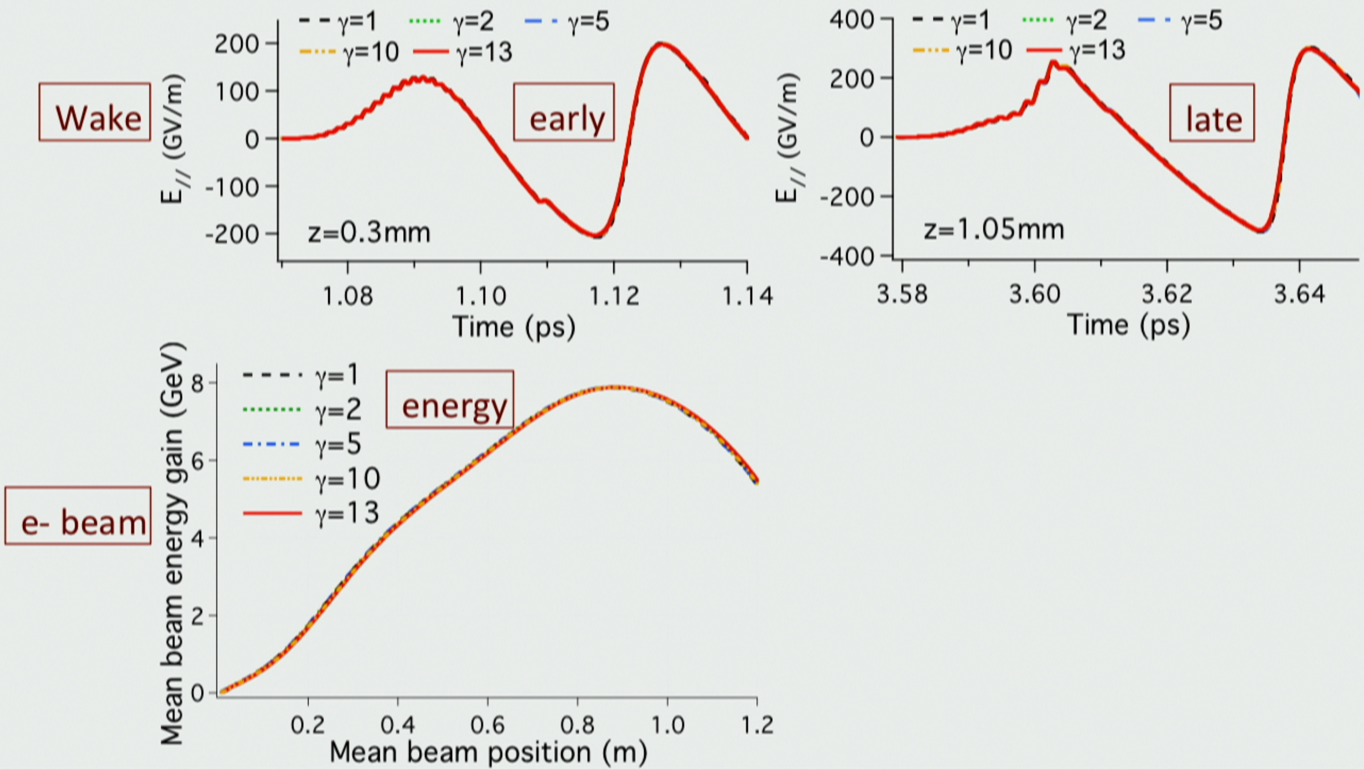
---

*J.-L. Vay, et al., *Phys. Plasmas* **18**, 123103 (2011)

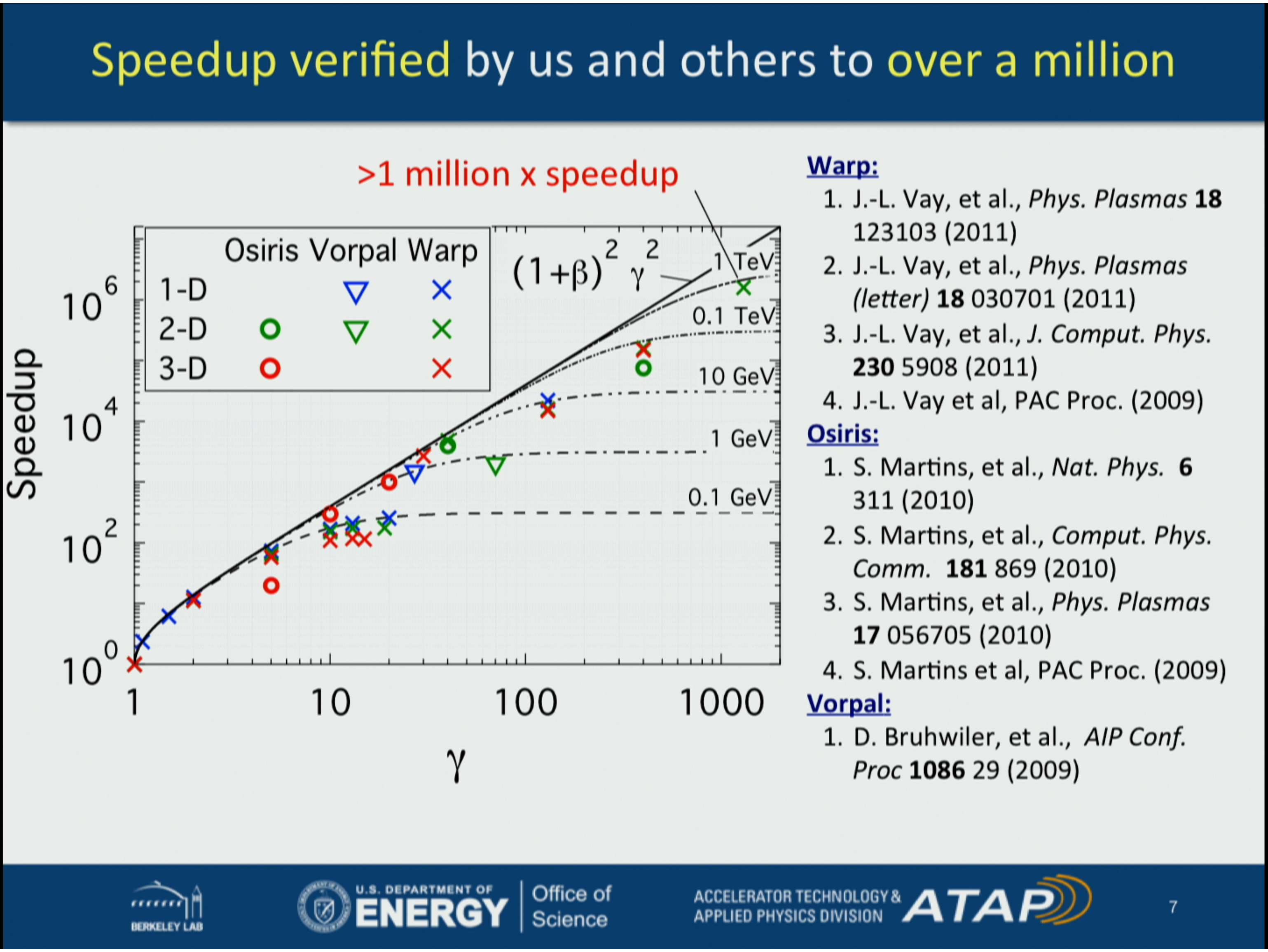
LBF method carefully validated in deeply depleted beam loaded stages

-- Excellent agreement between runs at various γ boost

Warp-3D – $a_0=1$, $n_0=10^{19}\text{cm}^{-3}$ (~100 MeV) scaled to 10^{17}cm^{-3} (~10 GeV)



*J.-L. Vay, et al., *Phys. Plasmas* **18**, 123103 (2011)



Speedup verified by us and others to over a million

>1 million x speedup

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:

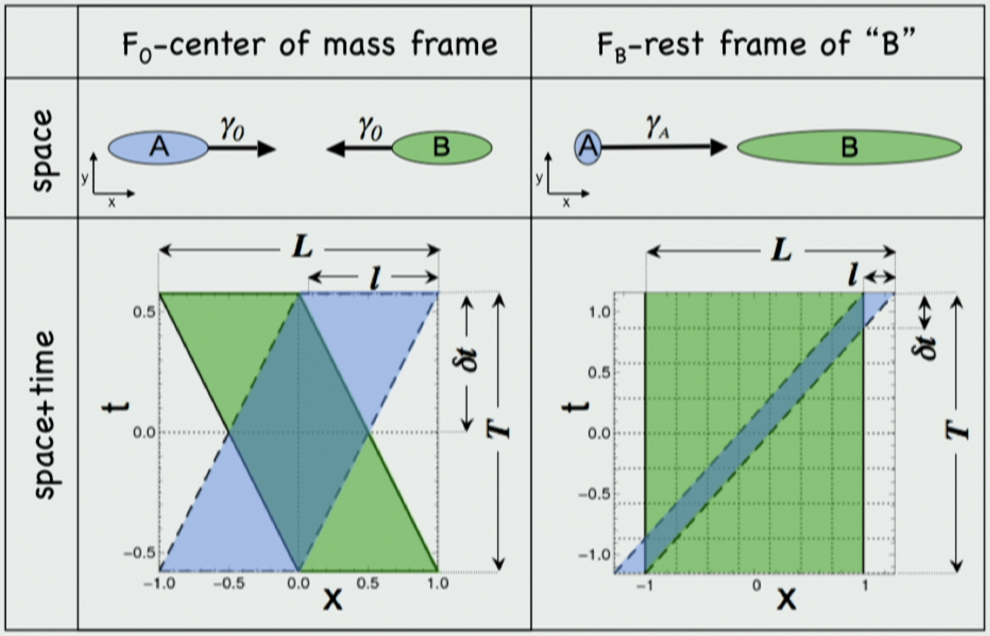
1. S. Martins, et al., *Nat. Phys.* **6** 311 (2010)
2. S. Martins, et al., *Comput. Phys. Comm.* **181** 869 (2010)
3. S. Martins, et al., *Phys. Plasmas* **17** 056705 (2010)
4. S. Martins et al, PAC Proc. (2009)

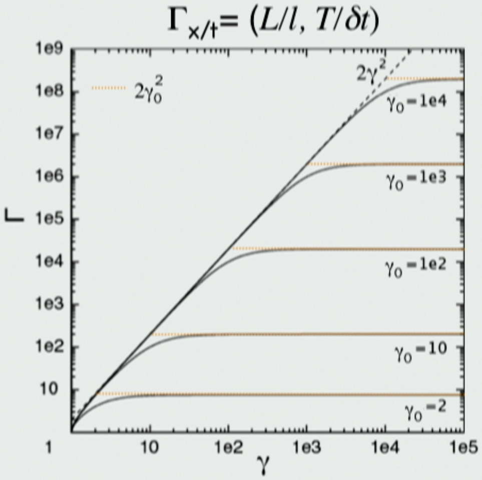
Vorpal:

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

Formulation is very general and applies to crossing relativistic objects

crossing of 2 relativistic objects



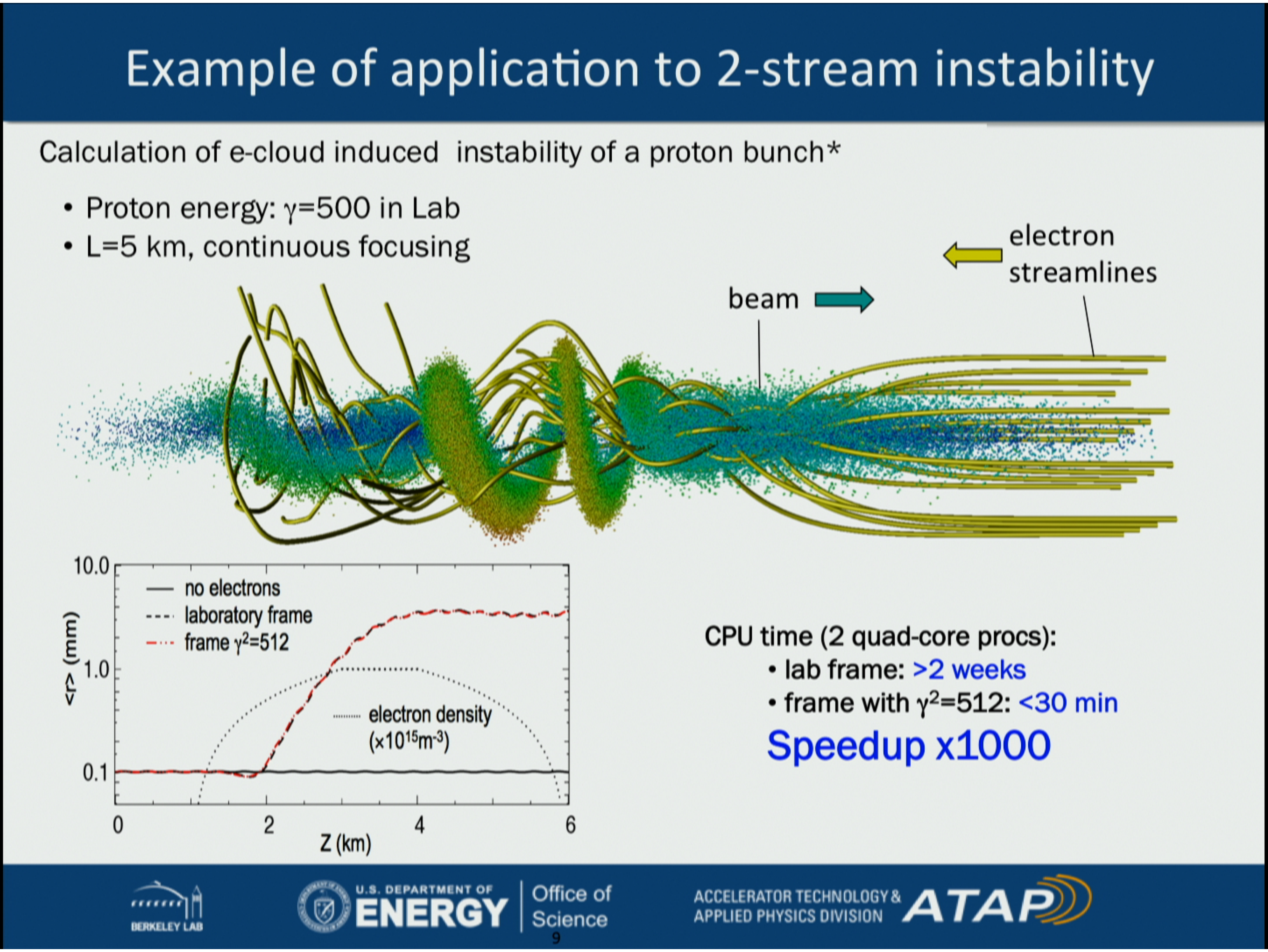


Γ is not invariant under a Lorentz transformation: $\Gamma_{x/t} \propto \gamma^2$.

γ^2 speedup demonstrated for 2-stream insta., plasma accelerators, FEL, ...

Can it apply to 2-stream insta of relevance to blazar studies?

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



Example of application to 2-stream instability

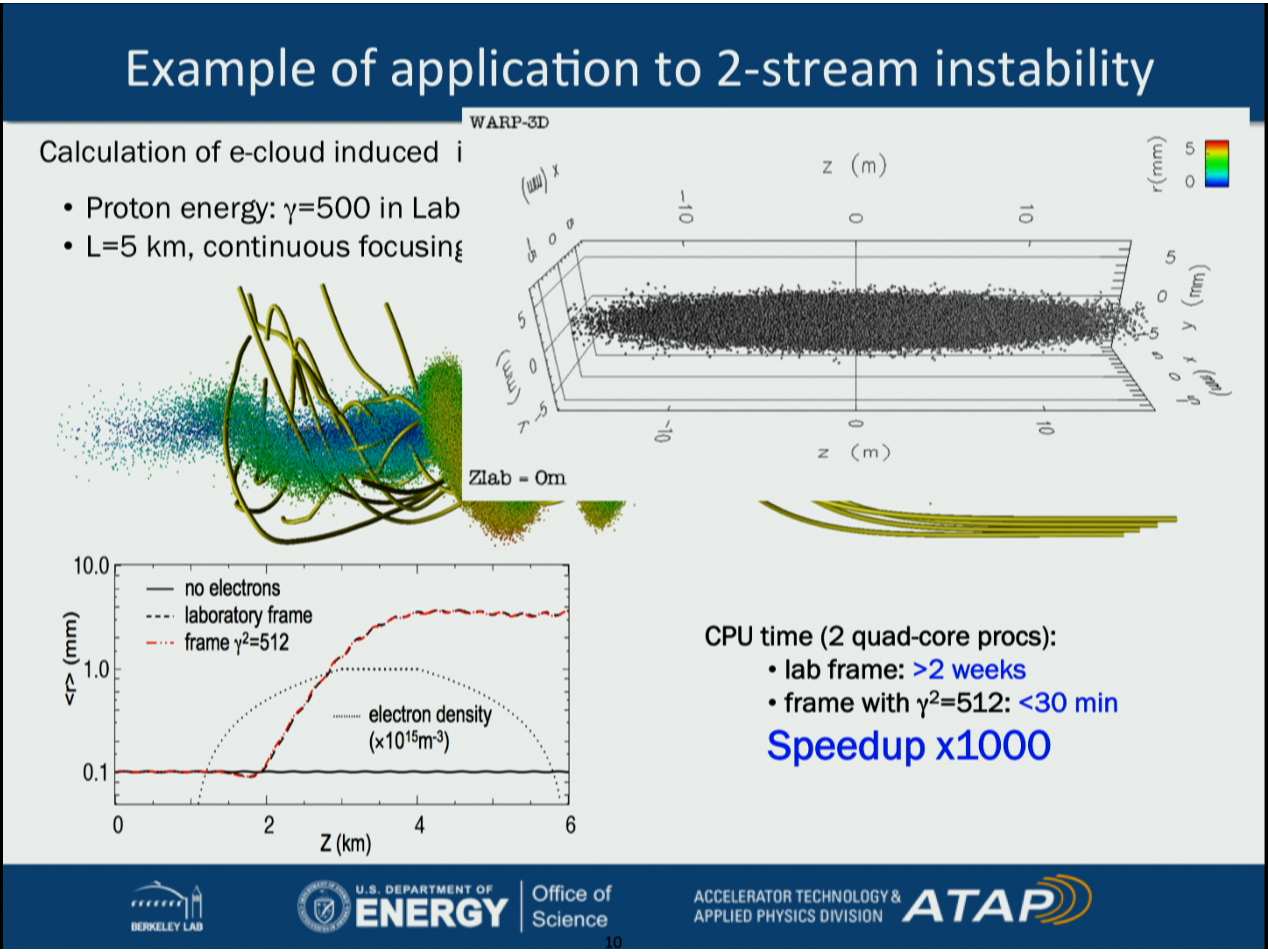
Calculation of e-cloud induced instability of a proton bunch*

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

CPU time (2 quad-core procs):
- lab frame: >2 weeks
- frame with γ^2=512: <30 min

Speedup x1000

Example of application to 2-stream instability



Calculation of e-cloud induced i

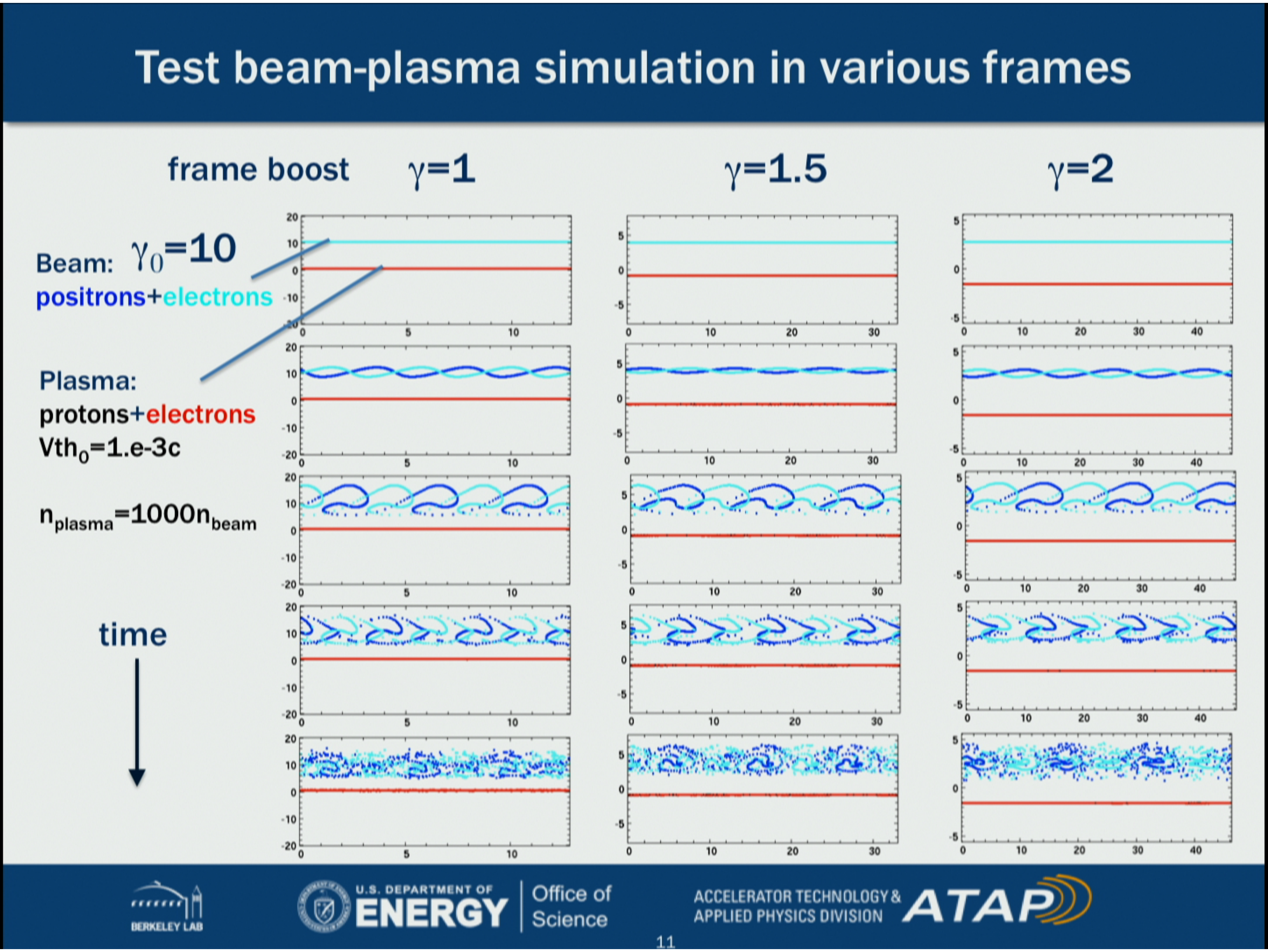
- Proton energy: γ=500 in Lab
- L=5 km, continuous focusin

