# Advanced Modeling of Beams & Accelerators

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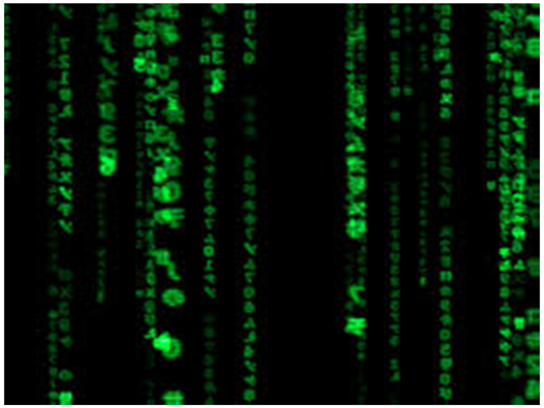
# Importance of computer modeling is on the rise

## with increasing:

**computers capacity**

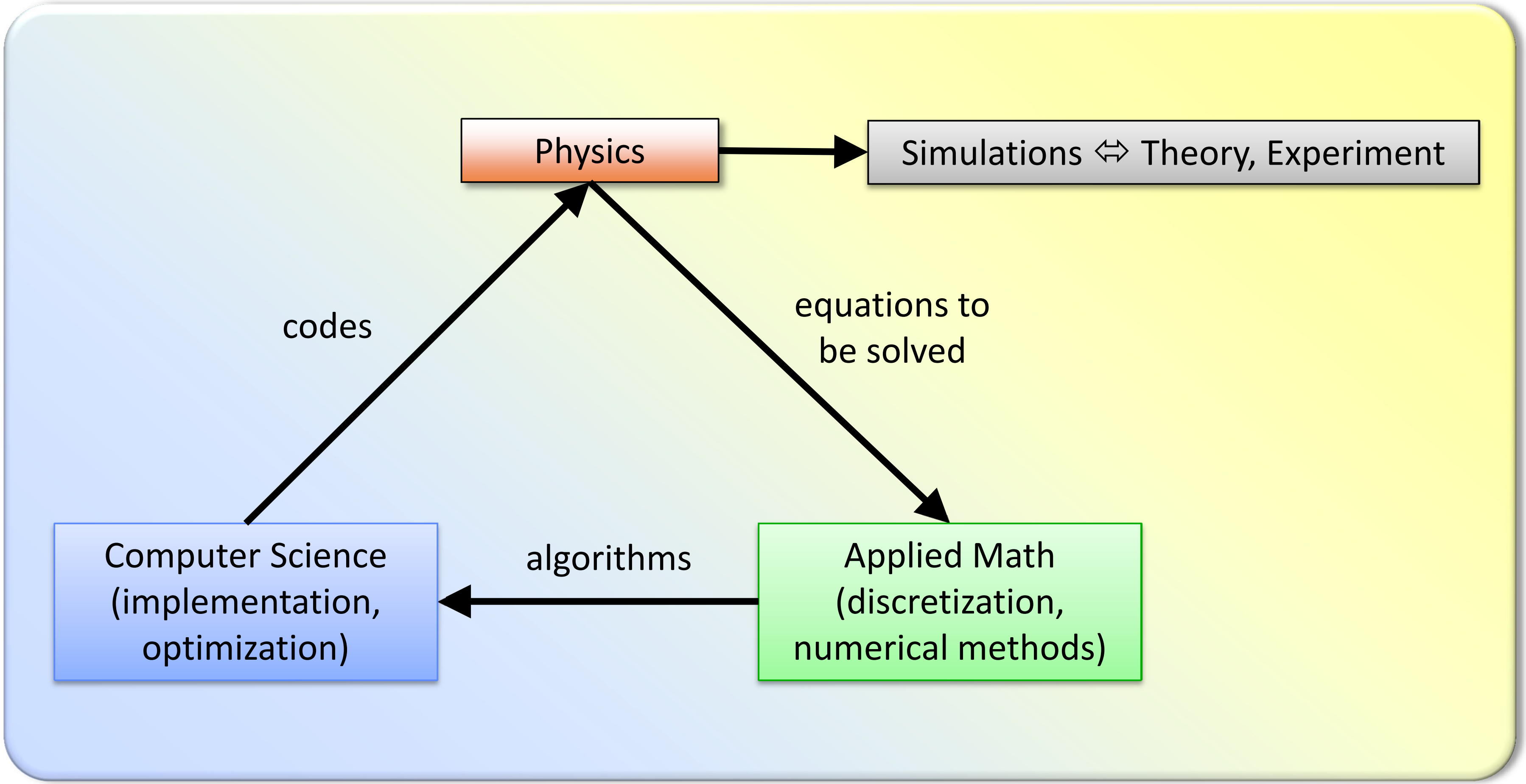
Top500 list, June 2013 #1: Tianhe-2, China (3.1 M cores)

accuracy of codes with **better algorithms** and **more physics**



pressure for **reducing uncertainties** and **cost** on development, construction & commissioning of accelerator

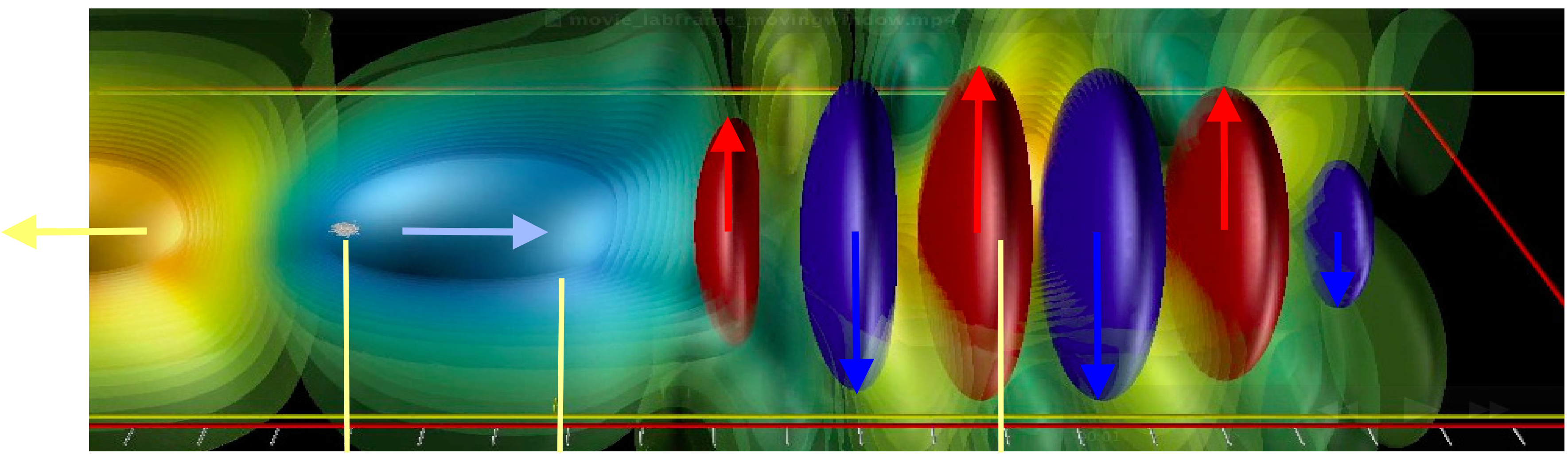
# Modeling of beams & accelerators




In practice, modeling activities can be significantly more complex.