CPU time (2 quad-core procs):

- lab frame: >2 weeks
- frame with γ^2=512: <30 min

Speedup x1000

Test beam-plasma simulation in various frames



Beam: γ_0=10

positrons+electrons

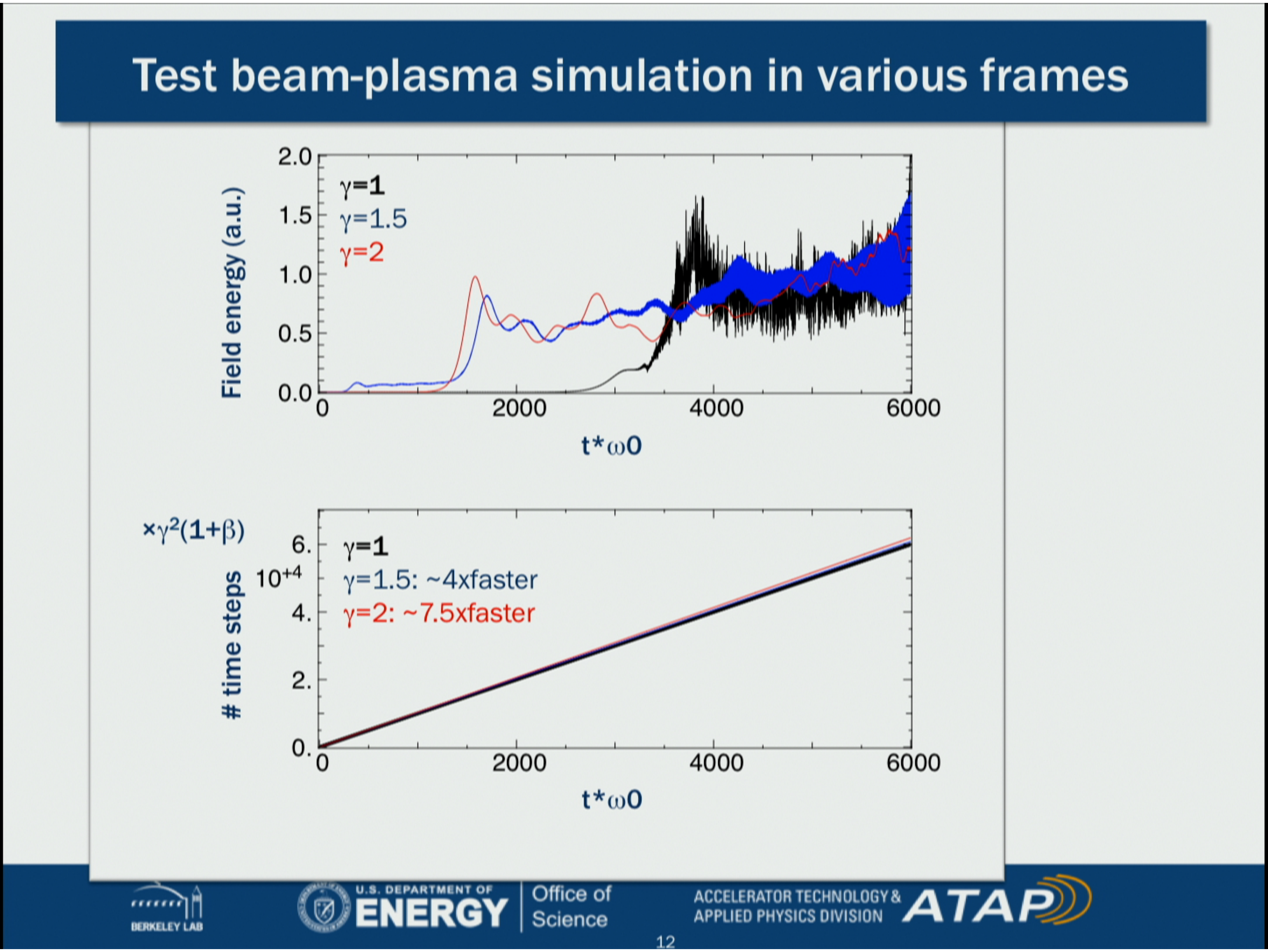
Plasma:

protons+electrons

Vth$_0$=1.e-3c

n$_{plasma}$=1000n$_{beam}$

time



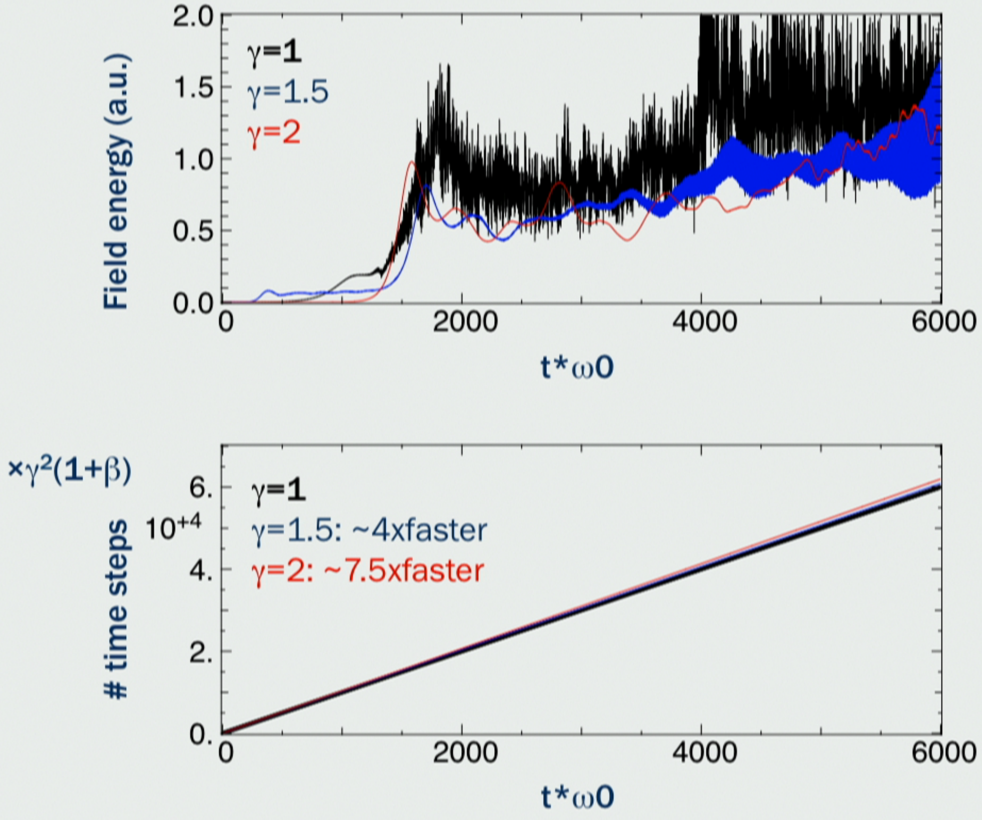
Test beam-plasma simulation in various frames

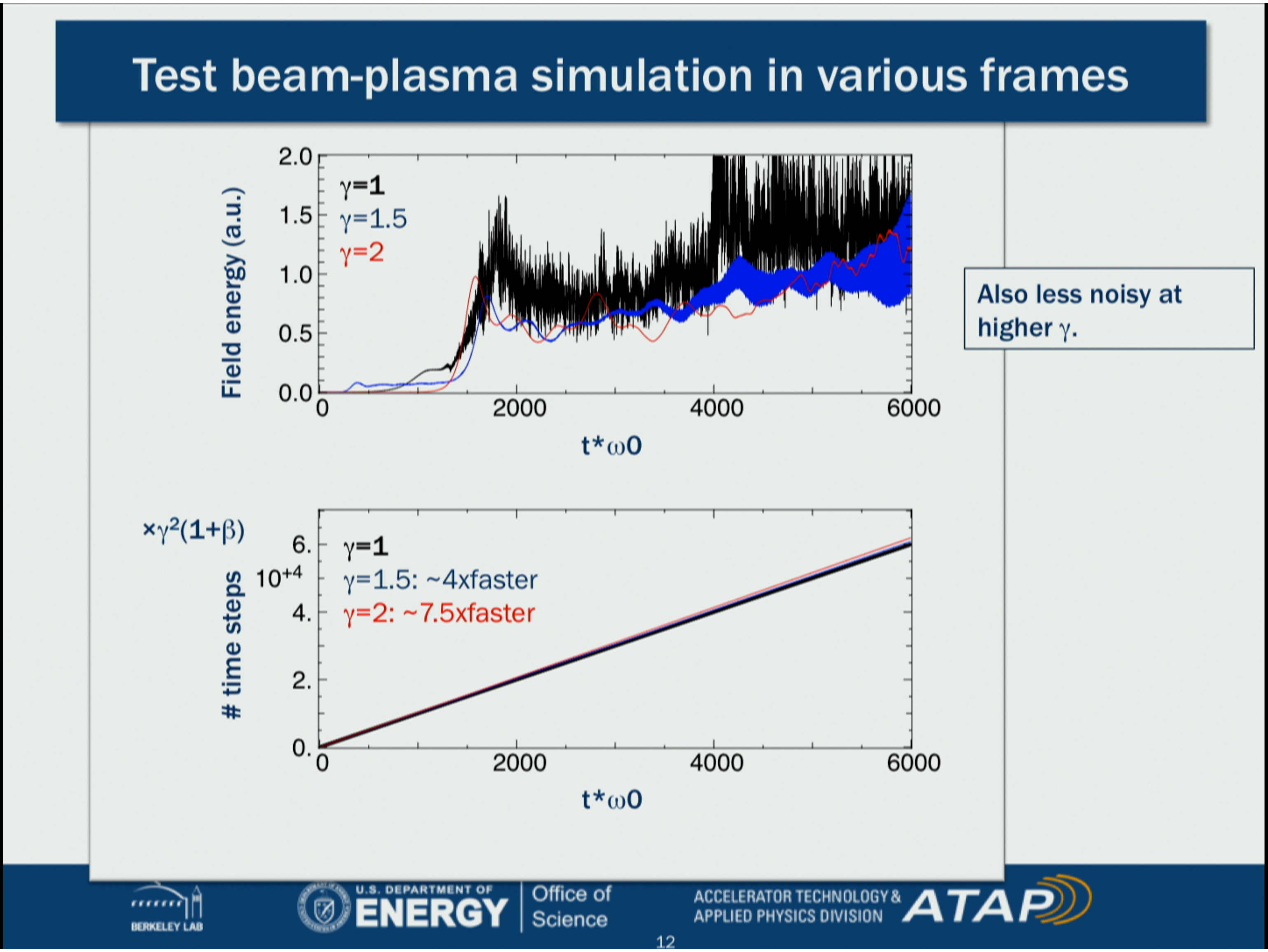
BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP

Test beam-plasma simulation in various frames



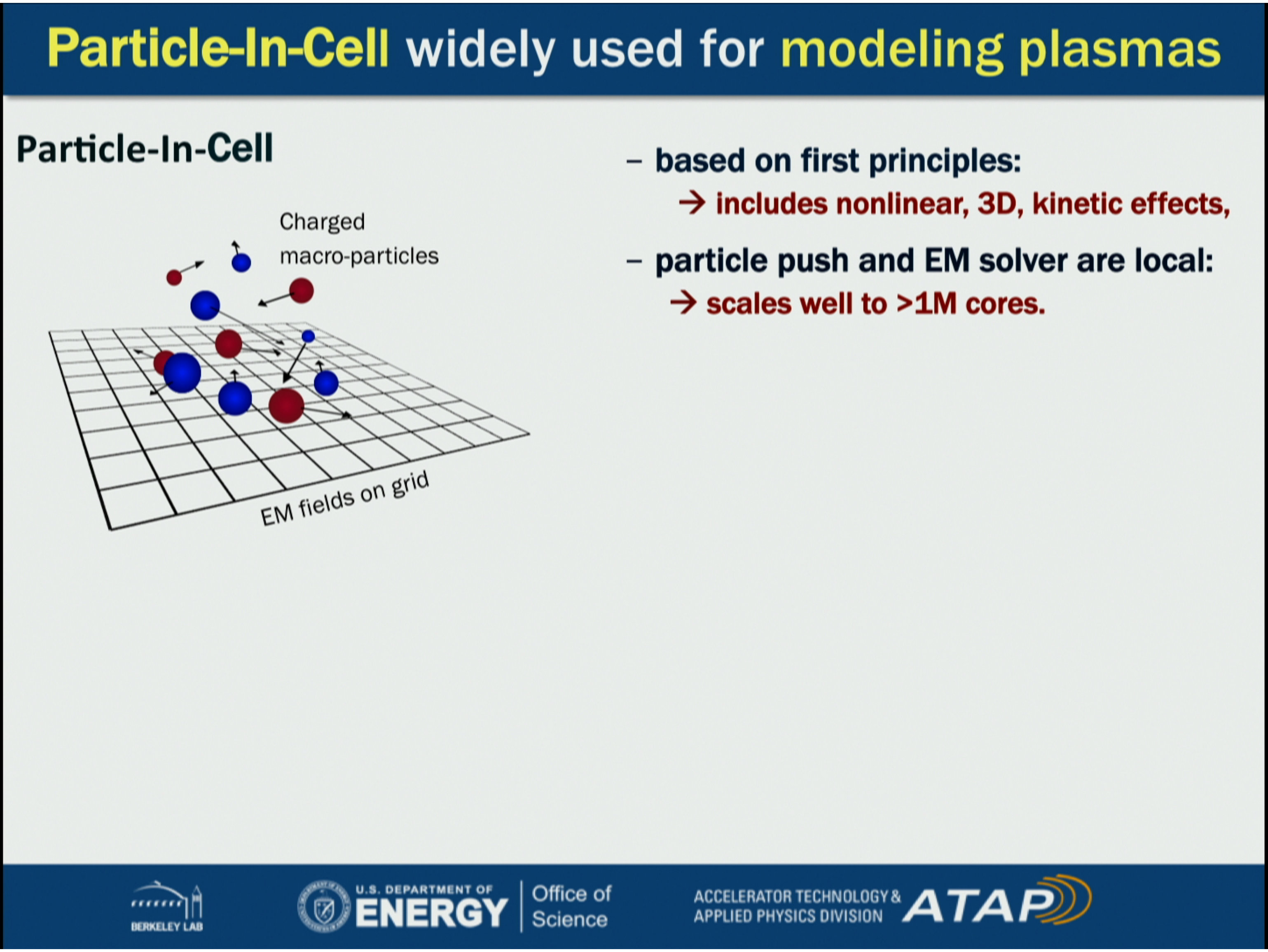


Test beam-plasma simulation in various frames

Also less noisy at higher γ.

Outline

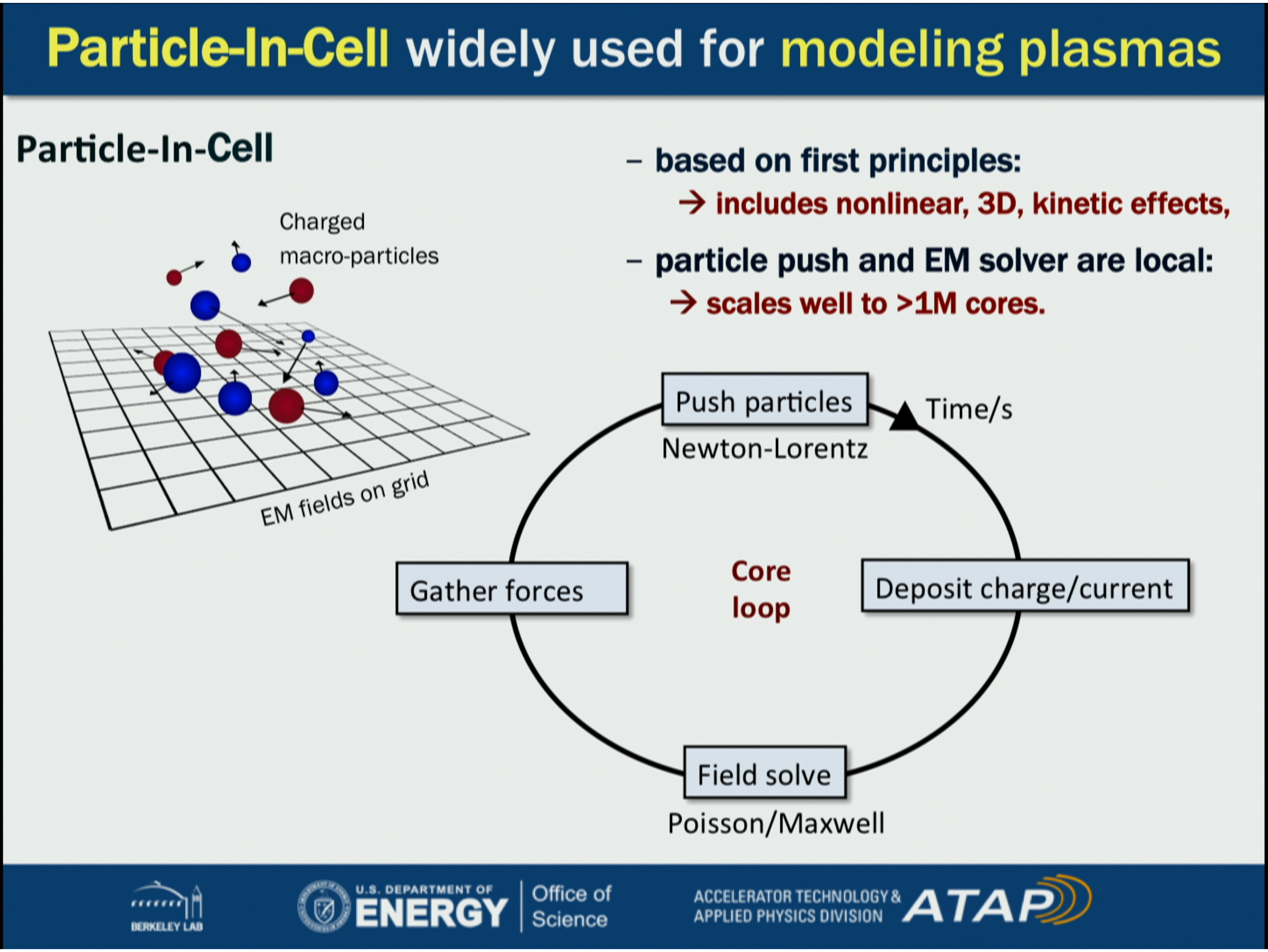
- Physics problems: astrophysical shocks, plasma accel.
    - choice of Lorentz frame for modeling of plasma accelerators
- Particle-in-Cell method basics
- Standard Boris & Lorentz invariant particle pusher
- Standard Yee & NSFDTD, high-order, spectral Maxwell solvers
- Numerical Cherenkov instability
- Conclusion



Particle-In-Cell widely used for **modeling plasmas**

Particle-In-Cell

- **based on first principles:**
  - **→ includes nonlinear, 3D, kinetic effects,**
- **particle push and EM solver are local:**
  - **→ scales well to >1M cores.**



Particle-In-Cell widely used for modeling plasmas

Particle-In-Cell

Charged macro-particles

EM fields on grid

- **based on first principles:**
  - **→ includes nonlinear, 3D, kinetic effects,**
- **particle push and EM solver are local:**
  - **→ scales well to >1M cores.**

Push particles
Newton-Lorentz

Time/s

Deposit charge/current

Field solve
Poisson/Maxwell

Gather forces

Core loop

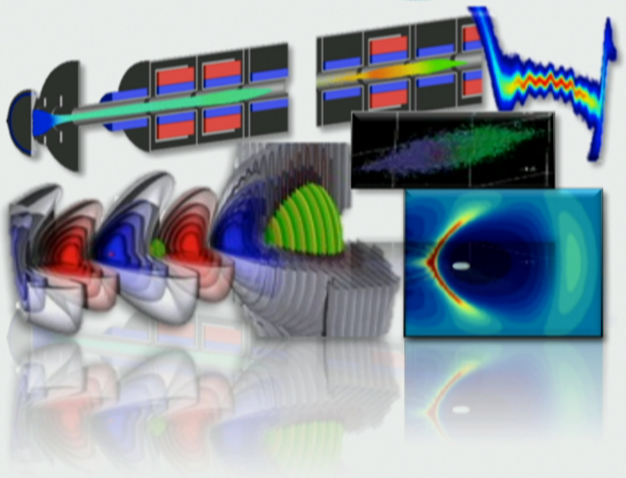
BERKELEY LAB   U.S. DEPARTMENT OF ENERGY | Office of Science   ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP

Berkeley Lab Accelerator Simulation Toolkit
Warp – open source PIC+accelerator framework

http://blast.lbl.gov

BLAST

BERKELEY LAB ACCELERATOR SIMULATION TOOLKIT



Warp

- 3-D, Circ, RZ, 2-D on structured meshes
- ***Ref. frames*** – lab, window, boost
- ***Poisson/Ampere*** – FFT, multigrid; AMR; implicit; arbitrary conductors (cut-cell)
- ***Maxwell*** – Yee mesh/node centered, arbitrary order, Yee/CK/Lehe, pseudo-spectral, PML, MR, arbitrary conductors/dielectric (grid-cell)
- ***Particle pushers*** – *Boris/Cohen/Vay/Maps*
- ***Accelerator*** – dipoles, quads, sextupoles, solenoids, acceleration gaps, arbitrary fields (gridded/functions), linear maps, ...
- ***Emission*** – particles: space charge limited, thermionic, prescribed, secondary; laser
- ***Monte Carlo collisions*** – ionization, capture, charge exchange
- ***Programming*** – *Python+FORTRAN, parallel MPI*

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP

Particle pusher

Boris pusher is most widely used

- Boris pusher: leapfrog second order in time
  - ○ Position push: $x^{n+1/2} = x^{n-1/2} + v^n \Delta t$
  - ○ Velocity push: $u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \frac{u^{n+1} + u^n}{2\gamma^{n+1/2}} \times B^{n+1/2}\right)$ $\qquad u = \gamma v$

Solved as follows:

$$u^- = u^n + \frac{\Delta t}{2}\frac{q}{m}E^{n+1/2}$$

← 1/2 electric field push

$$u^+ = u^- + \frac{q\Delta t}{m}\left(\frac{u^+ + u^-}{2\gamma^{n+1/2}} \times B^{n+1/2}\right)$$

← 1 magnetic field rotation

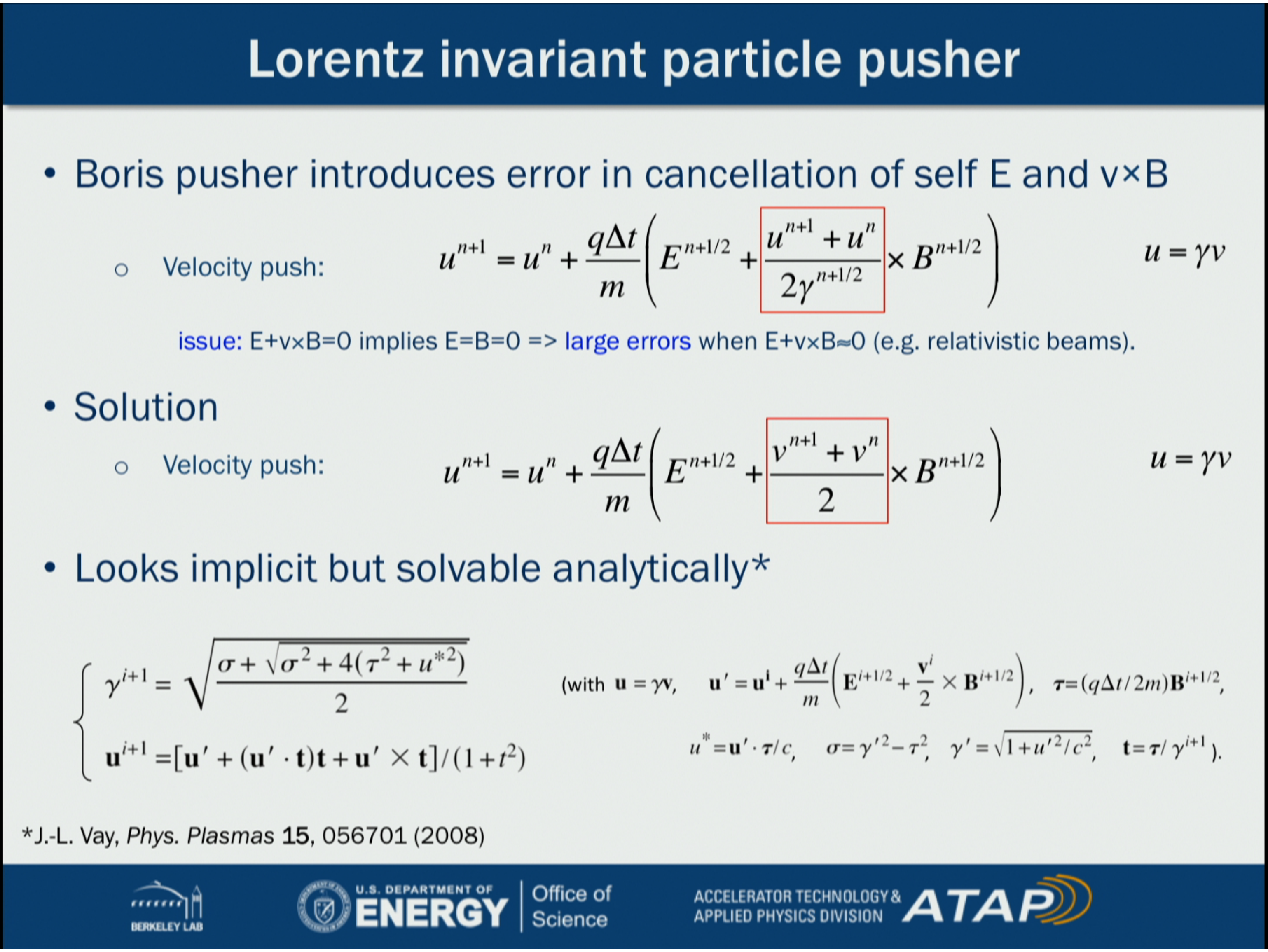
$$u^{n+1} = u^+ + \frac{\Delta t}{2}\frac{q}{m}E^{n+1/2}$$

← 1/2 electric field push

*J. P. Boris, *Proc. Fourth Conf. on Num. Sim. Plasmas* 3-67 (1970)

Recent developments in particle pusher

Problem with Boris pusher: not Lorentz invariant



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

- Looks implicit but solvable analytically*

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

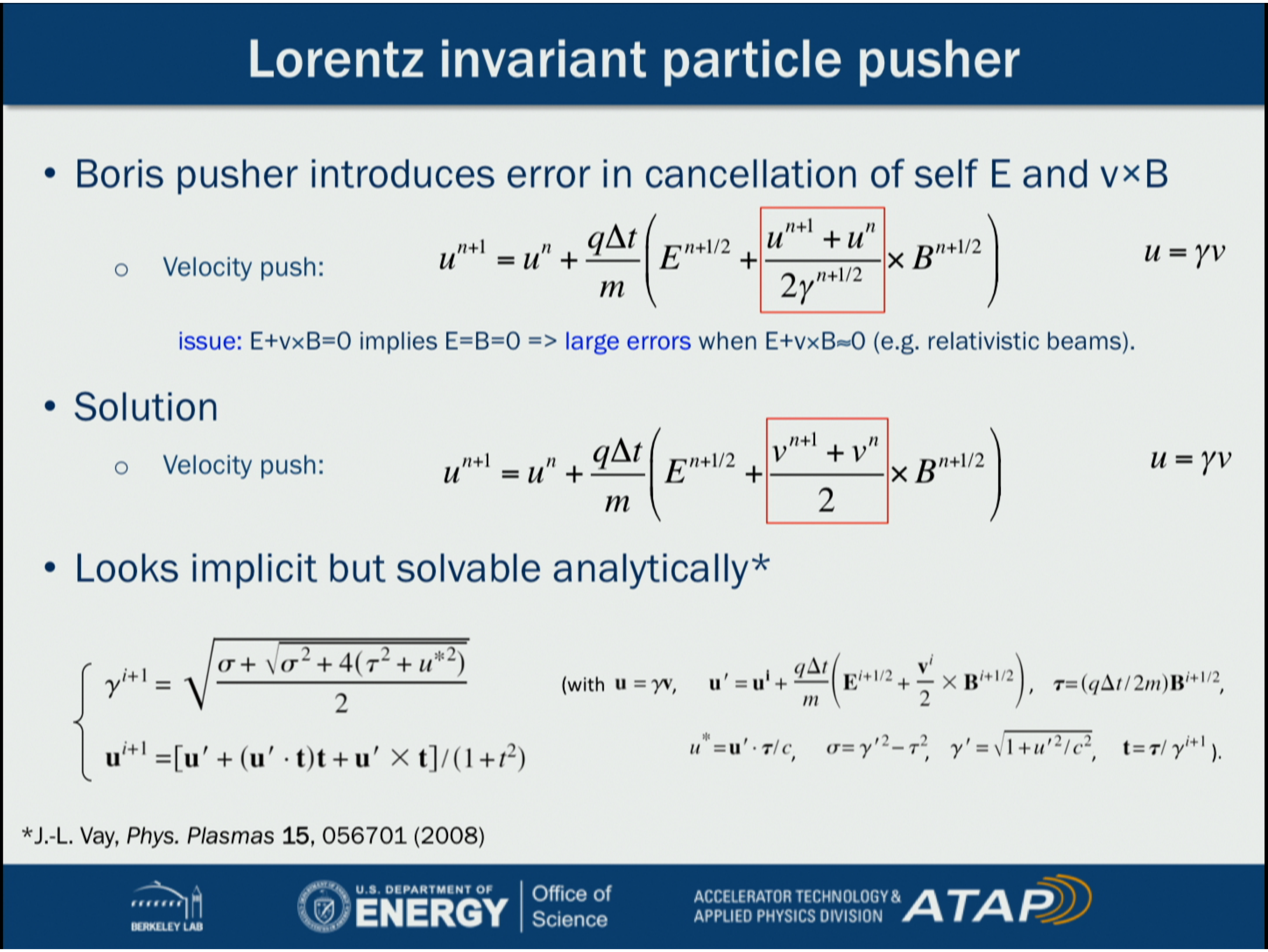
(with $\mathbf{u} = \gamma\mathbf{v}$, $\mathbf{u}' = \mathbf{u}^i + \frac{q\Delta t}{m}\left(\mathbf{E}^{i+1/2} + \frac{\mathbf{v}^i}{2} \times \mathbf{B}^{i+1/2}\right)$, $\boldsymbol{\tau} = (q\Delta t/2m)\mathbf{B}^{i+1/2}$, $u^* = \mathbf{u}' \cdot \boldsymbol{\tau}/c$, $\sigma = \gamma'^2 - \tau^2$,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

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

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP



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

BERKELEY LAB

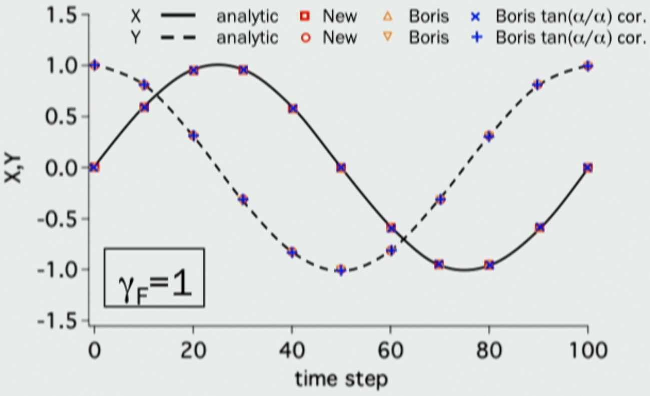
U.S. DEPARTMENT OF ENERGY | Office of Science

ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP

Single particle test of Lorentz invariant pusher

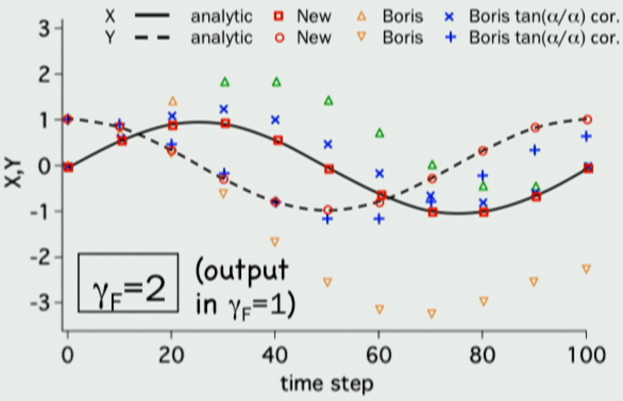
Lab frame

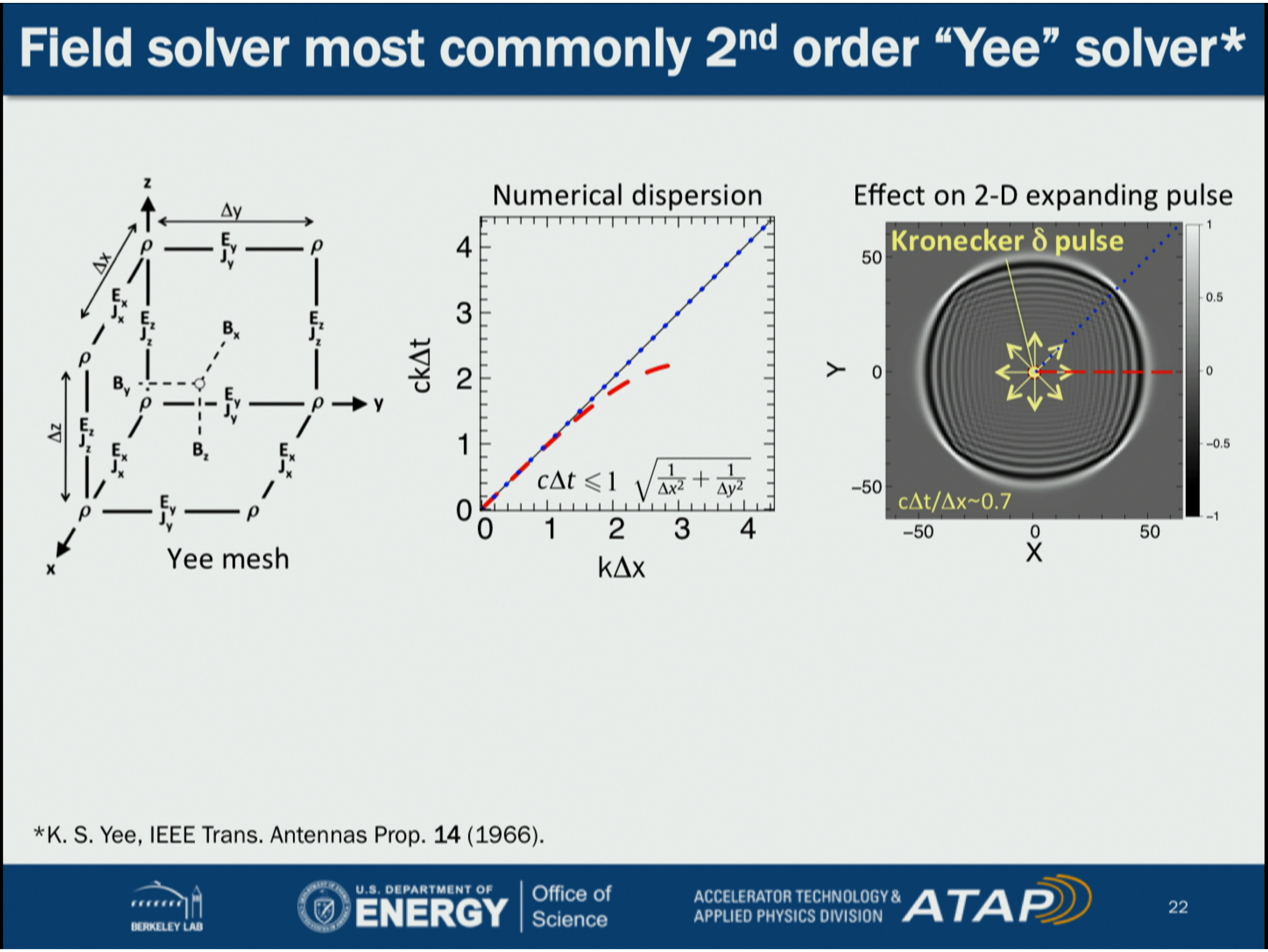
particle cycling in constant B field



Boosted frame γ=2

ExB drift adds to gyration



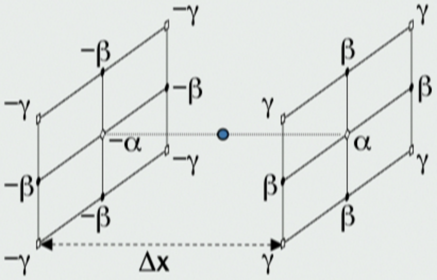


Field solver most commonly 2nd order "Yee" solver*

*K. S. Yee, IEEE Trans. Antennas Prop. **14** (1966).

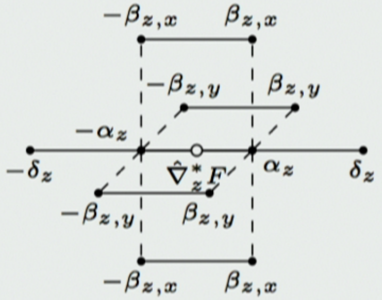
Non-Standard FD solvers offer some tunability

NSFD[1,2]: weighted average of quantities transverse to FD

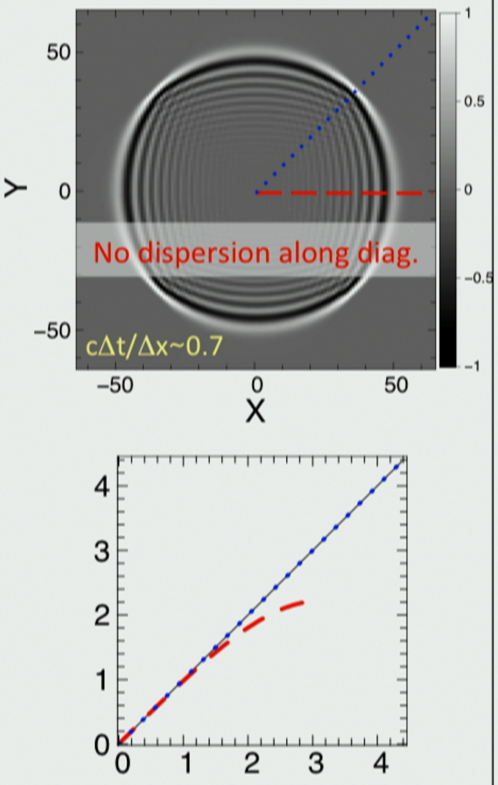


- Adaptations to PIC[3,4,5]

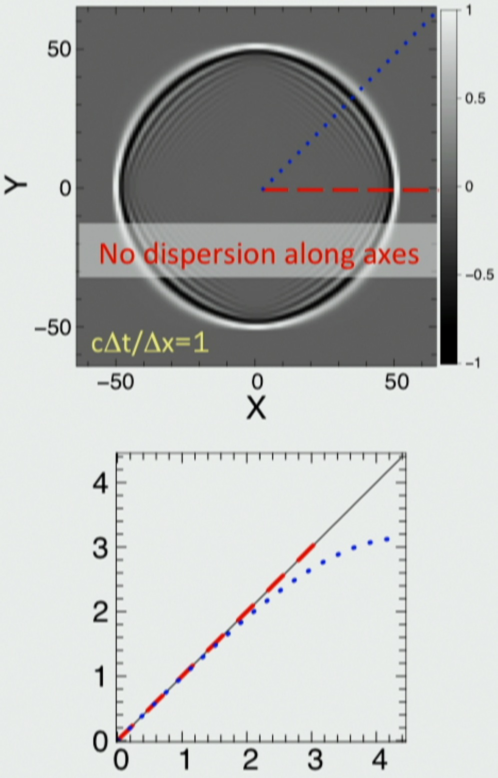
Lehe[6] algorithm:



FDTD (Yee)

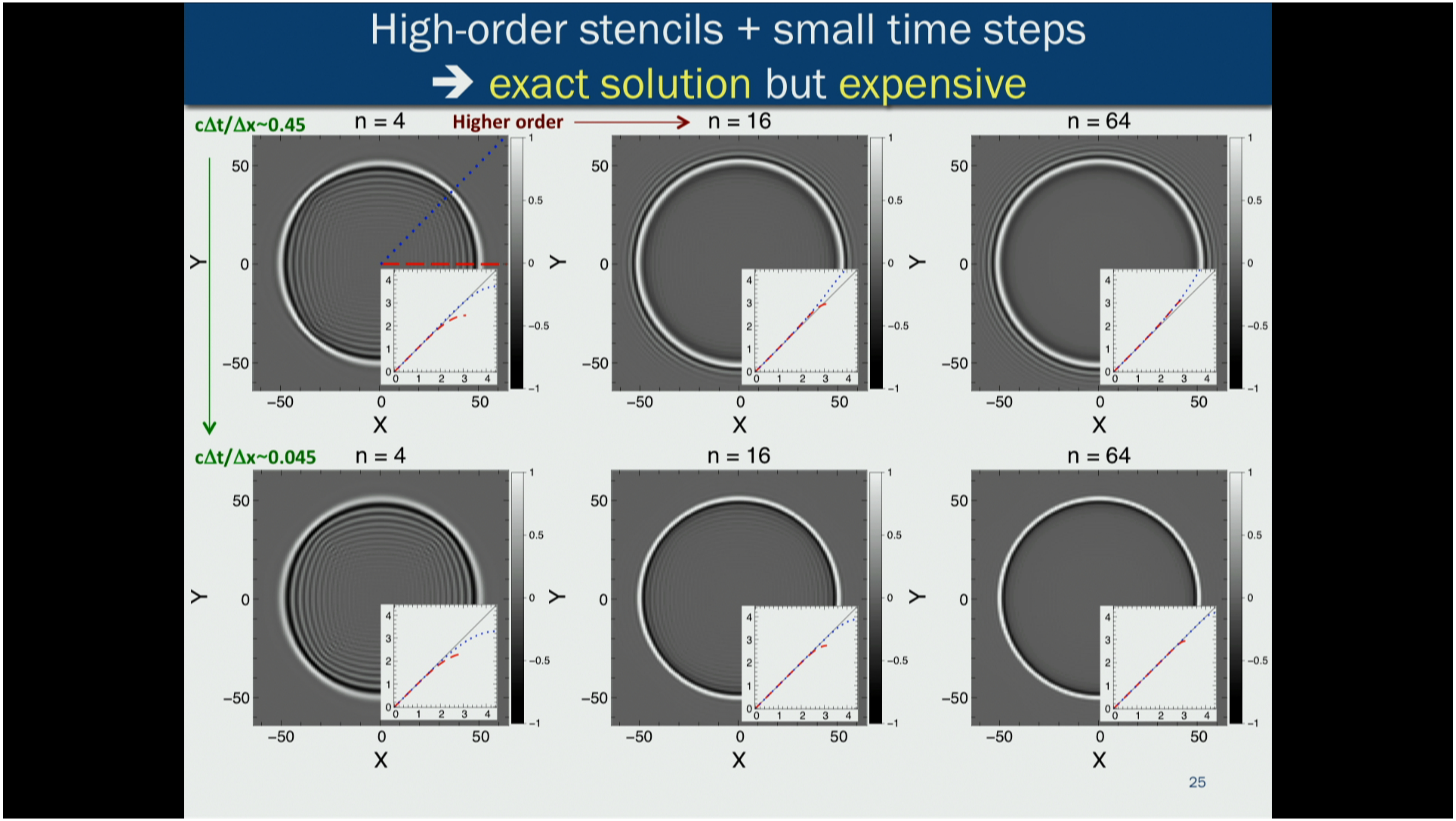


NS-FDTD (Karkkainen/Lehe)



---

[1] J. B. Cole, IEEE Trans. Microw. Theory Tech. **45** (1997).
[2] M. Karkkainen et al., Proc. ICAP, Chamonix, France (2006).
[3] A. Pukhov, J. Plasma Physics **61** (1999) 425.
[4] J.-L. Vay et al, J. Comput. Phys. **230** (2011) 5908.
[5] B. Cowan et al, PRST-AB **16** (2013) 041303.
[6] R. Lehe et al, PRST-AB **16** (2013) 021301.