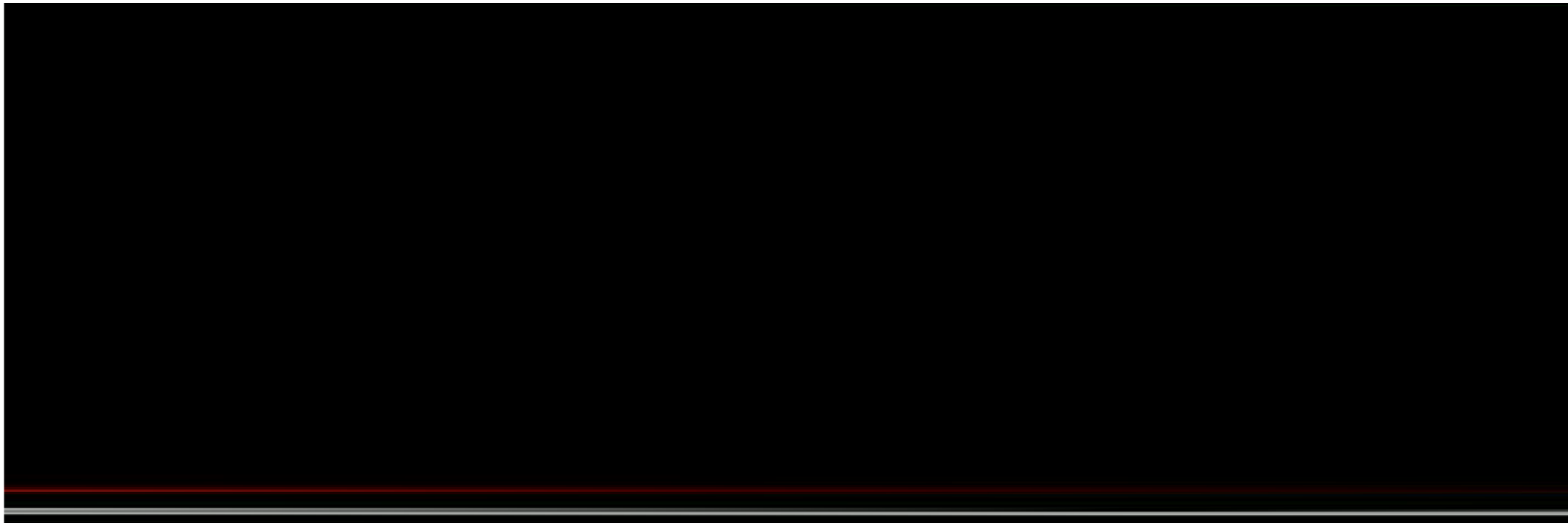
# Laser plasma acceleration (LPA)

surfer wake boat



e- beam wake laser

# Modeling from first principle is very challenging



**For a 10 GeV scale stage:**

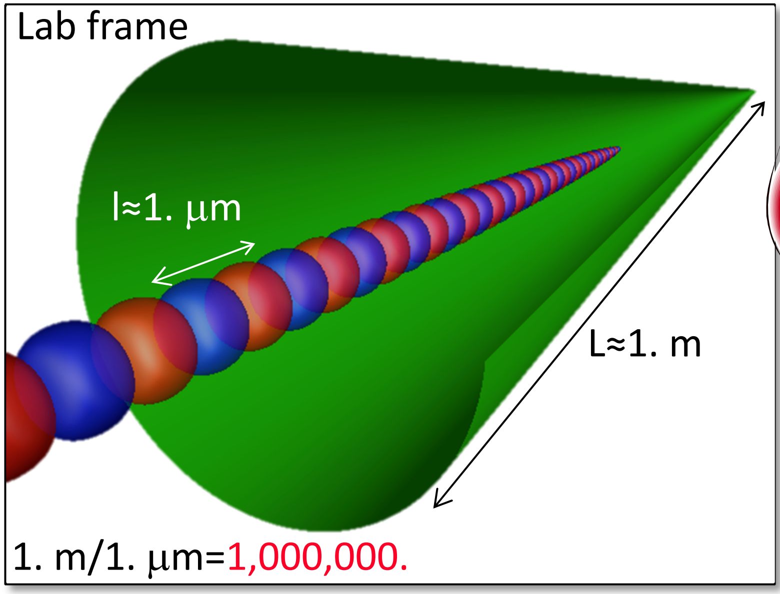
~1μm wavelength laser propagates into ~1m plasma

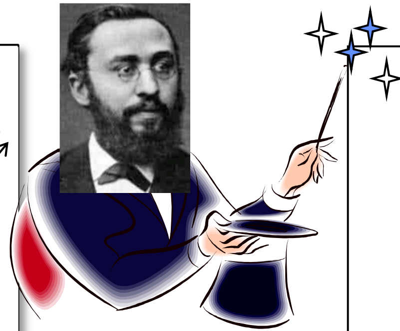
➔ millions of time steps needed

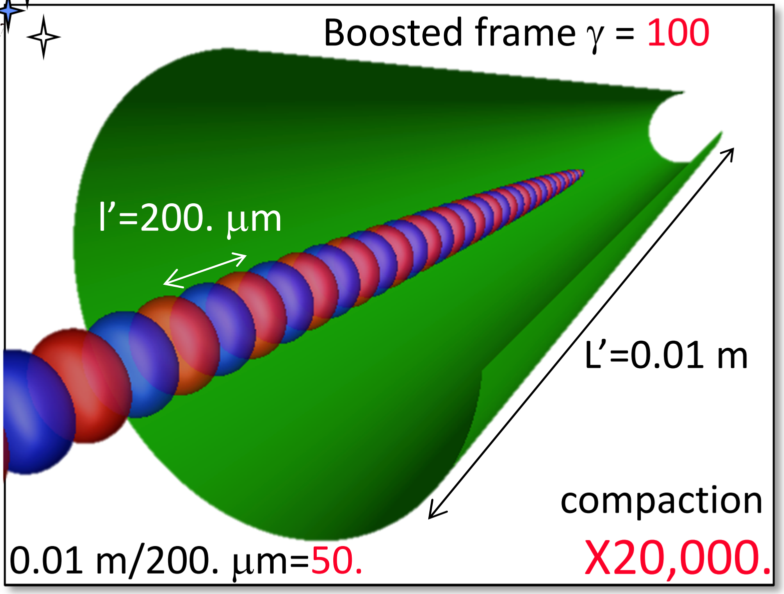
**Physics insight**

**Lorentz boosted frame ➔ lower # time steps**

# Lorentz boosted frame reduces scale range by orders of magnitude*

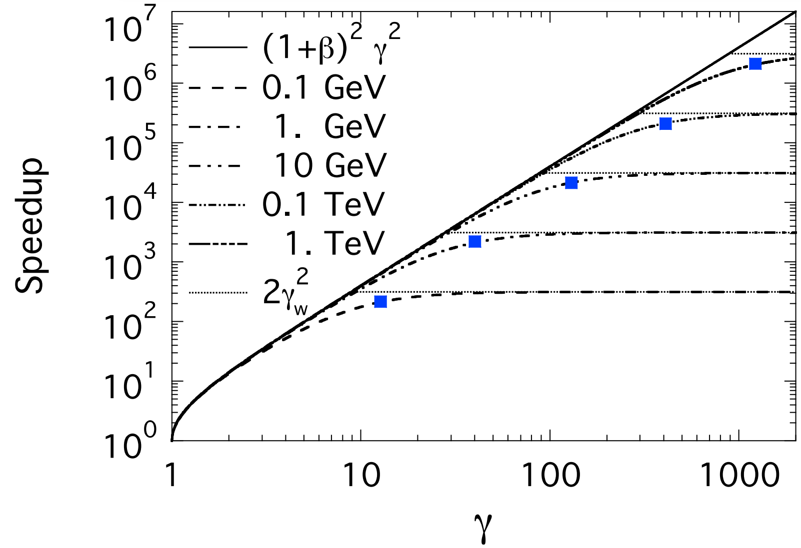



Predicted speedup*:

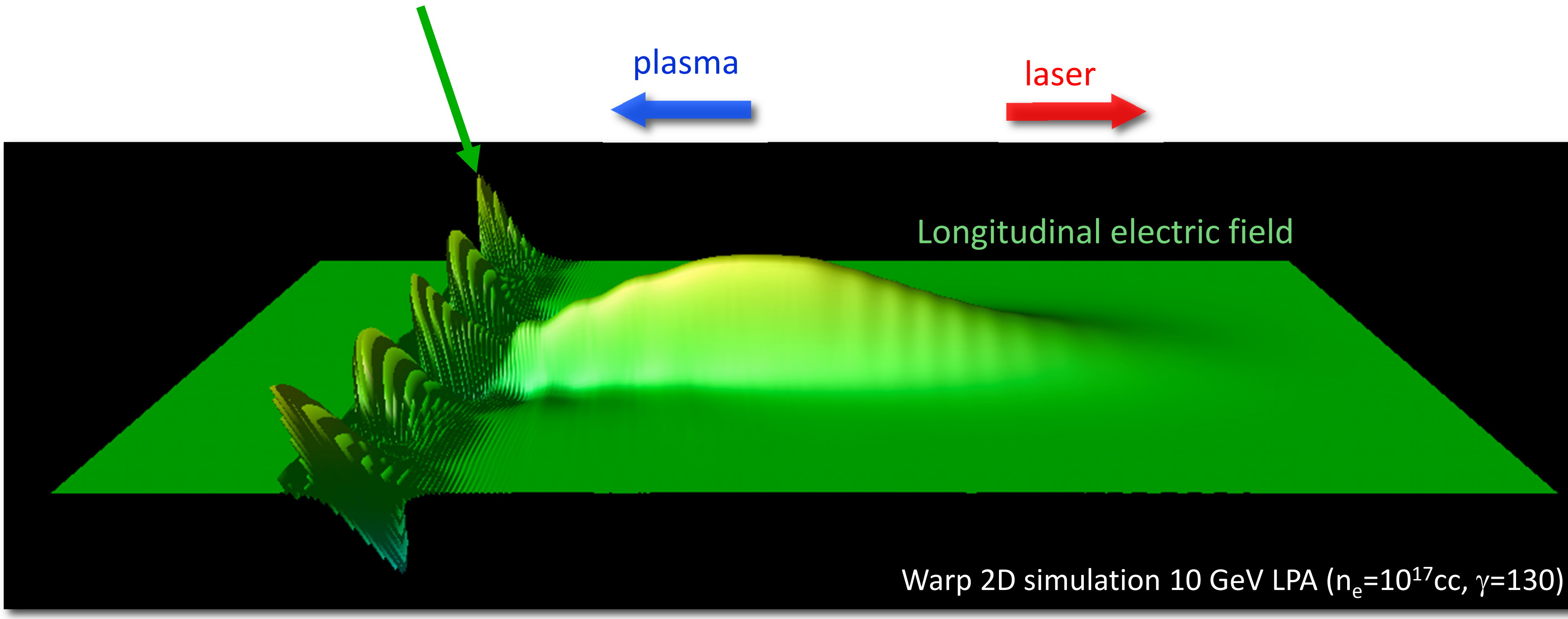
- > 10,000 for single 10 GeV (Bella) stage,
- > 1,000,000 for single 1 TeV stage.




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

# Complication

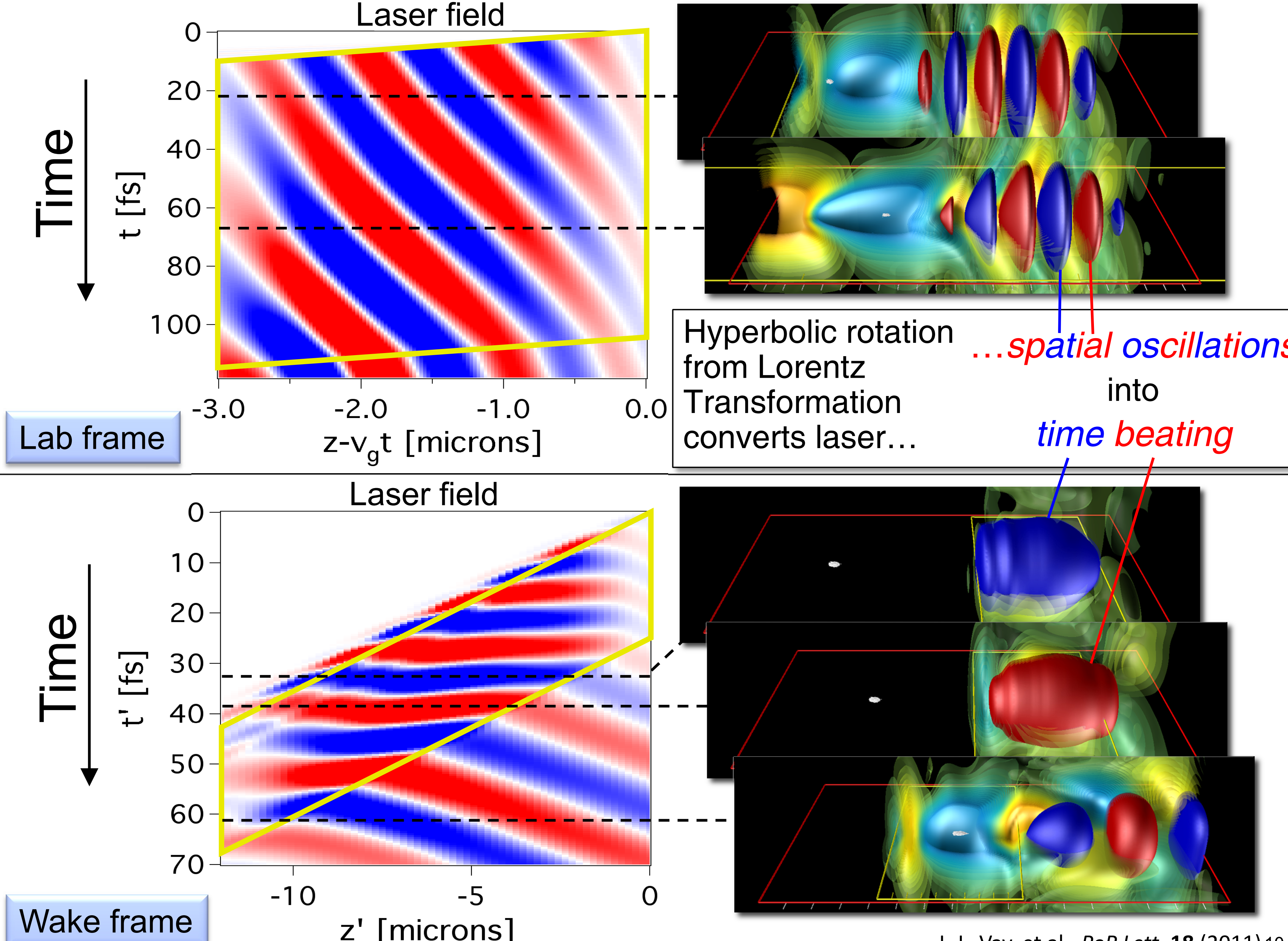
## Short wavelength instability observed at entrance of plasma for large $\gamma$ ($\varepsilon$ 100)