High-order stencils + small time steps

→ exact solution but expensive

Spectral solver offers "infinite order" but still needs small time steps

Finite-Difference Time-Domain (FDTD)

Pseudo-Spectral Time-Domain (PSTD)

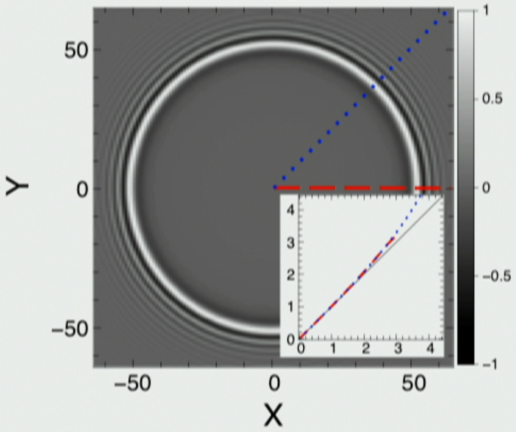
$\mathcal{F}$=FFT

$$B_z^{n+1} = B_z^n + \Delta t\left(\frac{\Delta E_x}{\Delta y} - \frac{\Delta E_y}{\Delta x}\right)$$

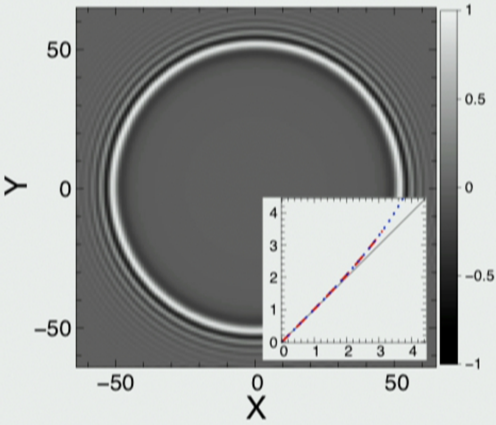
$$B_z^{n+1} = B_z^n + \Delta t\left[\mathcal{F}^{-1}\left(ik_y\,\mathcal{F}(E_x)\right) - \mathcal{F}^{-1}\left(ik_x\,\mathcal{F}(E_y)\right)\right]$$

FDTD cΔt/Δx~0.45

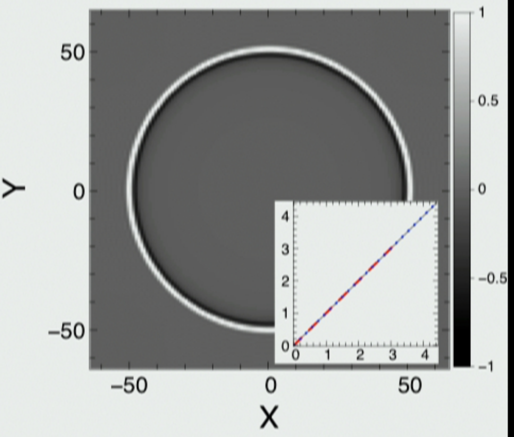
n = 64



PSTD cΔt/Δx~0.45



PSTD cΔt/Δx~0.045



PSTD is limit of high-order FDTD when n→infinity.

PSTD converges to exact solution (on grid) for Δt→0.

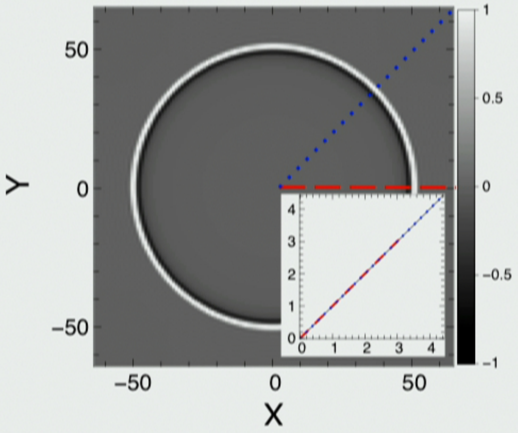
Analytical pseudo-spectral solver offers exact solution with no Courant condition

Pseudo-Spectral Analytical Time-Domain[1] (PSATD)

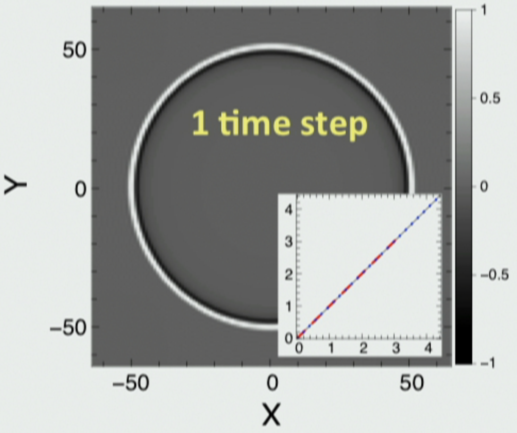
$$B_z^{n+1} = \mathcal{F}^{-1}\left(C\mathcal{F}\left(B_z^n\right)\right) + \mathcal{F}^{-1}\left(iSk_y\mathcal{F}\left(E_x\right)\right) - \mathcal{F}^{-1}\left(iSk_x\mathcal{F}\left(E_y\right)\right)$$

with $C = \cos\left(kc\Delta t\right);\quad S = \sin\left(kc\Delta t\right);\quad k = \sqrt{k_x^2 + k_y^2}$

PSTD cΔt/Δx~0.045

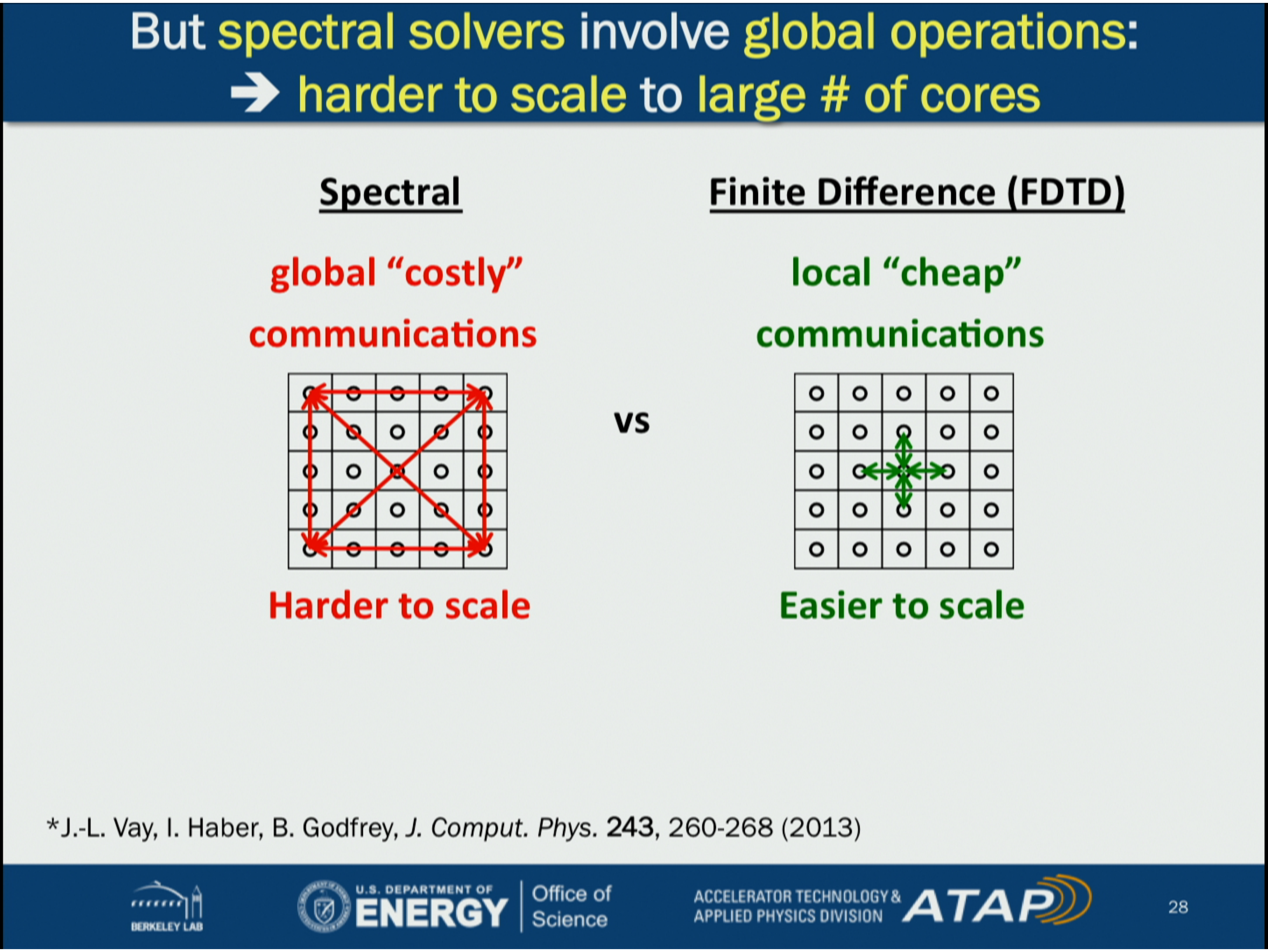


PSATD cΔt/Δx=50



---

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



But spectral solvers involve global operations:
➔ harder to scale to large # of cores

Spectral

global "costly"

communications

Harder to scale

vs

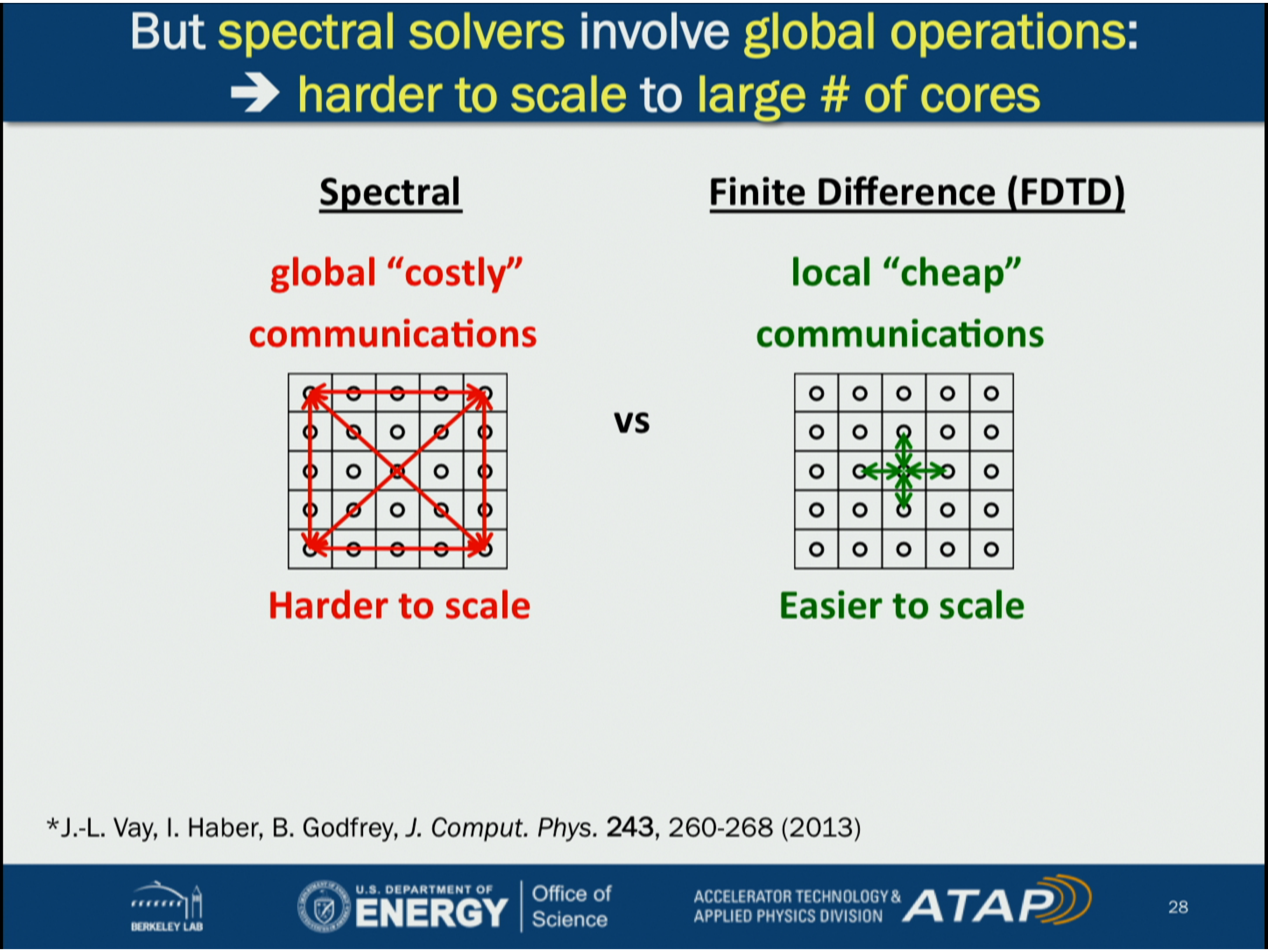
Finite Difference (FDTD)

local "cheap"

communications

Easier to scale

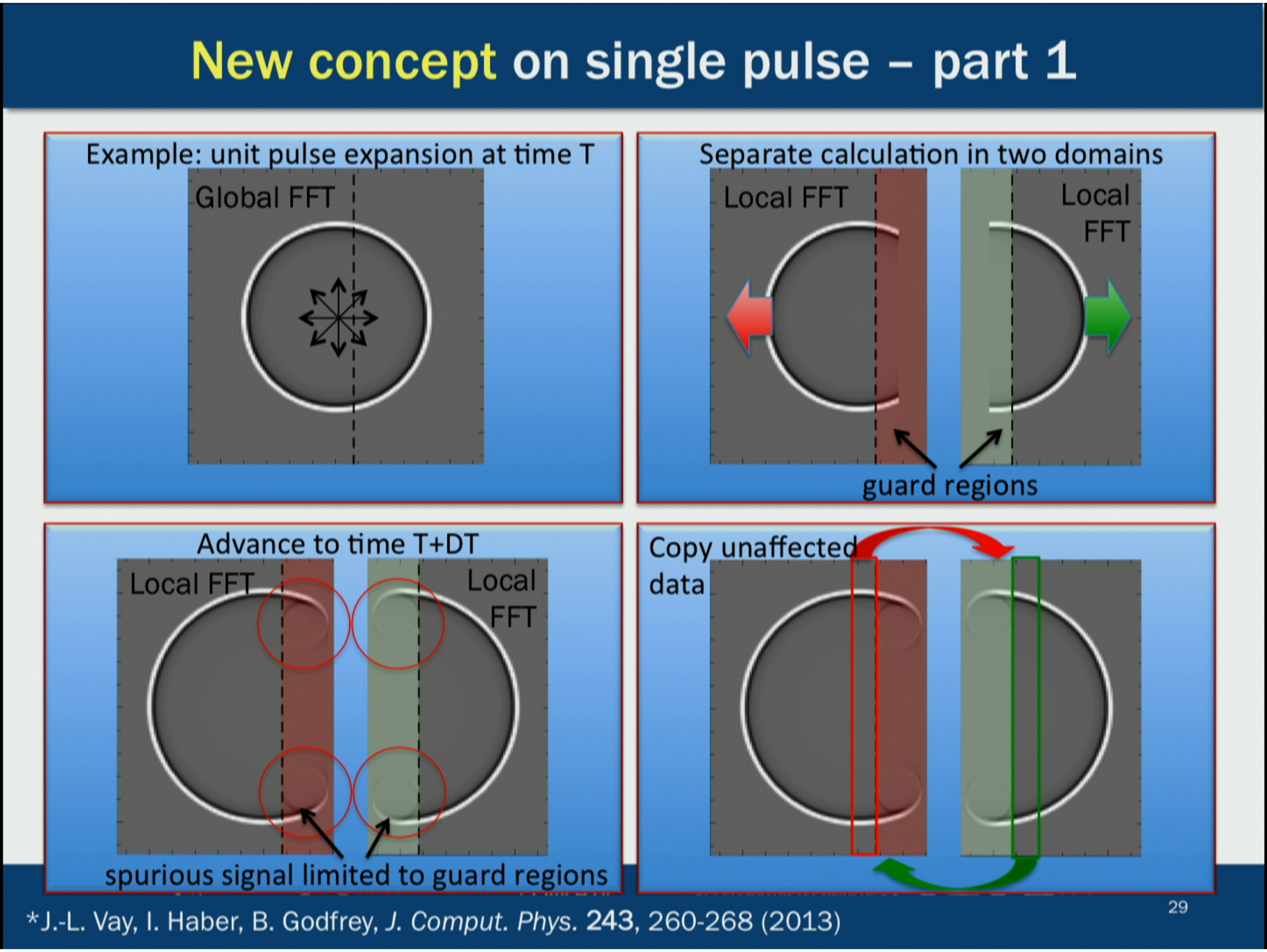
*J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)



But spectral solvers involve global operations: ➔ harder to scale to large # of cores

Spectral		**Finite Difference (FDTD)**
global “costly” communications	vs	local “cheap” communications
Harder to scale		Easier to scale

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



New concept on single pulse – part 1

Example: unit pulse expansion at time T

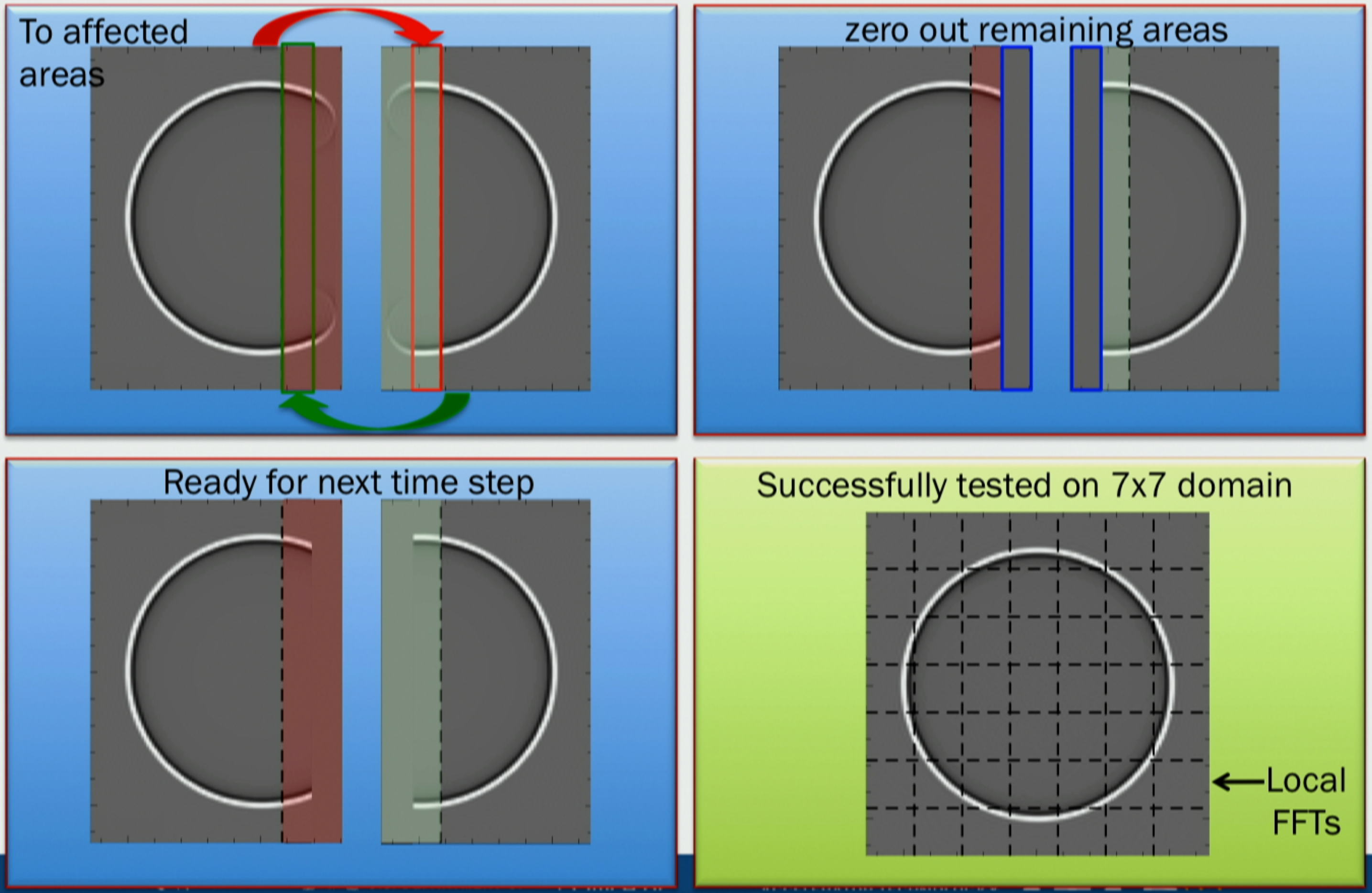
Separate calculation in two domains

Advance to time T+DT

Copy unaffected data

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

New concept on single pulse – part 2



To affected areas

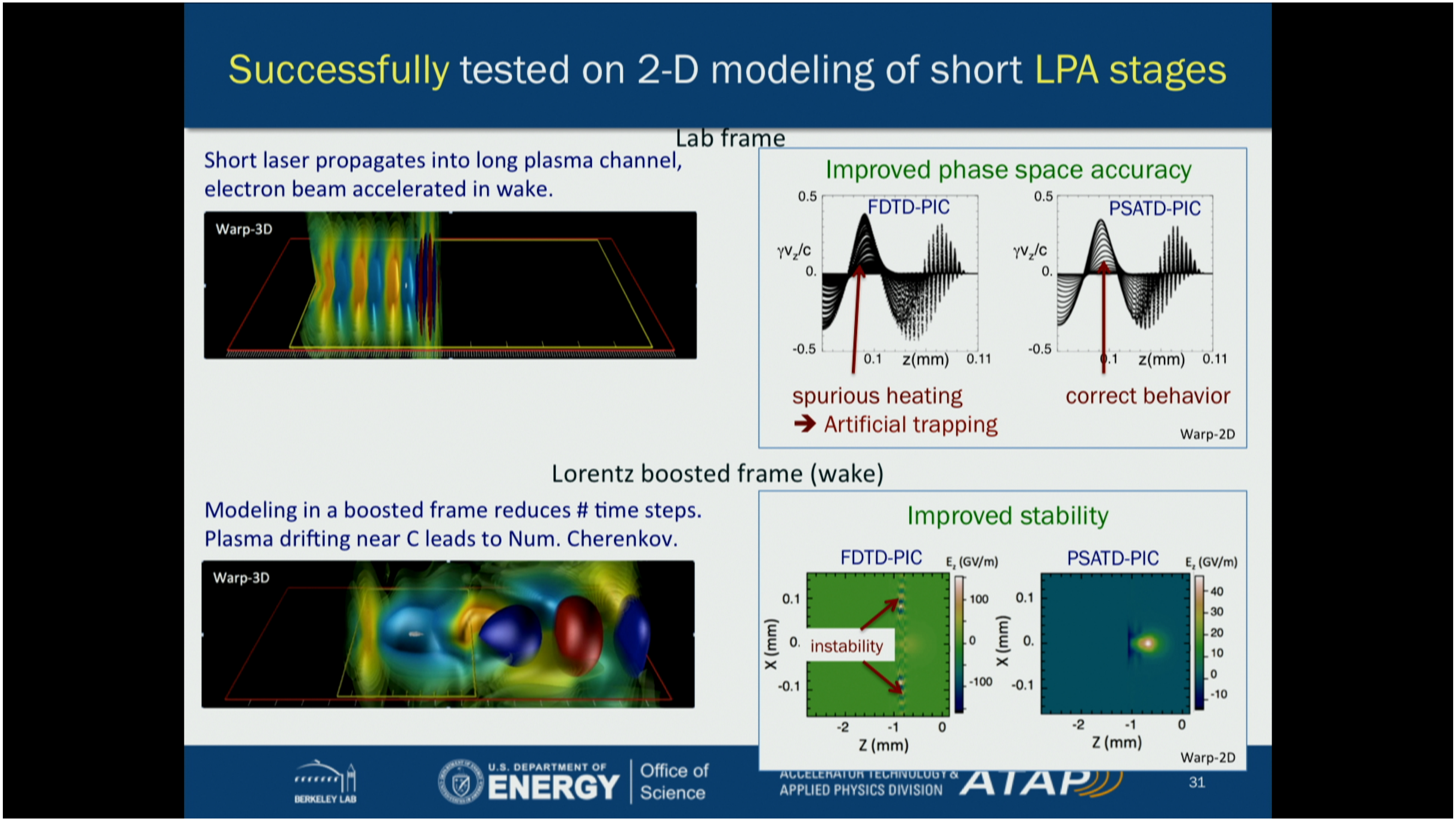
zero out remaining areas

Ready for next time step

Successfully tested on 7x7 domain

←Local FFTs

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



Successfully tested on 2-D modeling of short LPA stages

Lab frame

Short laser propagates into long plasma channel, electron beam accelerated in wake.

Improved phase space accuracy

spurious heating

➔ Artificial trapping

correct behavior

Lorentz boosted frame (wake)

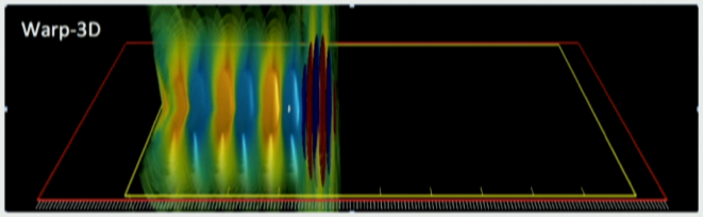
Modeling in a boosted frame reduces # time steps.
Plasma drifting near C leads to Num. Cherenkov.

Improved stability

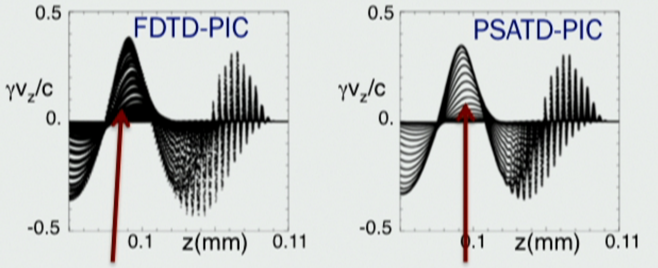
Successfully tested on 2-D modeling of short LPA stages

Lab frame

Short laser propagates into long plasma channel, electron beam accelerated in wake.



Improved phase space accuracy



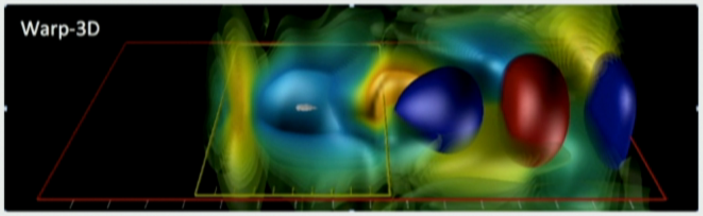
spurious heating
➔ Artificial trapping

correct behavior

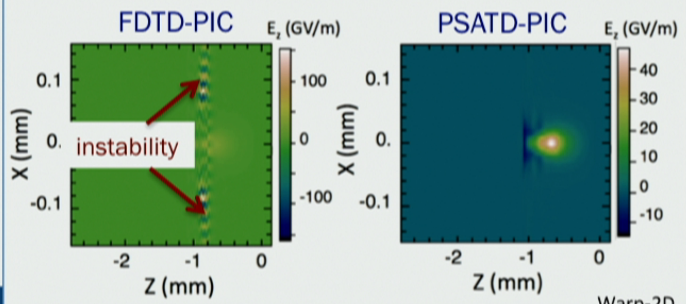
Warp-2D

Lorentz boosted frame (wake)

Modeling in a boosted frame reduces # time steps. Plasma drifting near C leads to Num. Cherenkov.

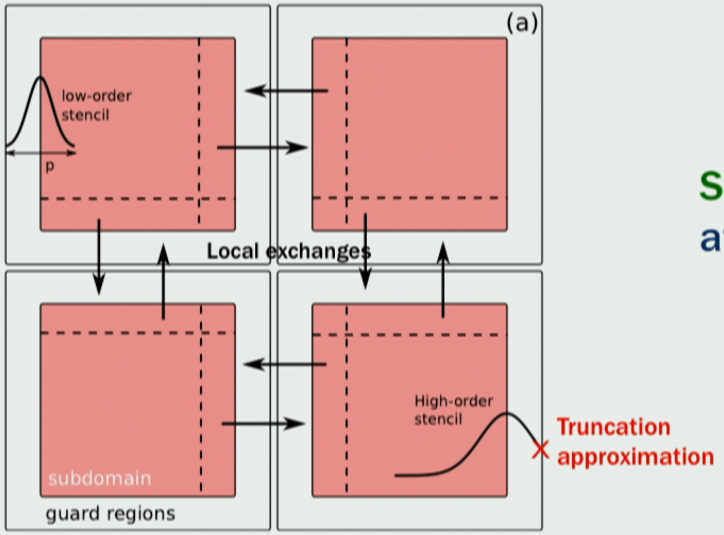


Improved stability



Warp-2D

Domain decomposition with high/infinite-order stencil implies stencil truncation



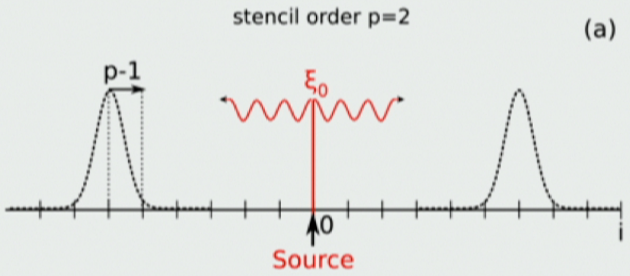
Scales but approximation at very high/infinite orders!

Need to characterize/mitigate truncation errors

to enable new method to scale to millions or billions of cores!

New error-predictive analytical model for stencil spatial variations/truncations

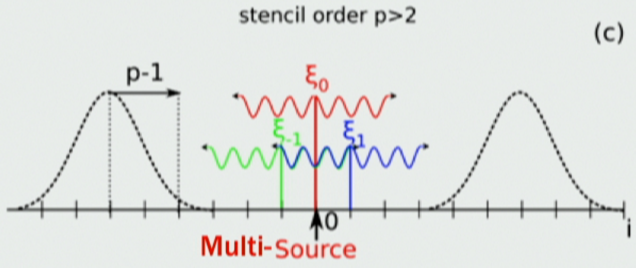
Order 2 stencil: stencil modification at one point accounted with a single source term*



- Yields inaccurate results for orders p>2
- Total truncation error amplitude:

$$\zeta = \xi_0$$

Higher order: stencil modification at one point accounted by multi-source error terms**

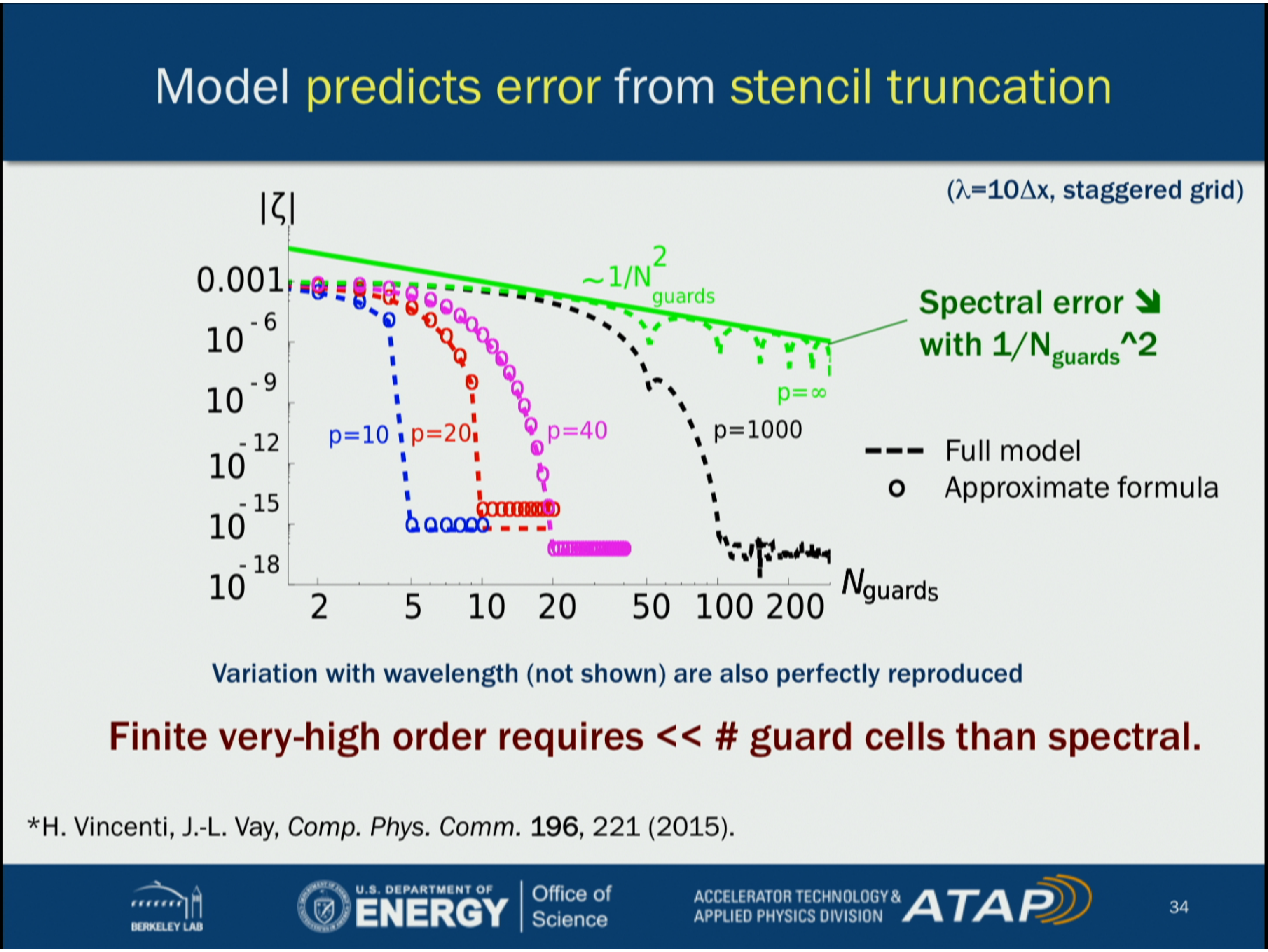


- Solves discrepancy at orders p>2
- Total truncation error amplitude:

$$\zeta = \sum_l \xi_l e^{jkl\delta x}$$

*J.-L. Vay, *J. Comput. Phys.* **183**, 367 (2002).

H. Vincenti, J.-L. Vay, *Comp. Phys. Comm.* **196, 221 (2015).



Model predicts error from stencil truncation

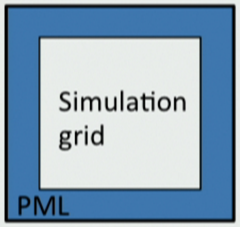
Variation with wavelength (not shown) are also perfectly reproduced

Finite very-high order requires << # guard cells than spectral.

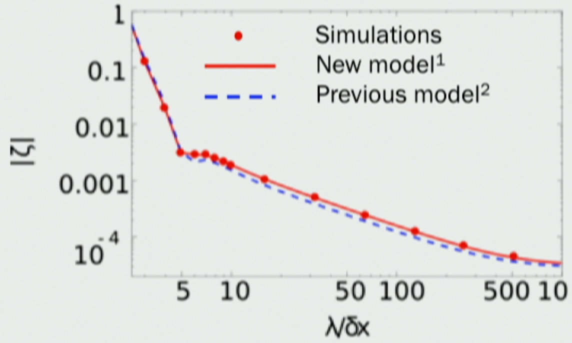
*H. Vincenti, J.-L. Vay, *Comp. Phys. Comm.* **196**, 221 (2015).

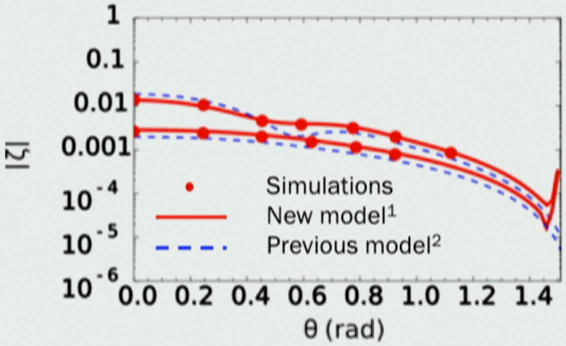
New analysis confirms efficacy of PML with spectral

Perfectly Matched Layer (PML) enables efficient open boundary conditions



New analysis predicts exact coefficients of reflections





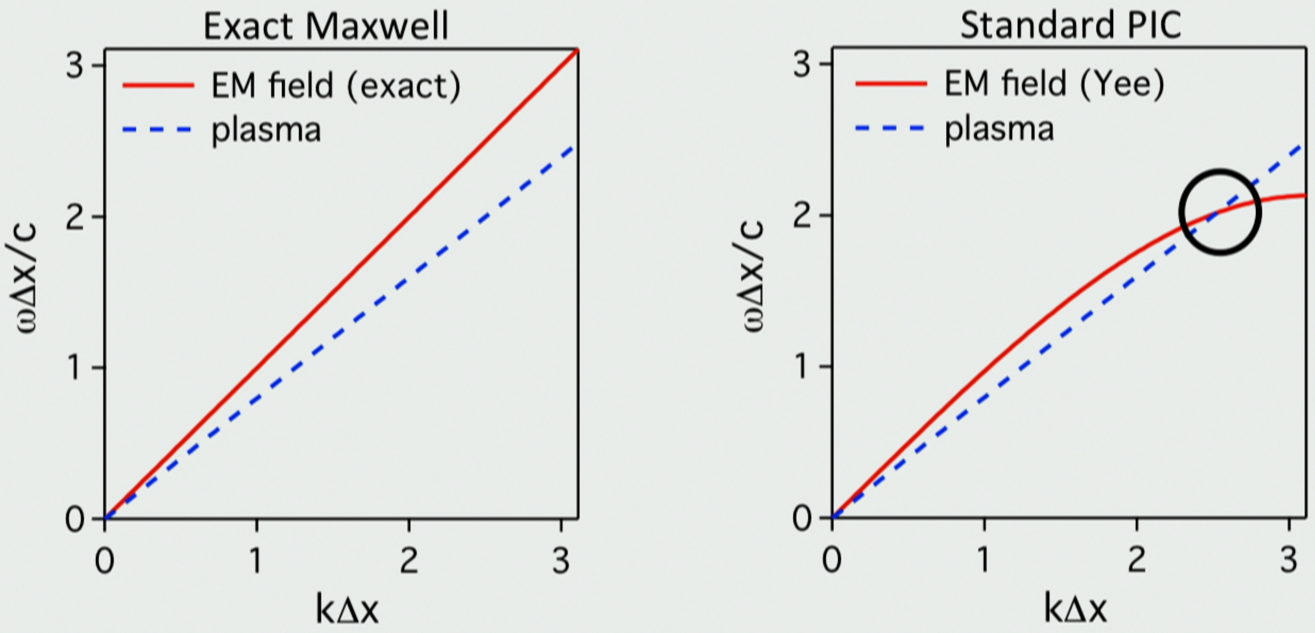
[1] H. Vincenti, J.-L. Vay, *Comp. Phys. Comm.* **196**, 221 (2015).