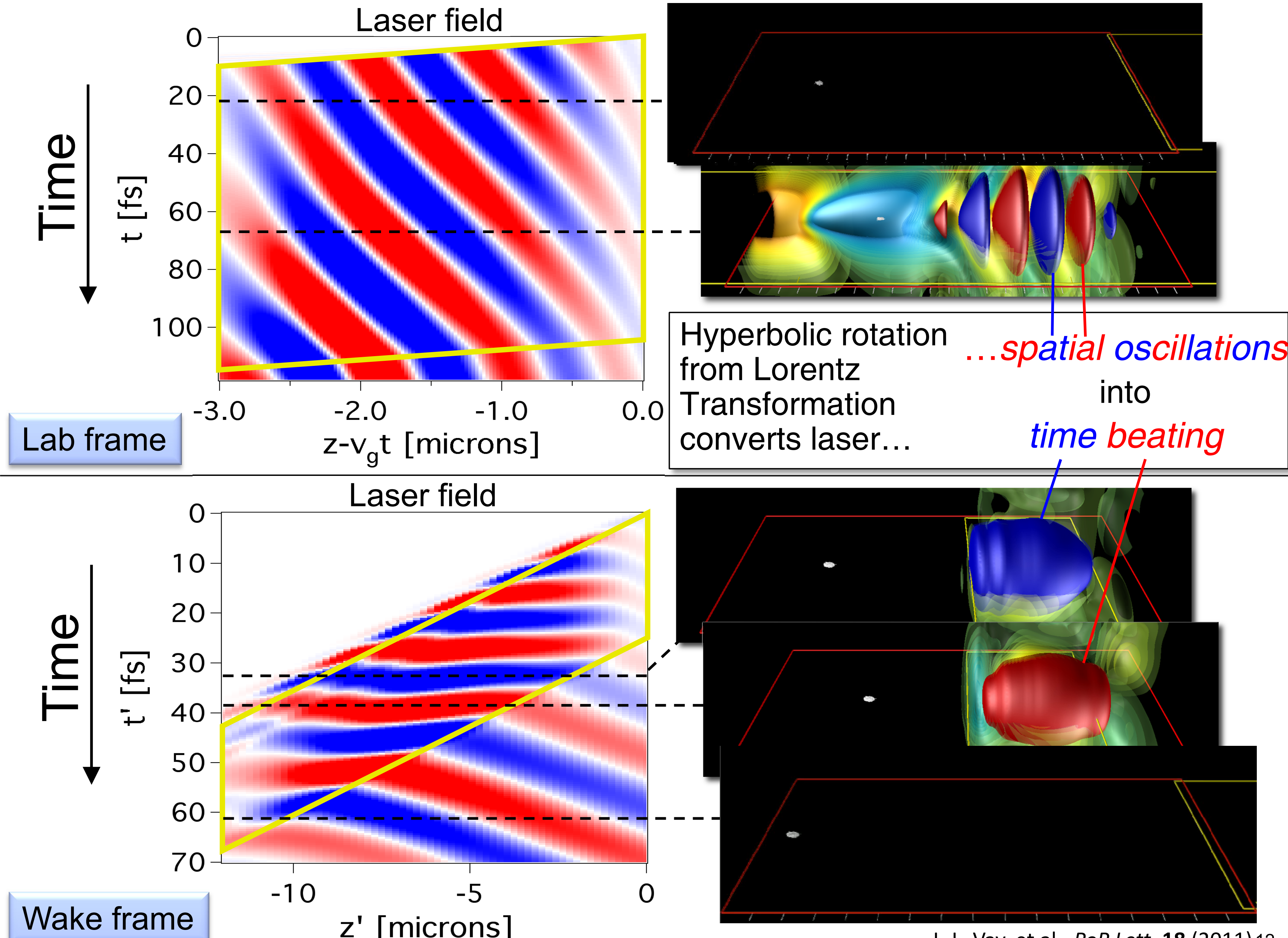

Instability at short wavelength: can it be filtered?

**Physics insight**

**Hyperbolic rotation → more filtering**




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

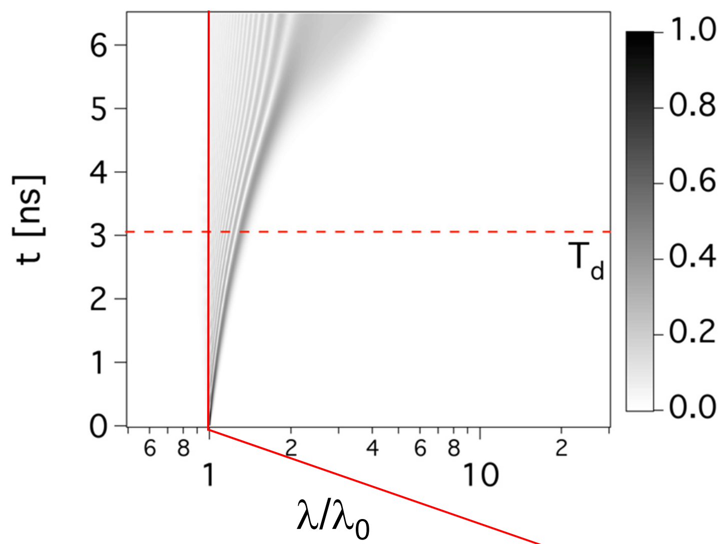



J.-L. Vay, et al., *PoP Lett.* **18** (2011).

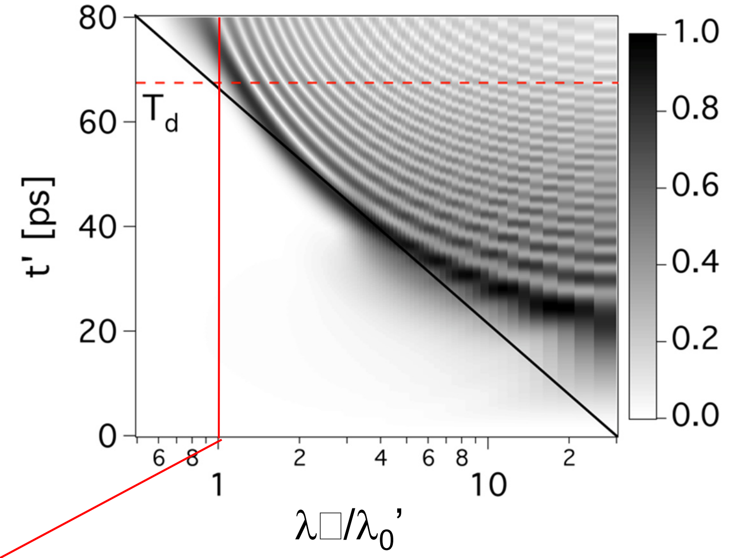
# More filtering is possible without altering physics

Laser spectrum on axis

**Lab frame**




**Frame of wake (γ=130)**



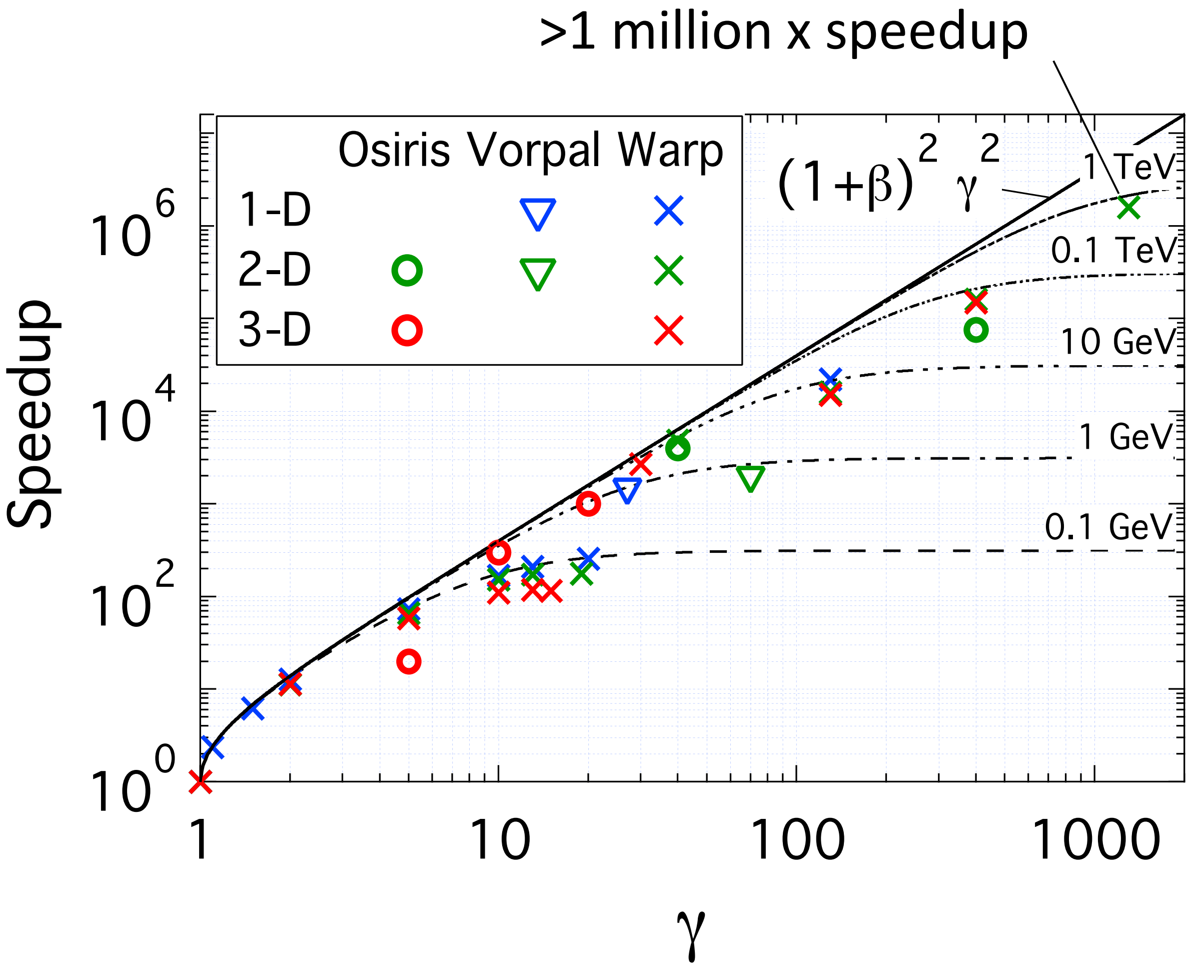

Laser in vacuum

Content concentrated around $\lambda_0$

Content concentrated at much larger $\lambda$

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

# 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 stage

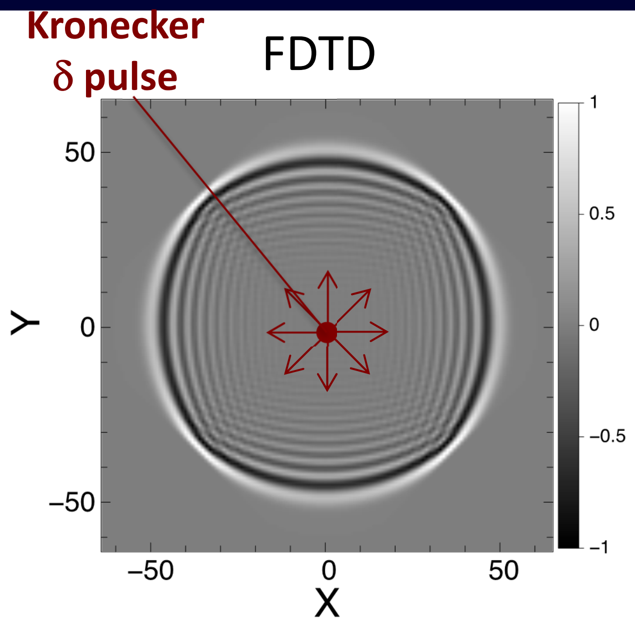
2006 (lab): in 1D ~ 5k CPU-hours ➔ 2011 (boost): in 3D ~ 1k CPU-hours

**Filtering the instability is good,**

**understanding the instability is better:**

**➔ stability analysis.**

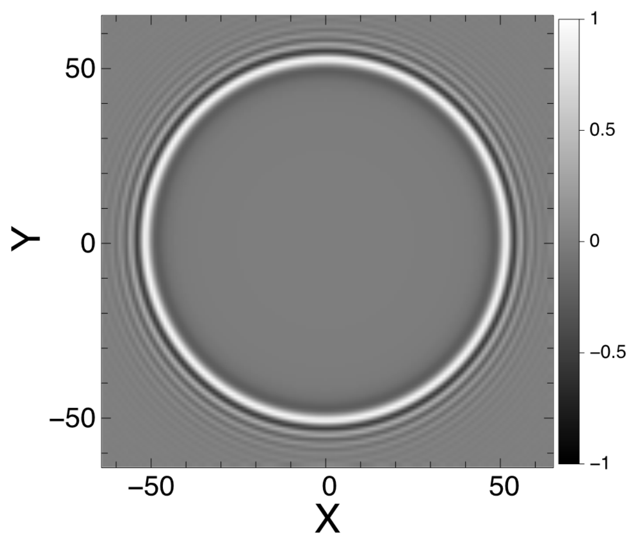
# Analysis performed for various field solvers