[2] P. Lee, J.-L. Vay, *Comp. Phys. Comm.* **194**, 1-9 (2015).

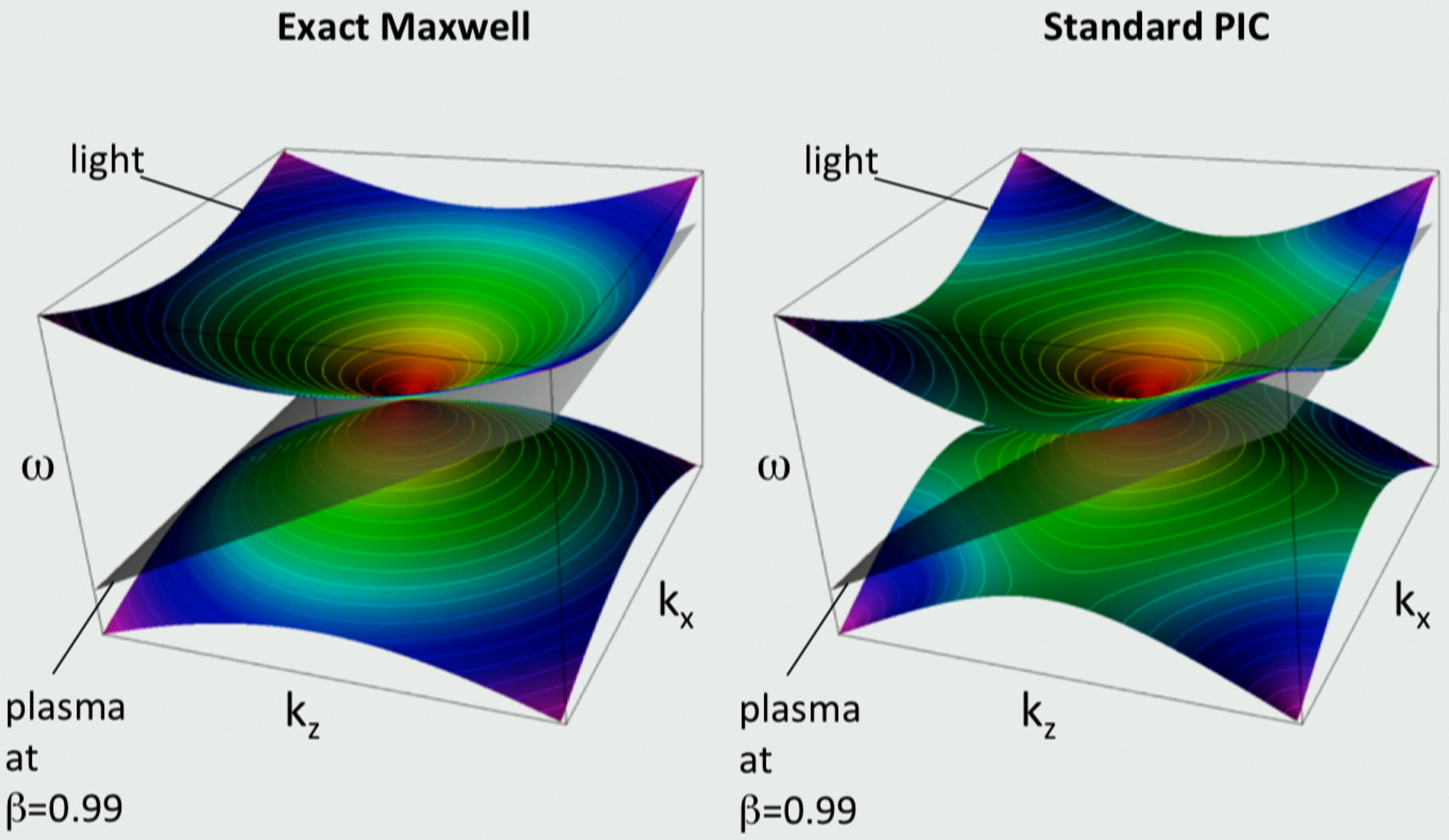
Relativistic plasmas PIC subject to "numerical Cherenkov"

B. B. Godfrey, "Numerical Cherenkov instabilities in electromagnetic particle codes", *J. Comput. Phys.* **15** (1974)

Numerical dispersion leads to crossing of EM field and plasma modes -> instability.

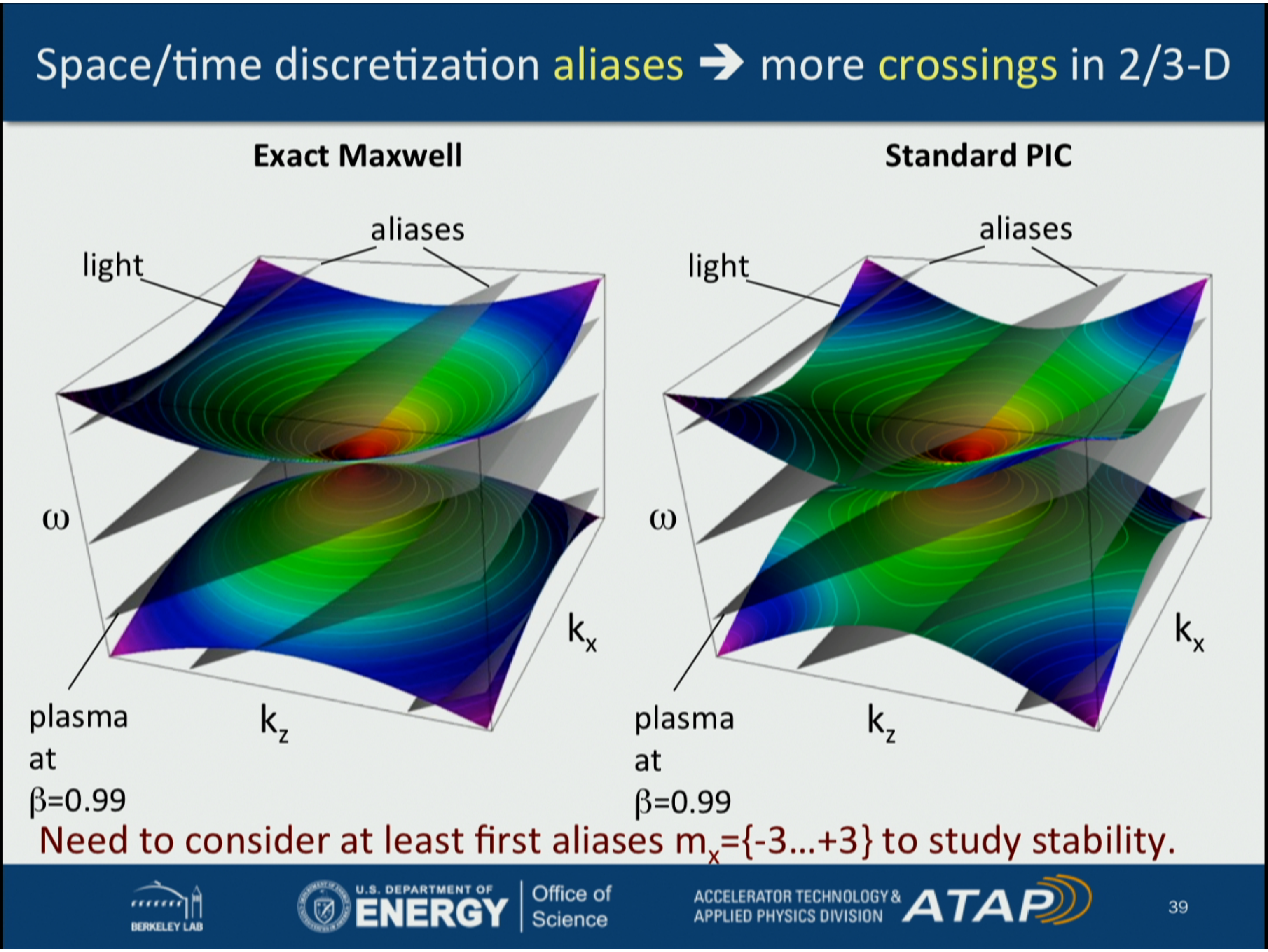


Space/time discretization aliases → more crossings in 2/3-D


Exact Maxwell

Standard PIC

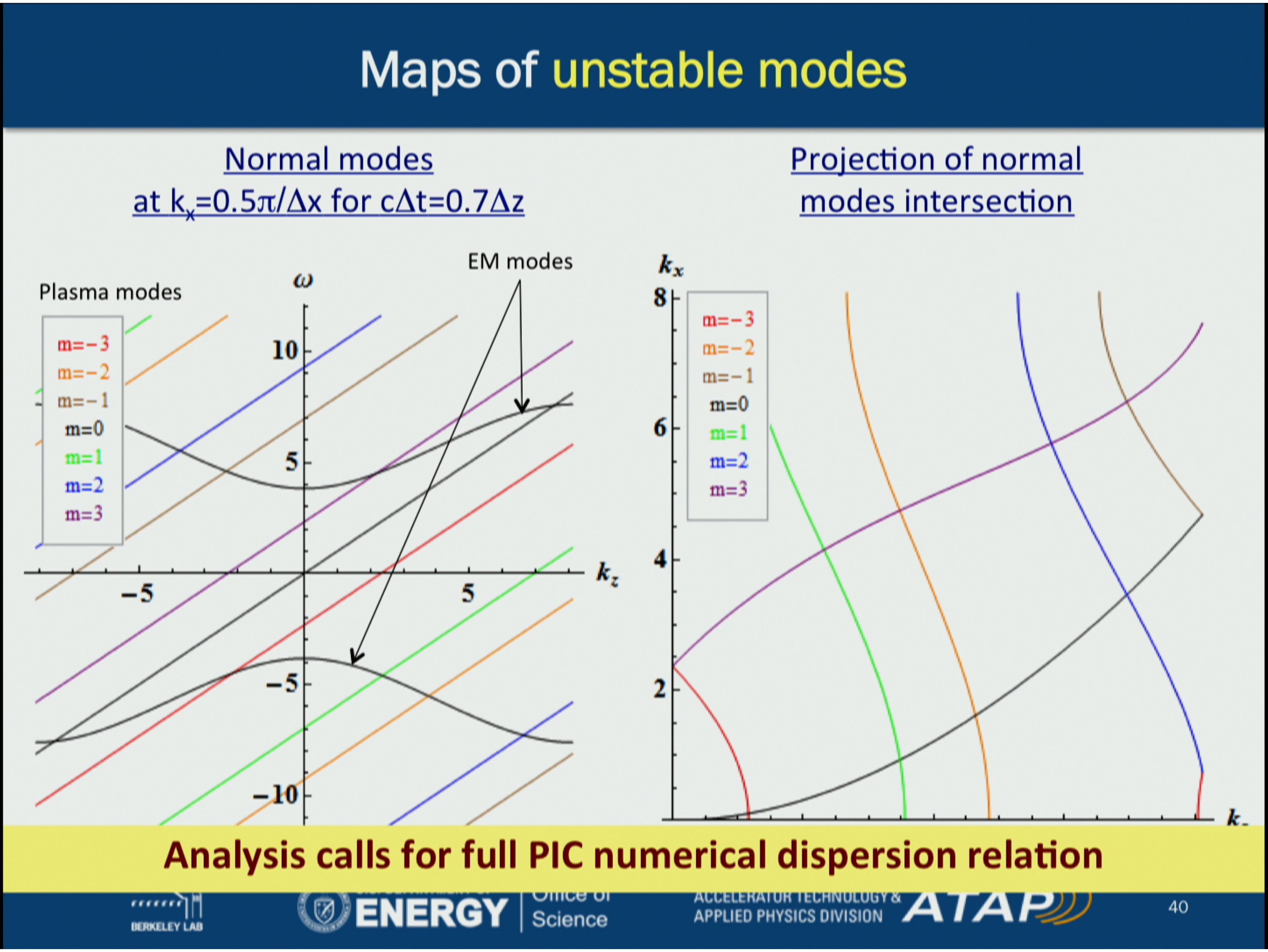
Space/time discretization aliases ➔ more crossings in 2/3-D



Exact Maxwell

Standard PIC

Need to consider at least first aliases m_x={-3…+3} to study stability.



Maps of unstable modes

Normal modes at $k_x=0.5\pi/\Delta x$ for $c\Delta t=0.7\Delta z$

Projection of normal modes intersection

Analysis calls for full PIC numerical dispersion relation

Numerical dispersion relation of full-PIC algorithm*

E.g.: 2-D relation (Fourier space):
$$\begin{pmatrix} \xi_{z,z}+[\omega] & \xi_{z,x} & \xi_{z,y}+[k_x] \\ \xi_{x,z} & \xi_{x,x}+[\omega] & \xi_{x,y}-[k_z] \\ [k_x] & -[k_z] & [\omega] \end{pmatrix} \begin{pmatrix} E_z \\ E_x \\ B_y \end{pmatrix} = 0.$$

$$[\omega] = \sin\left(\omega\frac{\Delta t}{2}\right)/\left(\frac{\Delta t}{2}\right) \quad [k_z] = k_z \sin\left(k\frac{\Delta t}{2}\right)/\left(k\frac{\Delta t}{2}\right) \quad [k_x] = k_x \sin\left(k\frac{\Delta t}{2}\right)/\left(k\frac{\Delta t}{2}\right)$$

$$S^J = \left[\sin\left(k'_z\frac{\Delta z}{2}\right)/\left(k'_z\frac{\Delta z}{2}\right)\right]^{\ell_z+1}\left[\sin\left(k'_x\frac{\Delta x}{2}\right)/\left(k'_x\frac{\Delta x}{2}\right)\right]^{\ell_x+1},$$

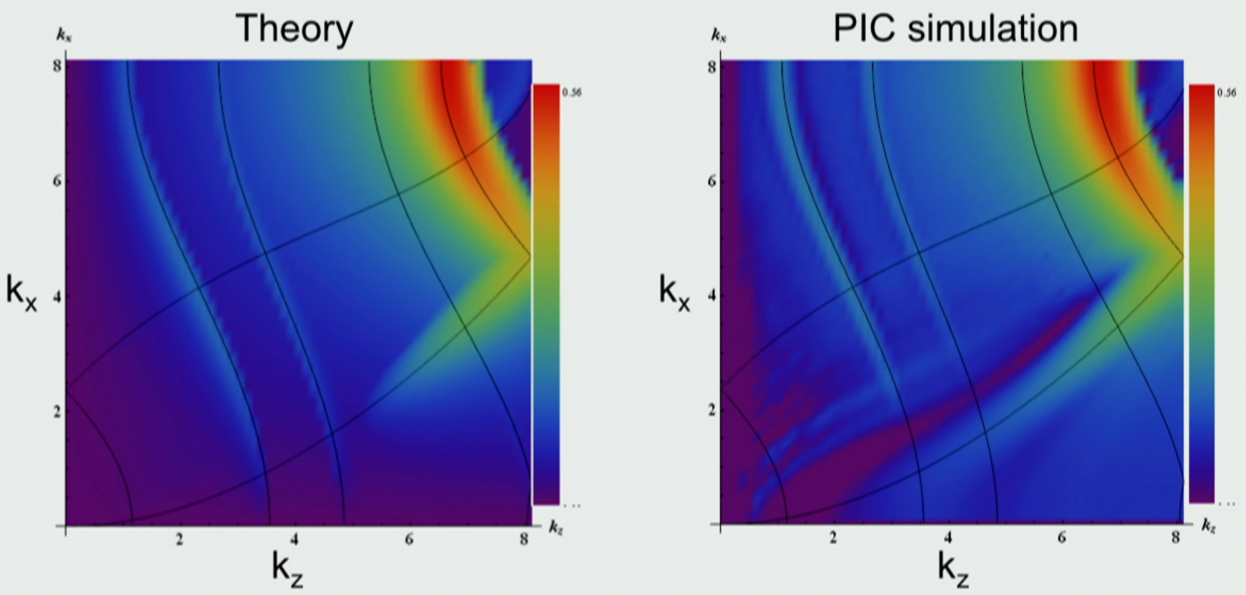
$$S^{E_z} = \left[\sin\left(k'_z\frac{\Delta z}{2}\right)/\left(k'_z\frac{\Delta z}{2}\right)\right]^{\ell_z}\left[\sin\left(k'_x\frac{\Delta x}{2}\right)/\left(k'_x\frac{\Delta x}{2}\right)\right]^{\ell_x+1}(-1)^{m_z},$$

$$S^{E_x} = \left[\sin\left(k'_z\frac{\Delta z}{2}\right)/\left(k'_z\frac{\Delta z}{2}\right)\right]^{\ell_z+1}\left[\sin\left(k'_x\frac{\Delta x}{2}\right)/\left(k'_x\frac{\Delta x}{2}\right)\right]^{\ell_x}(-1)^{m_x},$$

$$S^{B_y} = \cos\left(\omega\frac{\Delta t}{2}\right)\left[\sin\left(k'_z\frac{\Delta z}{2}\right)/\left(k'_z\frac{\Delta z}{2}\right)\right]^{\ell_z}\left[\sin\left(k'_x\frac{\Delta x}{2}\right)/\left(k'_x\frac{\Delta x}{2}\right)\right]^{\ell_x}(-1)^{m_z+m_x}.$$

*B. B. Godfrey, J. L. Vay, I. Haber, J. Comp. Phys. 248 (2013)

Growth rates from theory match PIC simulations

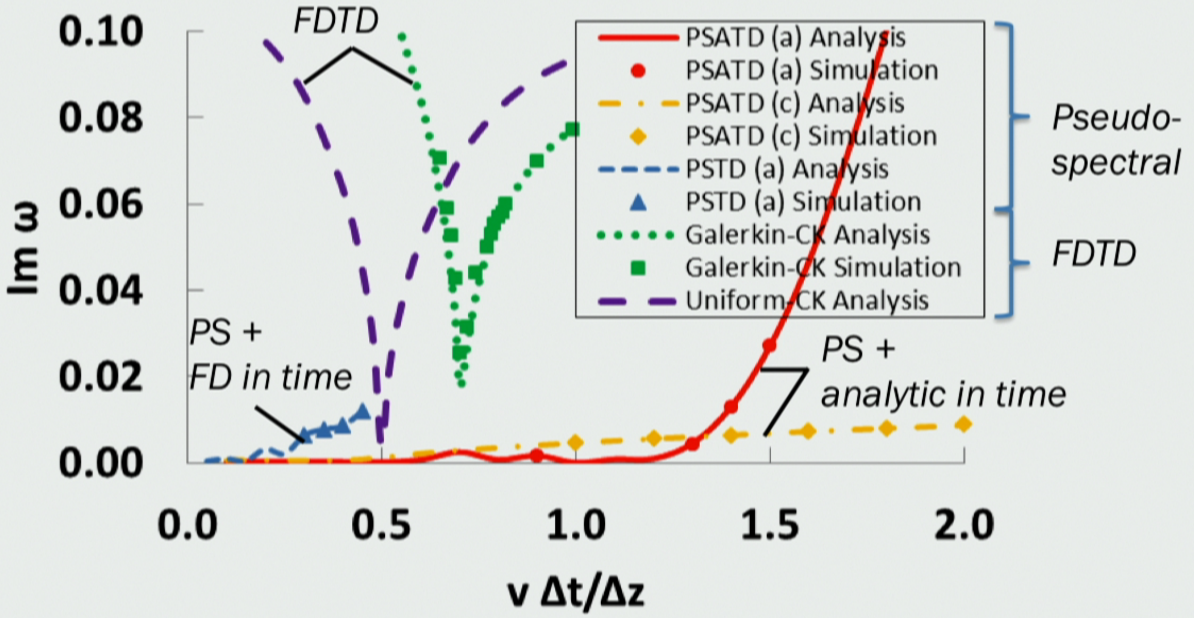

Theory

PIC simulation

PIC: uniform drifting plasma
with periodic BC.