- Numerical dispersion,
- anisotropy,
- Courant condition:

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

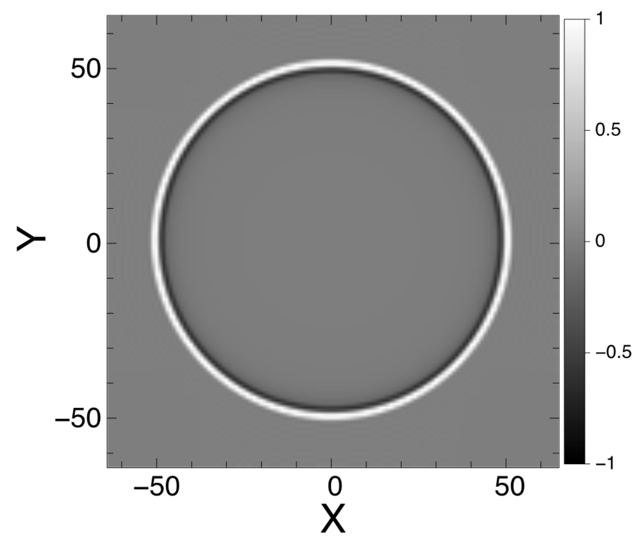
## PSTD




- Numerical dispersion,
- isotropy,
- Courant condition:

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

## PSATD




- Exact dispersion,
- isotropy,
- Courant condition:

**None**

FDTD = Finite-Difference Time Domain: Warp[1] (LBNL/LLNL/U. Maryland), Osiris[2] (UCLA)
PSTD = Pseudo-Spectral Time Domain: UPIC-EMMA[2] (UCLA)
PSATD = Pseudo-Spectral Analytical Time Domain: Warp[3] (LBNL/LLNL/U. Maryland)

[1]B. B. Godfrey, J.-L. Vay, "Numerical stability of relativistic beam multidimensional PIC simulations employing the Esirkepov algorithm" J. Comp. Phys. 248 (2013)
[2]X. Xu, et al, "Numerical instability due to relativistic plasma drift in EM-PIC simulations", Comp. Comm. Phys. 184 (2013)
[3]B. B. Godfrey, J. L. Vay, I. Haber, "Numerical stability analysis of the PSATD-PIC algorithm", *submitted*

# Numerical dispersion relation of spectral-PIC algorithm*

**2-D numerical dispersion relation (Fourier space):**

$$\begin{pmatrix} \xi_{z,z} + [\omega] & \xi_{z,x} & \xi_{z,y} + [k_x] \\ \xi_{x,z} & \xi_{x,x} + [\omega] & \xi_{x,y} - [k_z] \\ [k_x] & -[k_z] & [\omega] \end{pmatrix} \begin{pmatrix} E_z \\ E_x \\ B_y \end{pmatrix} = 0.$$

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

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

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

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

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

*B. B. Godfrey, J. L. Vay, I. Haber, "Numerical stability analysis of the Pseudo-Spectral Analytical Time-Domain PIC algorithm", *submitted*

# Numerical dispersion relation of spectral PIC algorithm (II)

$$\xi_{z,z} = -n\gamma^{-2} \sum_m S^J S^{E_z} \csc^2 \left[ \left( \omega - k'_z v \right) \frac{\Delta t}{2} \right] \left( k k_z^2 \Delta t + \zeta_z k_x^2 \sin\left( k \Delta t \right) \right) \Delta t \left[ \omega \right] k'_z / 4k^3 k_z,$$

$$\xi_{z,x} = -n \sum_m S^J S^{E_x} \csc \left[ \left( \omega - k'_z v \right) \frac{\Delta t}{2} \right] \eta_z k'_x / 2k^3 k_z,$$

$$\xi_{z,y} = nv \sum_m S^J S^{B_y} \csc \left[ \left( \omega - k'_z v \right) \frac{\Delta t}{2} \right] \eta_z k'_x / 2k^3 k_z,$$

$$\xi_{x,z} = -n\gamma^{-2} \sum_m S^J S^{E_z} \csc^2 \left[ \left( \omega - k'_z v \right) \frac{\Delta t}{2} \right] \left( k \Delta t - \zeta_z \sin\left( k \Delta t \right) \right) \Delta t \left[ \omega \right] k_x k'_z / 4k^3,$$

$$\xi_{x,x} = -n \sum_m S^J S^{E_x} \csc \left[ \left( \omega - k'_z v \right) \frac{\Delta t}{2} \right] \eta_x k'_x / 2k^3 k_x,$$

$$\xi_{x,y} = nv \sum_m S^J S^{B_y} \csc \left[ \left( \omega - k'_z v \right) \frac{\Delta t}{2} \right] \eta_x k'_x / 2k^3 k_x,$$

# Numerical dispersion relation of spectral PIC algorithm (III)

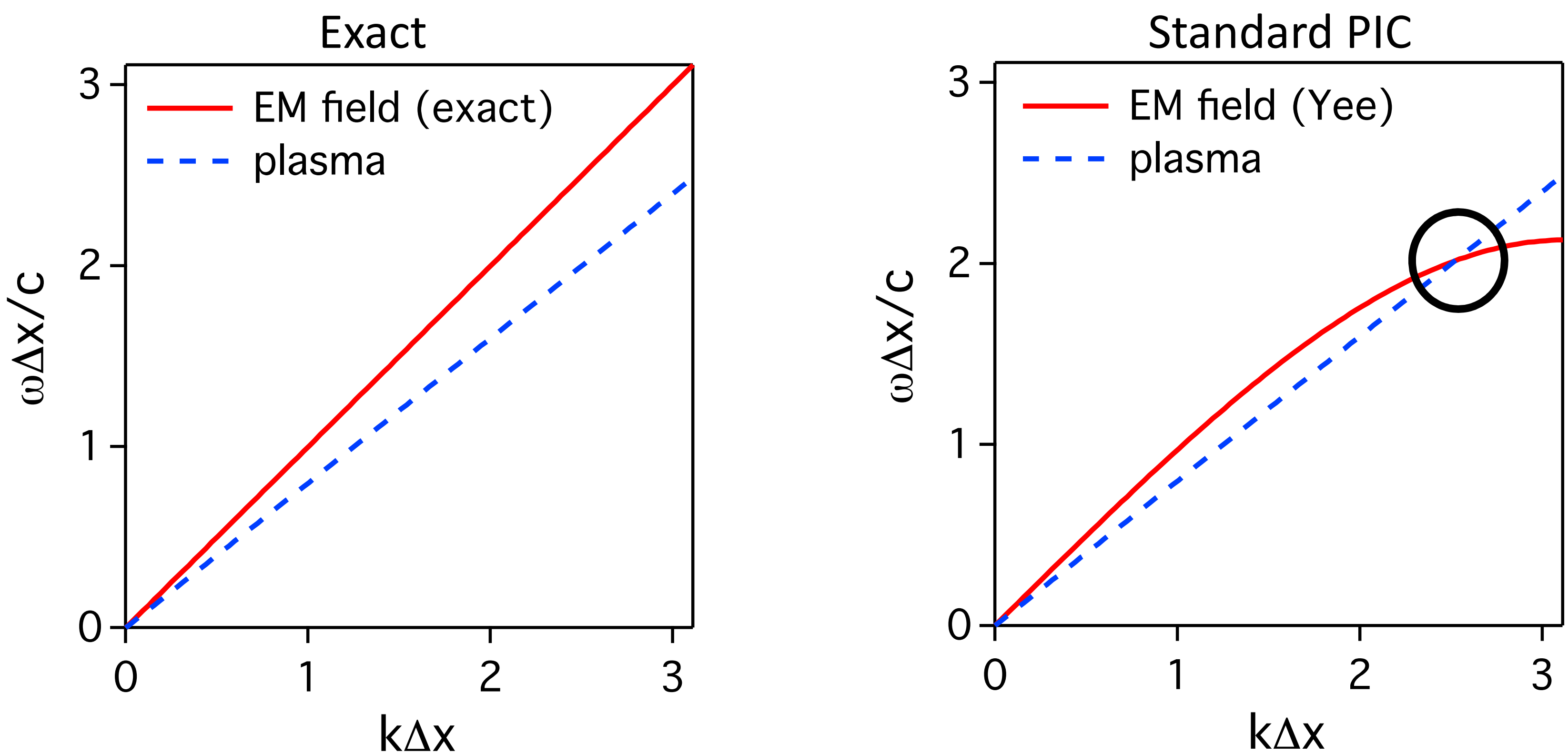
$$\eta_z = \cot\left[\left(\omega - k'_z v\right)\frac{\Delta t}{2}\right]\left(k k_z^2 \Delta t + \zeta_z k_x^2 \sin\left(k\Delta t\right)\right)\sin\left(k'_z v \frac{\Delta t}{2}\right) + \left(k\Delta t - \zeta_x \sin\left(k\Delta t\right)\right) k_z^2 \cos\left(k'_z v \frac{\Delta t}{2}\right),$$

$$\eta_x = \cot\left[\left(\omega - k'_z v\right)\frac{\Delta t}{2}\right]\left(k\Delta t - \zeta_z \sin\left(k\Delta t\right)\right) k_x^2 \sin\left(k'_z v \frac{\Delta t}{2}\right) + \left(k k_x^2 \Delta t + \zeta_x k_z^2 \sin\left(k\Delta t\right)\right)\cos\left(k'_z v \frac{\Delta t}{2}\right).$$

Then simplify and solve with Mathematica…

# Numerical Cherenkov in 1-D*

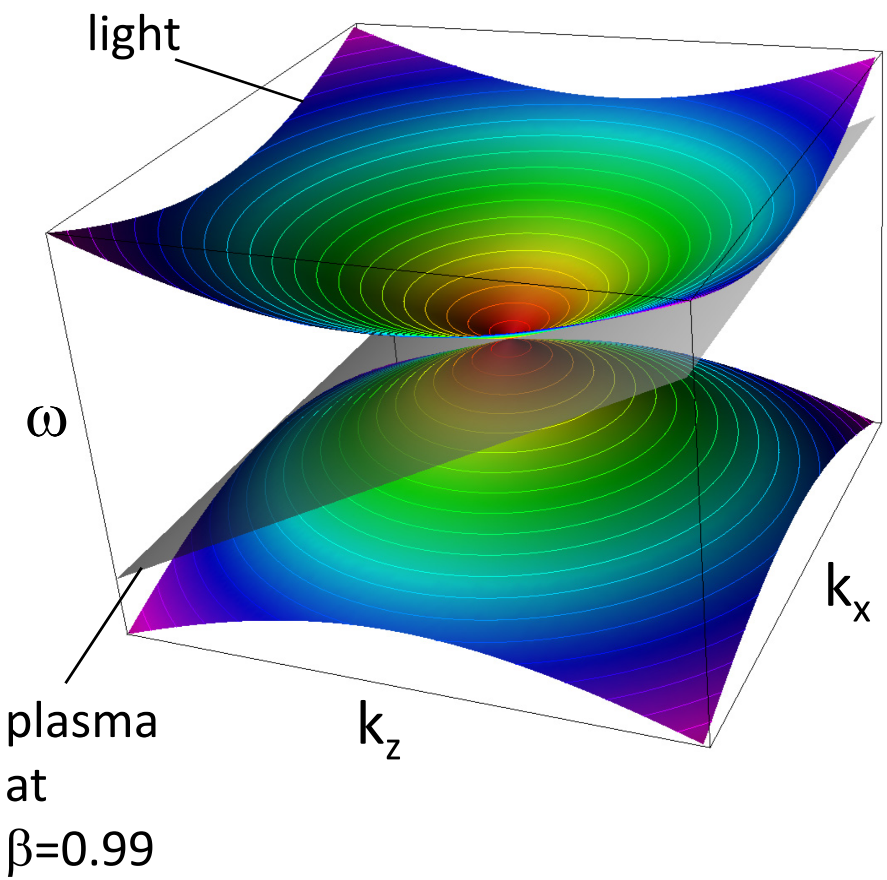
Numerical dispersion leads to crossing of EM field and plasma modes -> instability.



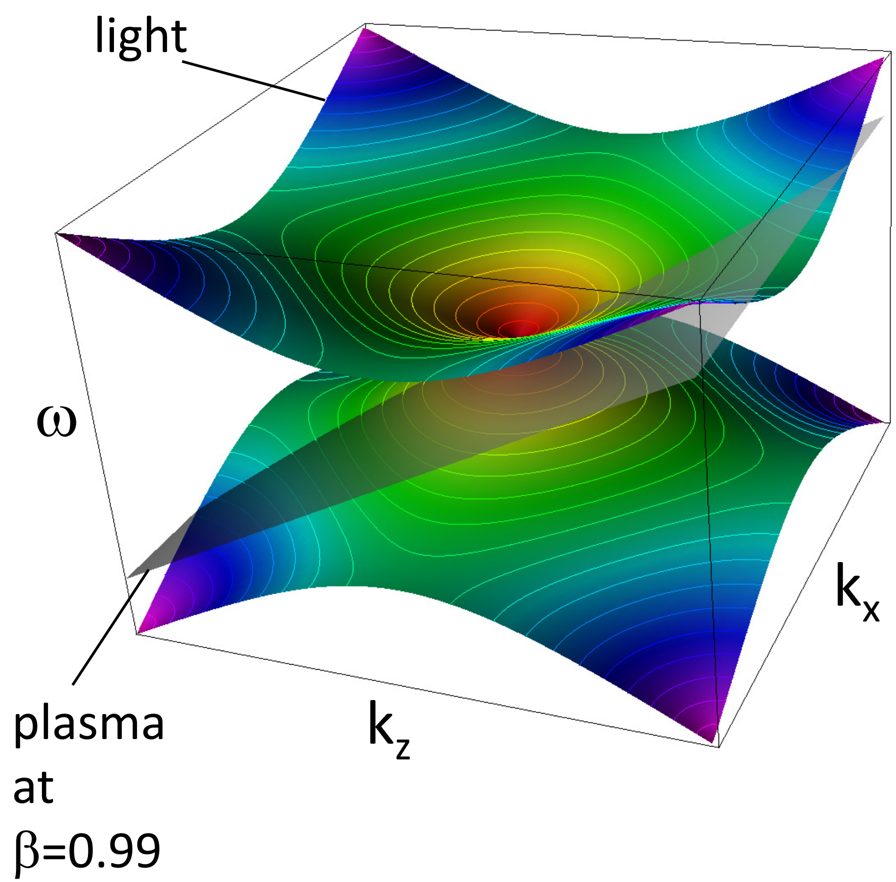

*B. B. Godfrey, “Numerical Cherenkov instabilities in electromagnetic particle codes”, *J. Comput. Phys.* **15** (1974)