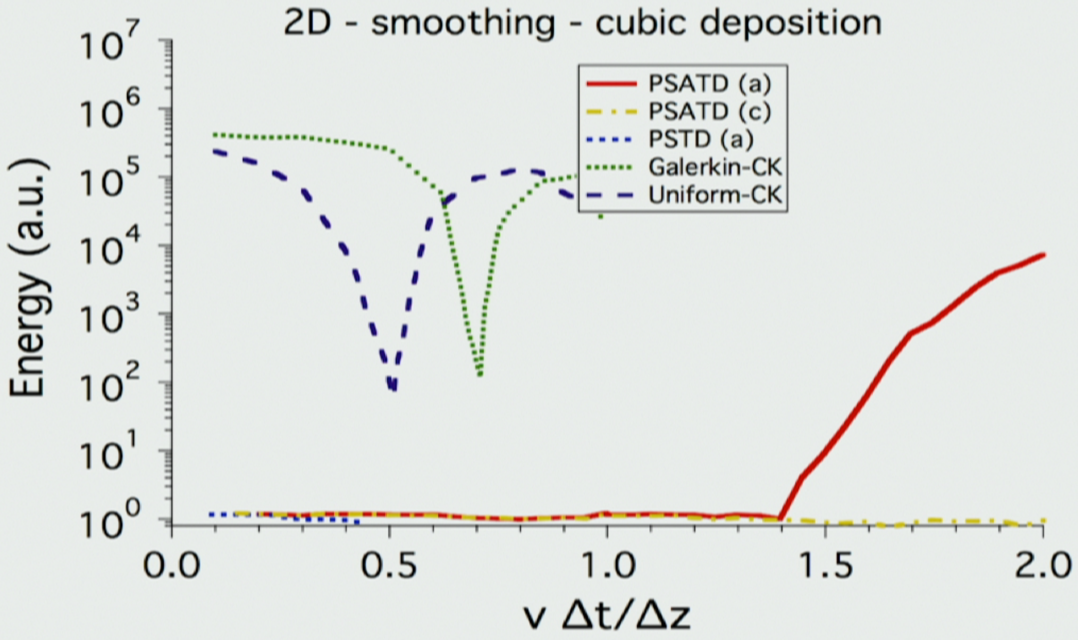
Yee finite difference, energy conserving gather ($c\Delta t/\Delta x=0.7$)

Stability analysis also shows that pseudo-spectral algorithms are more stable*

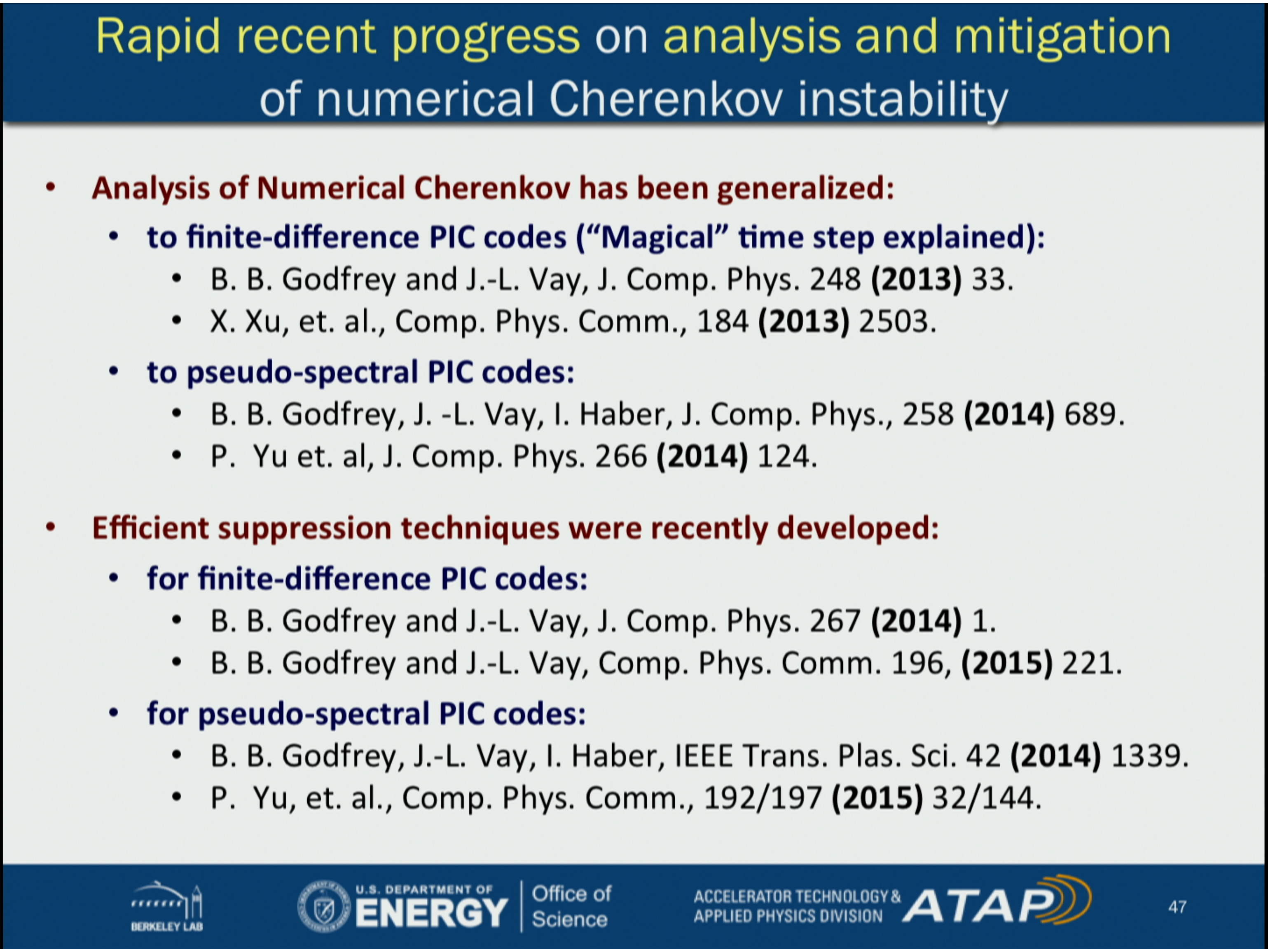


*B. B. Godfrey, J.-L. Vay, I. Haber, "Numerical stability analysis of the Pseudo-Spectral Analytical Time-Domain PIC algorithm", *J. Comp. Phys.* **258** (2014) 689.

Stability over wide range of time steps confirmed with Warp*

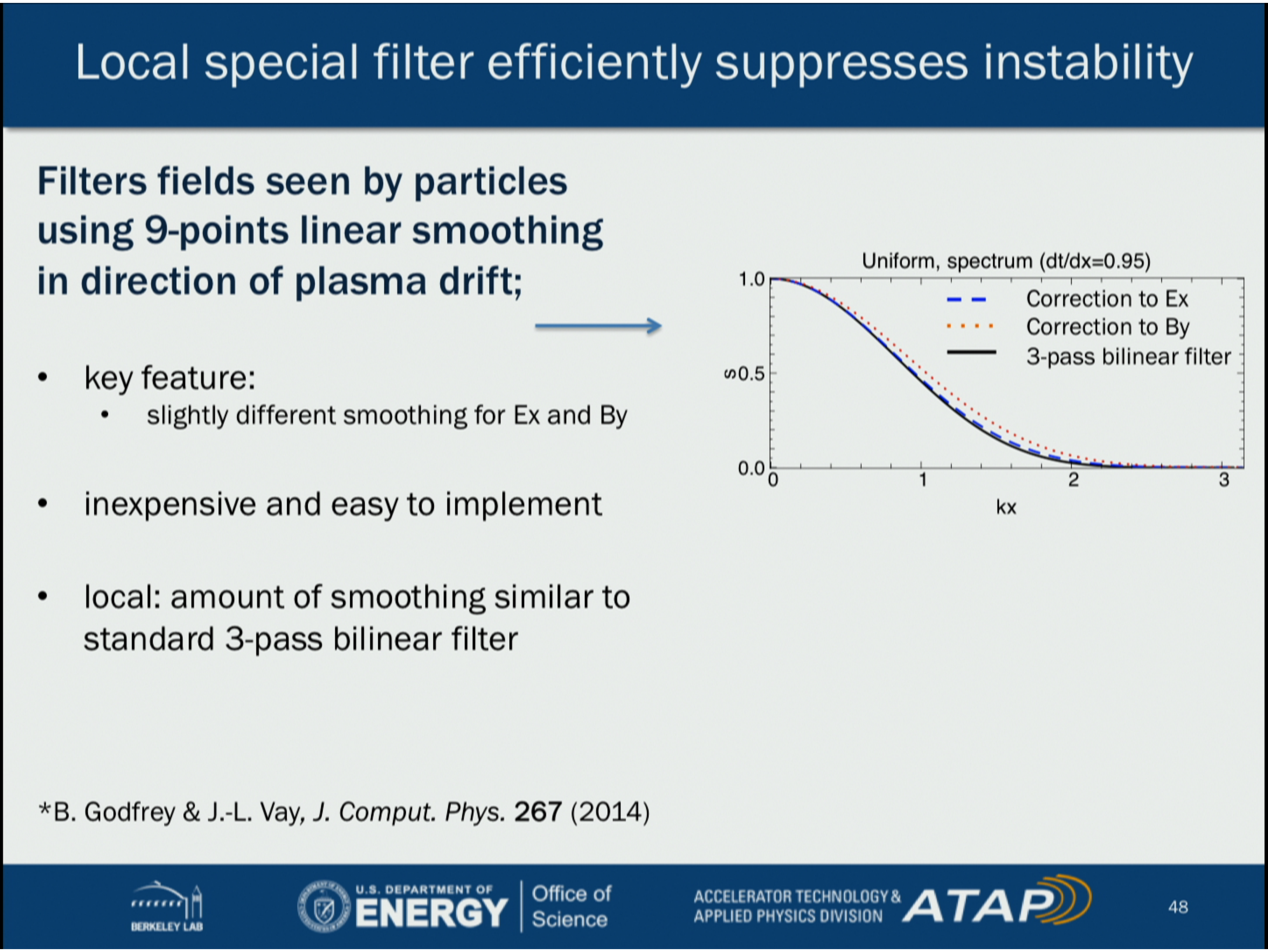


*B. B. Godfrey, J.-L. Vay, I. Haber, "Numerical stability analysis of the Pseudo-Spectral Analytical Time-Domain PIC algorithm", *J. Comp. Phys.* **258** (2014) 689.



Rapid recent progress on analysis and mitigation of numerical Cherenkov instability

- **Analysis of Numerical Cherenkov has been generalized:**
    - **to finite-difference PIC codes ("Magical" time step explained):**
        - B. B. Godfrey and J.-L. Vay, J. Comp. Phys. 248 **(2013)** 33.
        - X. Xu, et. al., Comp. Phys. Comm., 184 **(2013)** 2503.
    - **to pseudo-spectral PIC codes:**
        - B. B. Godfrey, J. -L. Vay, I. Haber, J. Comp. Phys., 258 **(2014)** 689.
        - P. Yu et. al, J. Comp. Phys. 266 **(2014)** 124.
- **Efficient suppression techniques were recently developed:**
    - **for finite-difference PIC codes:**
        - B. B. Godfrey and J.-L. Vay, J. Comp. Phys. 267 **(2014)** 1.
        - B. B. Godfrey and J.-L. Vay, Comp. Phys. Comm. 196, **(2015)** 221.
    - **for pseudo-spectral PIC codes:**
        - B. B. Godfrey, J.-L. Vay, I. Haber, IEEE Trans. Plas. Sci. 42 **(2014)** 1339.
        - P. Yu, et. al., Comp. Phys. Comm., 192/197 **(2015)** 32/144.



Local special filter efficiently suppresses instability

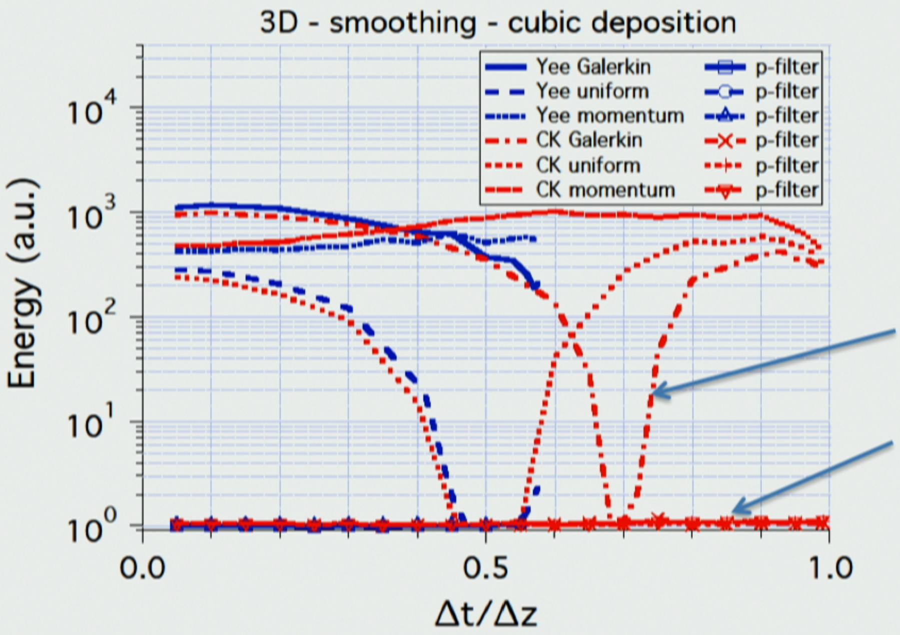
Filters fields seen by particles using 9-points linear smoothing in direction of plasma drift;

- key feature:
    - slightly different smoothing for Ex and By
- inexpensive and easy to implement
- local: amount of smoothing similar to standard 3-pass bilinear filter

*B. Godfrey & J.-L. Vay, *J. Comput. Phys.* **267** (2014)

Filtering scheme yields excellent stability

Warp simulations of LPA



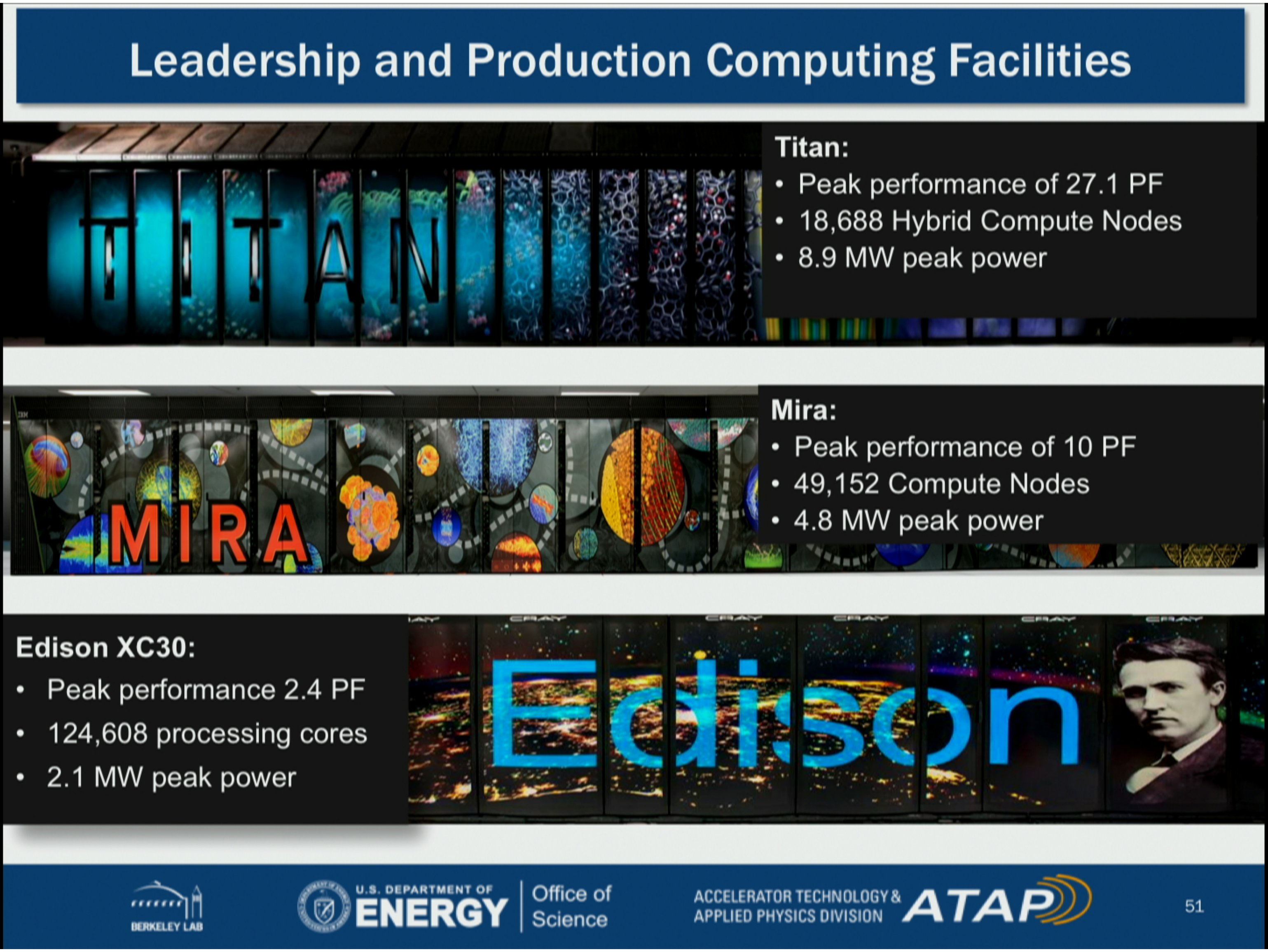
*Without filtering, stability only around "magical time steps"**

*New filter** enables stability at all time steps.*

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

B. Godfrey & J.-L. Vay, *J. Comput. Phys.* **267 (2014)

Exascale Supercomputing



Leadership and Production Computing Facilities

Titan:

- Peak performance of 27.1 PF
- 18,688 Hybrid Compute Nodes
- 8.9 MW peak power

Mira:

- Peak performance of 10 PF
- 49,152 Compute Nodes
- 4.8 MW peak power

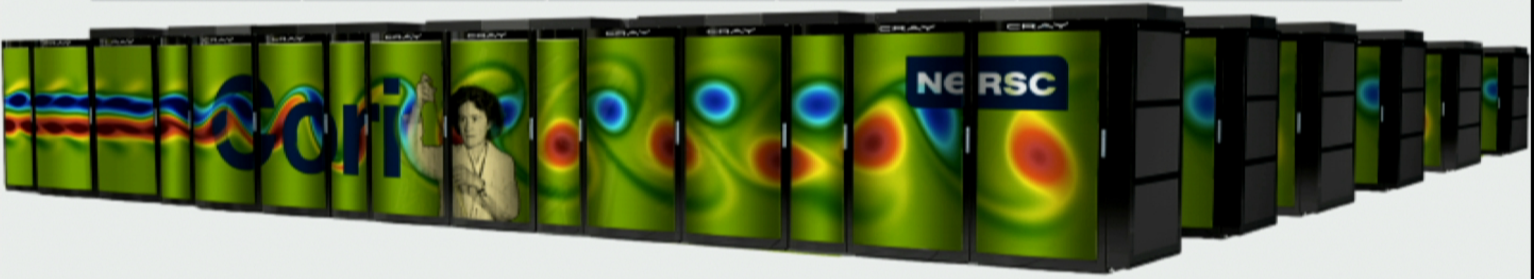
Edison XC30:

- Peak performance 2.4 PF
- 124,608 processing cores
- 2.1 MW peak power

NERSC systems to reach 1 ExaFlops by 2024

NERSC Systems Timeline

2007/2009	NERSC-5	Franklin	Cray XT4	102/352 TF
2010	NERSC-6	Hopper	Cray XE6	1.28 PF
2014	NERSC-7	Edison	Cray XC30	2.57 PF
2016	NERSC-8	Cori	Cray XC	30 PF
2020	NERSC-9			100PF-300PF
2024	NERSC-10			1EF
2028	NERSC-11			5-10EF

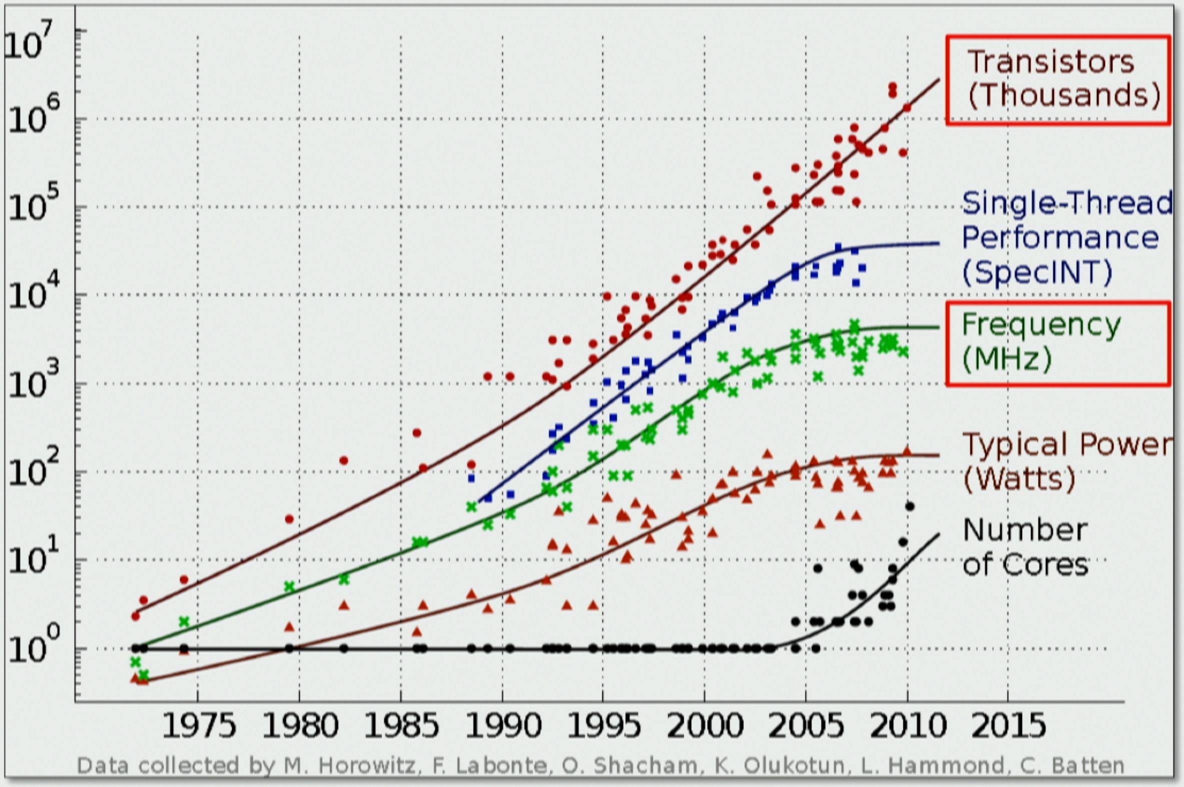


Courtesy Sudip Dosanjh, IXPUG 2015

Computing Sciences Area

ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION

Progress in CMOS CPU Technology



Data collected by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, C. Batten

Moore's Law continues

- Transistor count still doubles every 24 months

Dennard scaling stalls

- Voltage
- Clock Speed
- Power
- Performance/clock

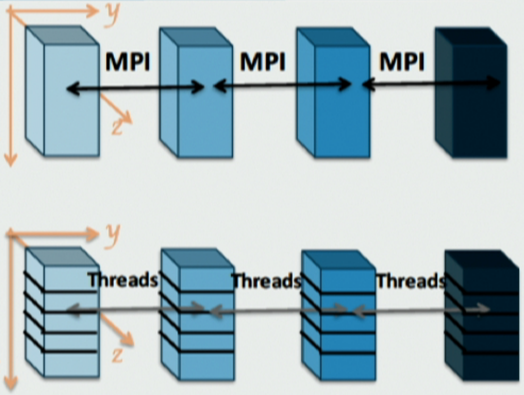
BESAC Briefing February 11, 2016

Courtesy Steve Binkley, BESAC 2016

Novel exascale supercomputers require restructuration with "multi-level parallelism"

To run effectively on future systems

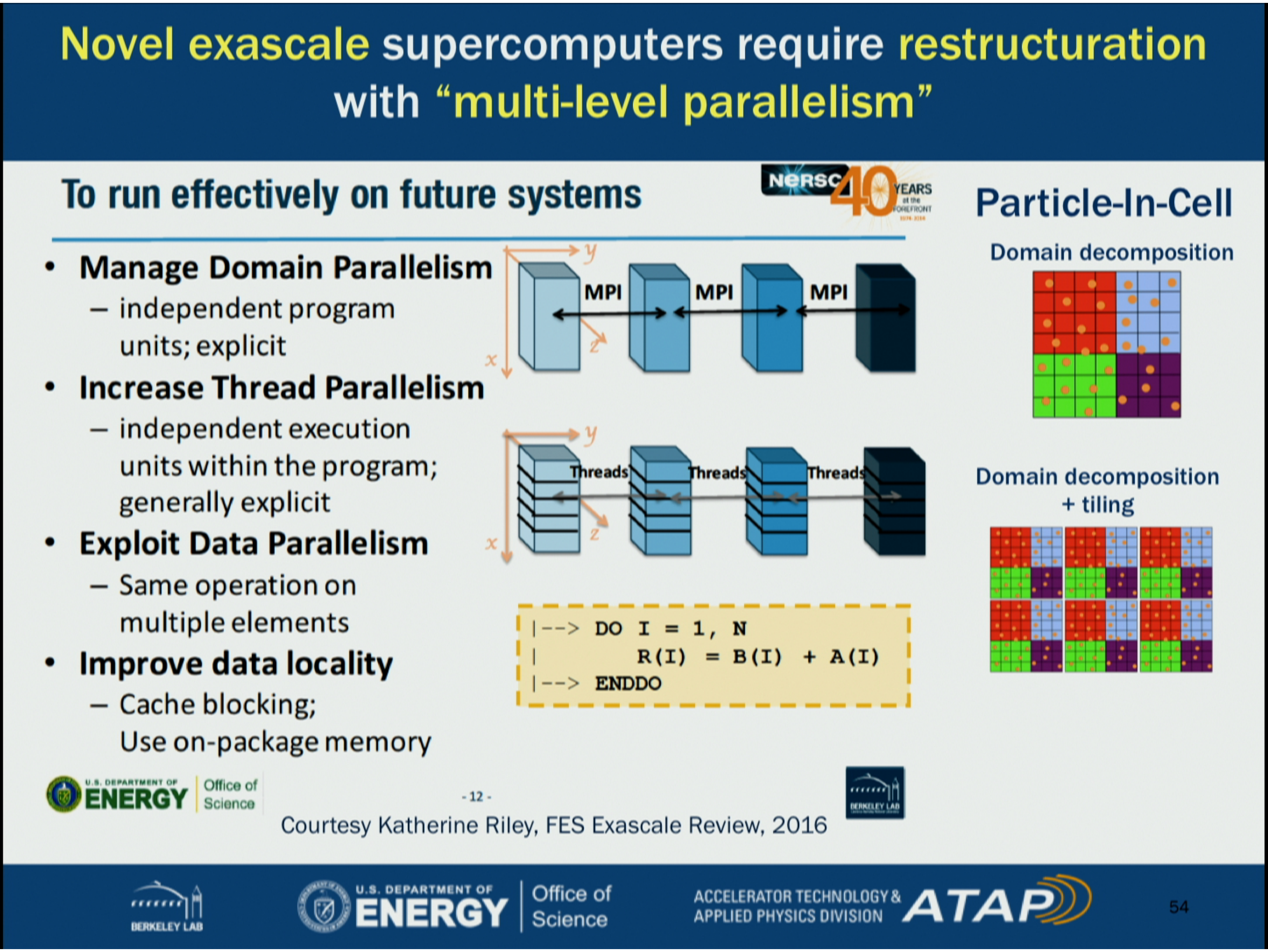
- **Manage Domain Parallelism**
  - independent program units; explicit
- **Increase Thread Parallelism**
  - independent execution units within the program; generally explicit
- **Exploit Data Parallelism**
  - Same operation on multiple elements
- **Improve data locality**
  - Cache blocking; Use on-package memory



```
|--> DO I = 1, N
|        R(I)  = B(I)  + A(I)
|--> ENDDO
```

Courtesy Katherine Riley, FES Exascale Review, 2016

ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION



Novel exascale supercomputers require restructuration with "multi-level parallelism"

To run effectively on future systems

- **Manage Domain Parallelism**
  - independent program units; explicit
- **Increase Thread Parallelism**
  - independent execution units within the program; generally explicit
- **Exploit Data Parallelism**
  - Same operation on multiple elements
- **Improve data locality**
  - Cache blocking; Use on-package memory

```
|--> DO I = 1, N
|        R(I) = B(I) + A(I)
|--> ENDDO
```

Particle-In-Cell

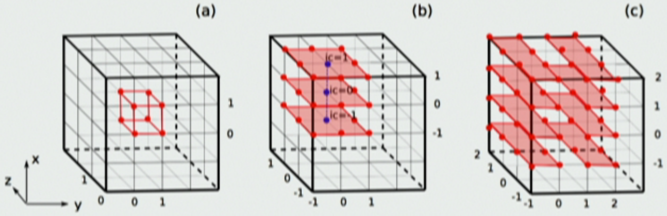
Domain decomposition

Domain decomposition + tiling

Courtesy Katherine Riley, FES Exascale Review, 2016

Novel vectorization algorithm leads to >2x speedup on charge/current deposition routines

- Previous algorithms developped on vector supercomputers in 70s-90s do not work
- Novel algorithm developped* (implemented in Warp/PICSAR)

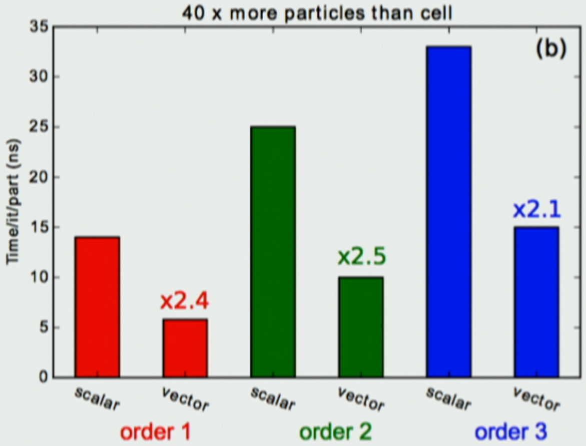


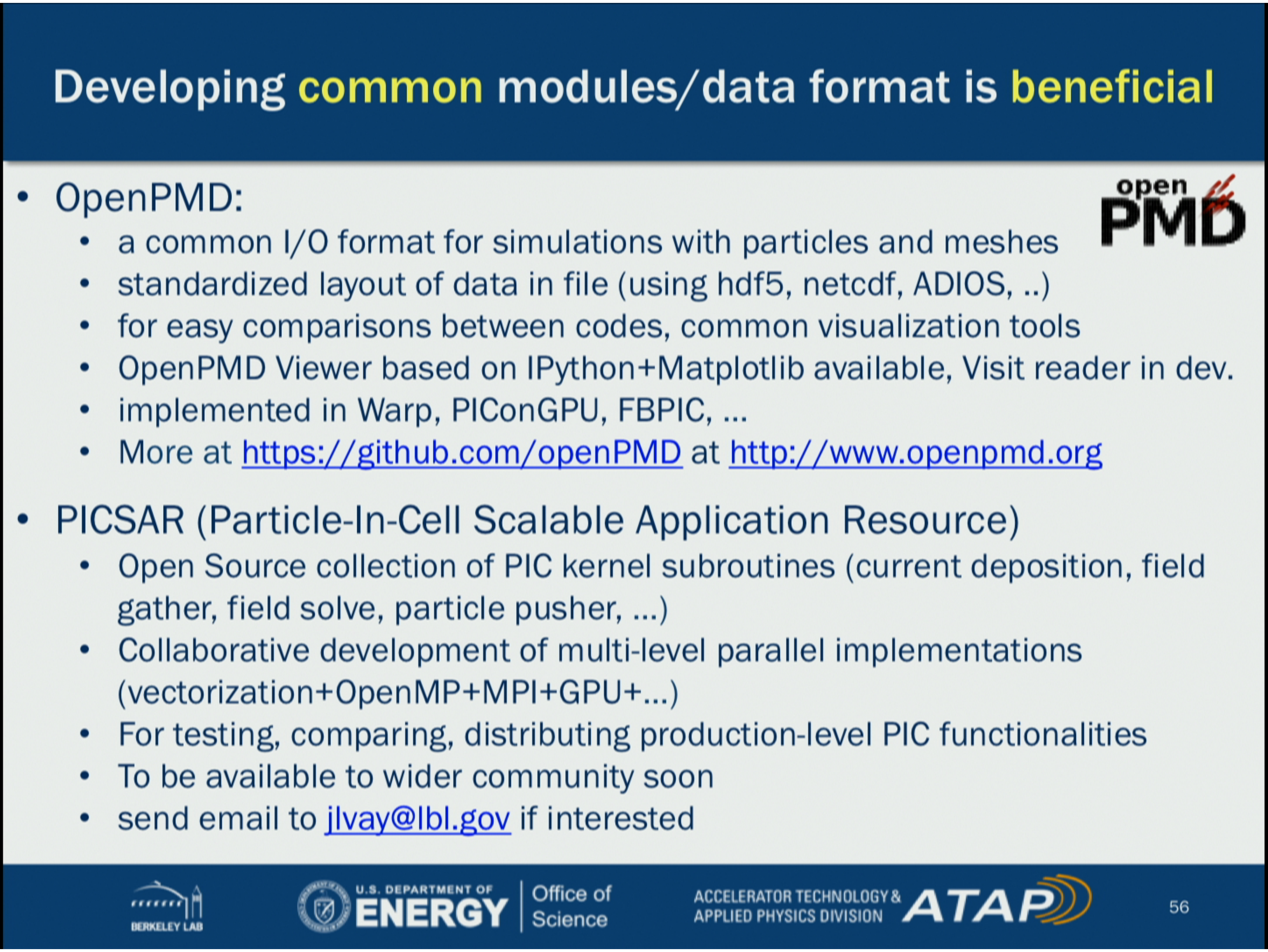
linear quadratic cubic

*H. Vincenti, R. Lehe, R. Sasanka, J-L. Vay, « An efficient and portable SIMD algorithm for charge/current deposition in Particle-In-Cell codes », arXiv:1601.02056, submitted to Comp. Phys. Comm.

➢ Benchmarks on Cori (Haswell CPU)

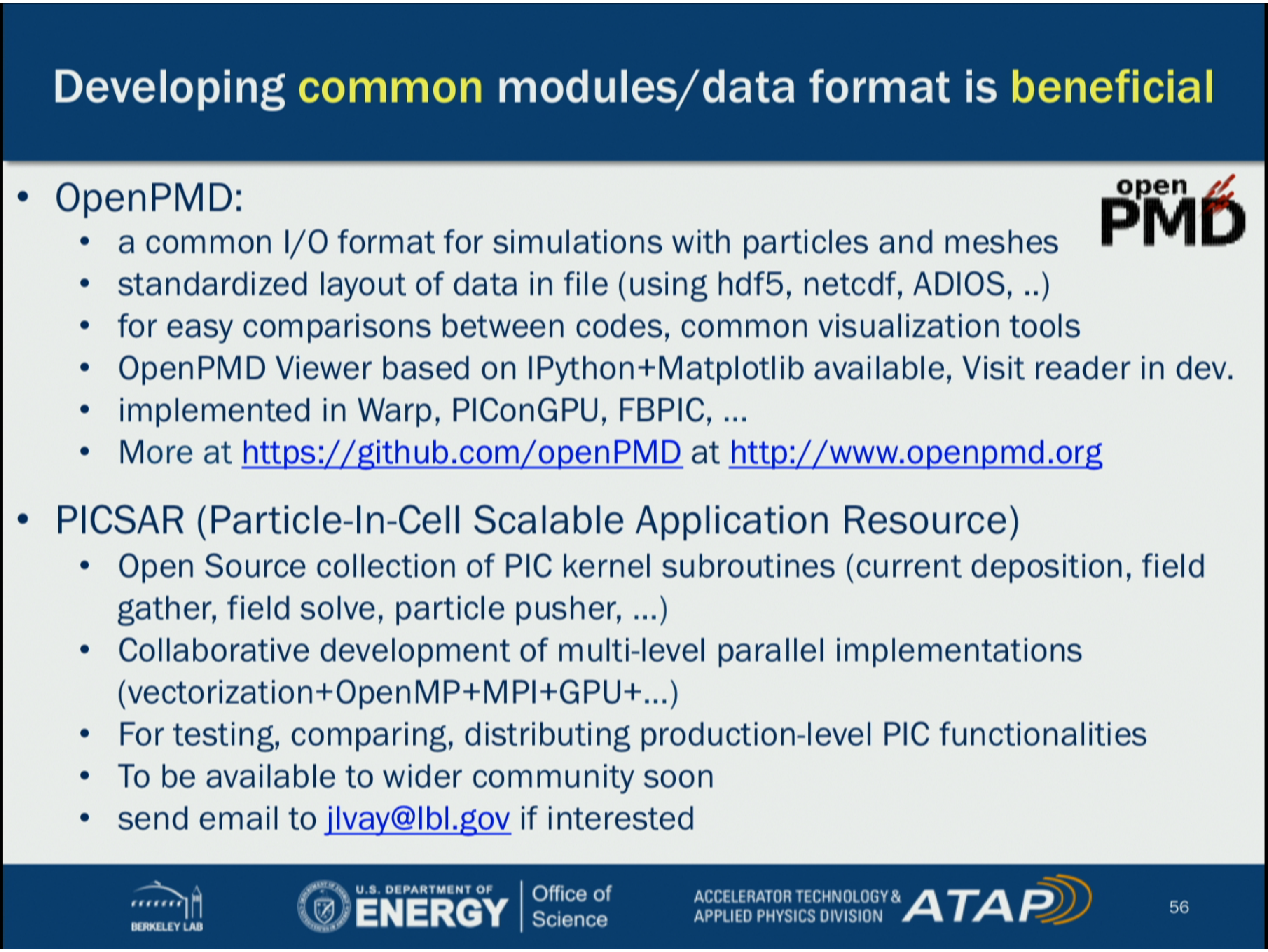
Tests demonstrate speedups >2x (max. theoretical=4)





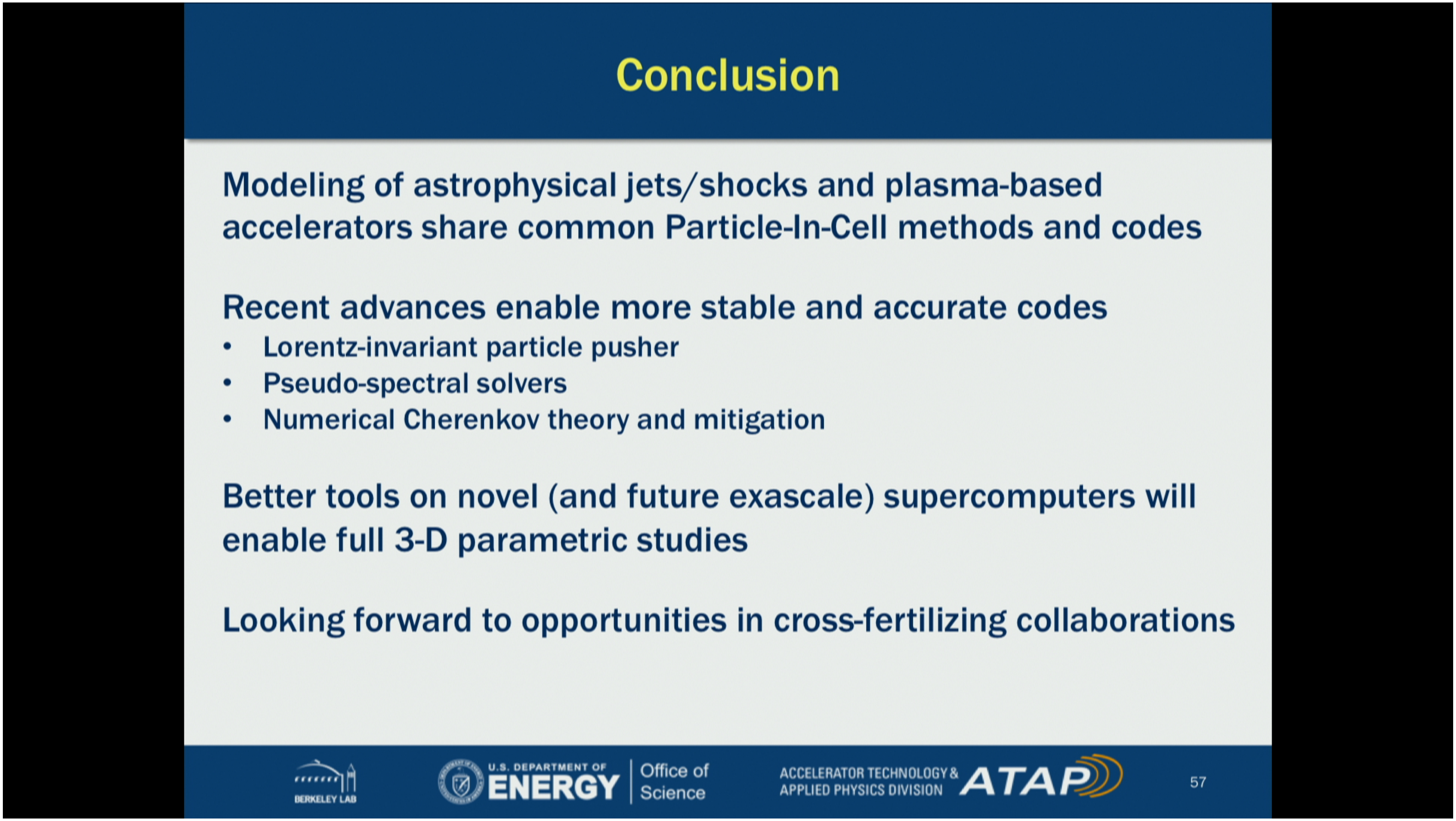
Developing common modules/data format is beneficial

- OpenPMD:
  - a common I/O format for simulations with particles and meshes
  - standardized layout of data in file (using hdf5, netcdf, ADIOS, ..)
  - for easy comparisons between codes, common visualization tools
  - OpenPMD Viewer based on IPython+Matplotlib available, Visit reader in dev.
  - implemented in Warp, PIConGPU, FBPIC, ...
  - More at https://github.com/openPMD at http://www.openpmd.org
- PICSAR (Particle-In-Cell Scalable Application Resource)
  - Open Source collection of PIC kernel subroutines (current deposition, field gather, field solve, particle pusher, ...)
  - Collaborative development of multi-level parallel implementations (vectorization+OpenMP+MPI+GPU+...)
  - For testing, comparing, distributing production-level PIC functionalities
  - To be available to wider community soon
  - send email to jlvay@lbl.gov if interested



Developing common modules/data format is beneficial

- OpenPMD:
  - a common I/O format for simulations with particles and meshes
  - standardized layout of data in file (using hdf5, netcdf, ADIOS, ..)
  - for easy comparisons between codes, common visualization tools
  - OpenPMD Viewer based on IPython+Matplotlib available, Visit reader in dev.
  - implemented in Warp, PIConGPU, FBPIC, ...
  - More at https://github.com/openPMD at http://www.openpmd.org
- PICSAR (Particle-In-Cell Scalable Application Resource)
  - Open Source collection of PIC kernel subroutines (current deposition, field gather, field solve, particle pusher, ...)
  - Collaborative development of multi-level parallel implementations (vectorization+OpenMP+MPI+GPU+...)
  - For testing, comparing, distributing production-level PIC functionalities
  - To be available to wider community soon
  - send email to jlvay@lbl.gov if interested



Conclusion

Modeling of astrophysical jets/shocks and plasma-based accelerators share common Particle-In-Cell methods and codes

Recent advances enable more stable and accurate codes

- Lorentz-invariant particle pusher
- Pseudo-spectral solvers
- Numerical Cherenkov theory and mitigation

Better tools on novel (and future exascale) supercomputers will enable full 3-D parametric studies

Looking forward to opportunities in cross-fertilizing collaborations