# Numerical Cherenkov in 2-D (for $c\Delta t=\Delta x/\mathrm{sqrt}(2)$)

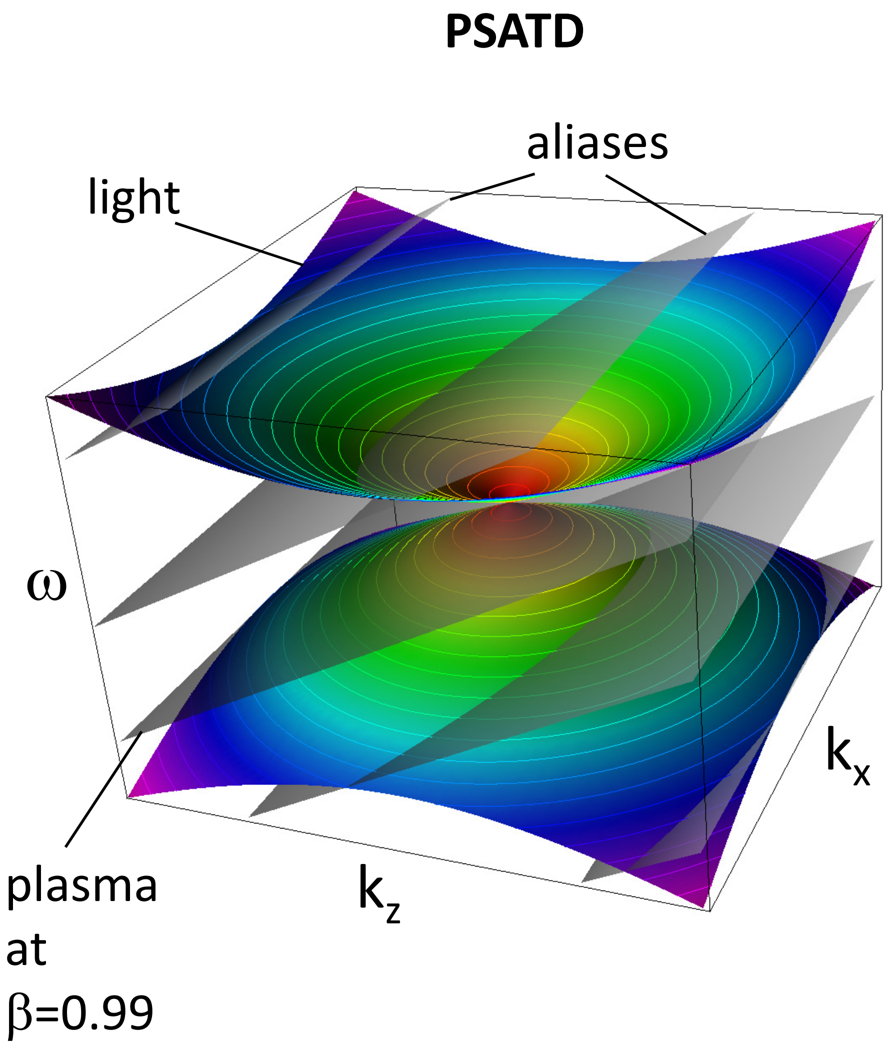
**PSATD**

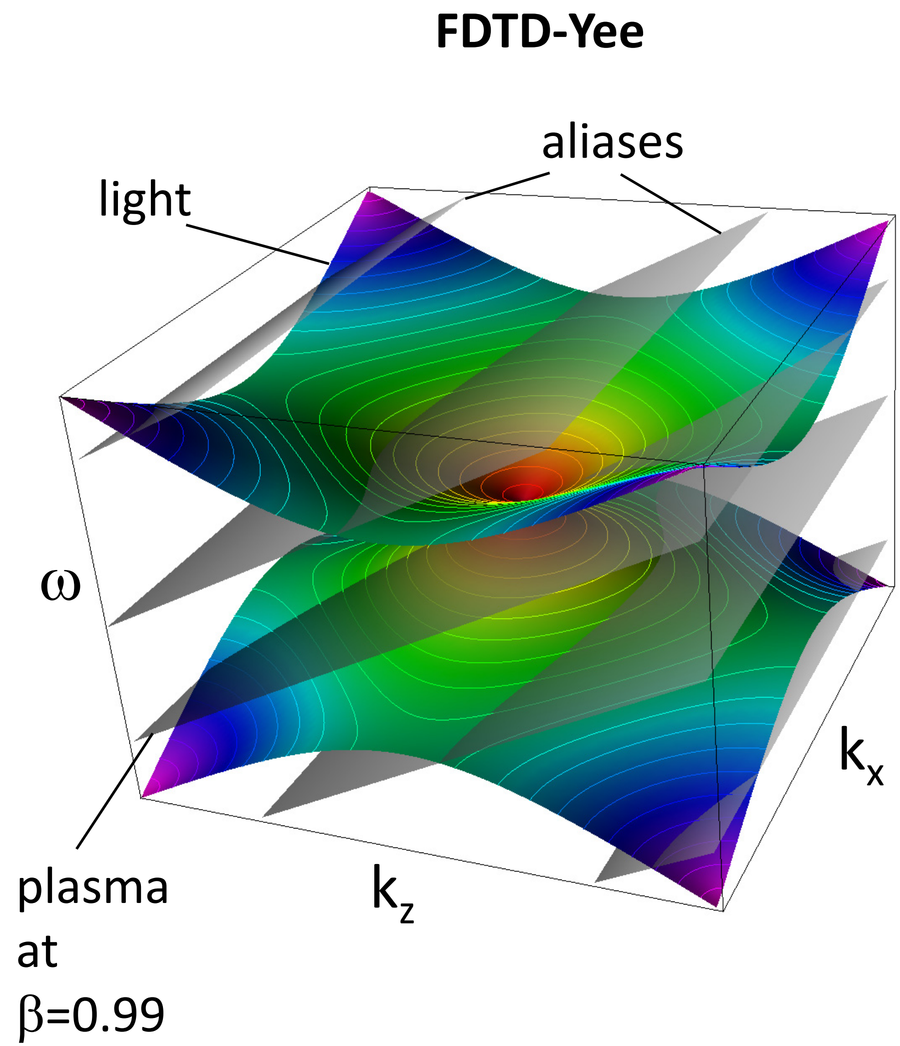



**FDTD-Yee**



# Need to take aliases into account in 2-D

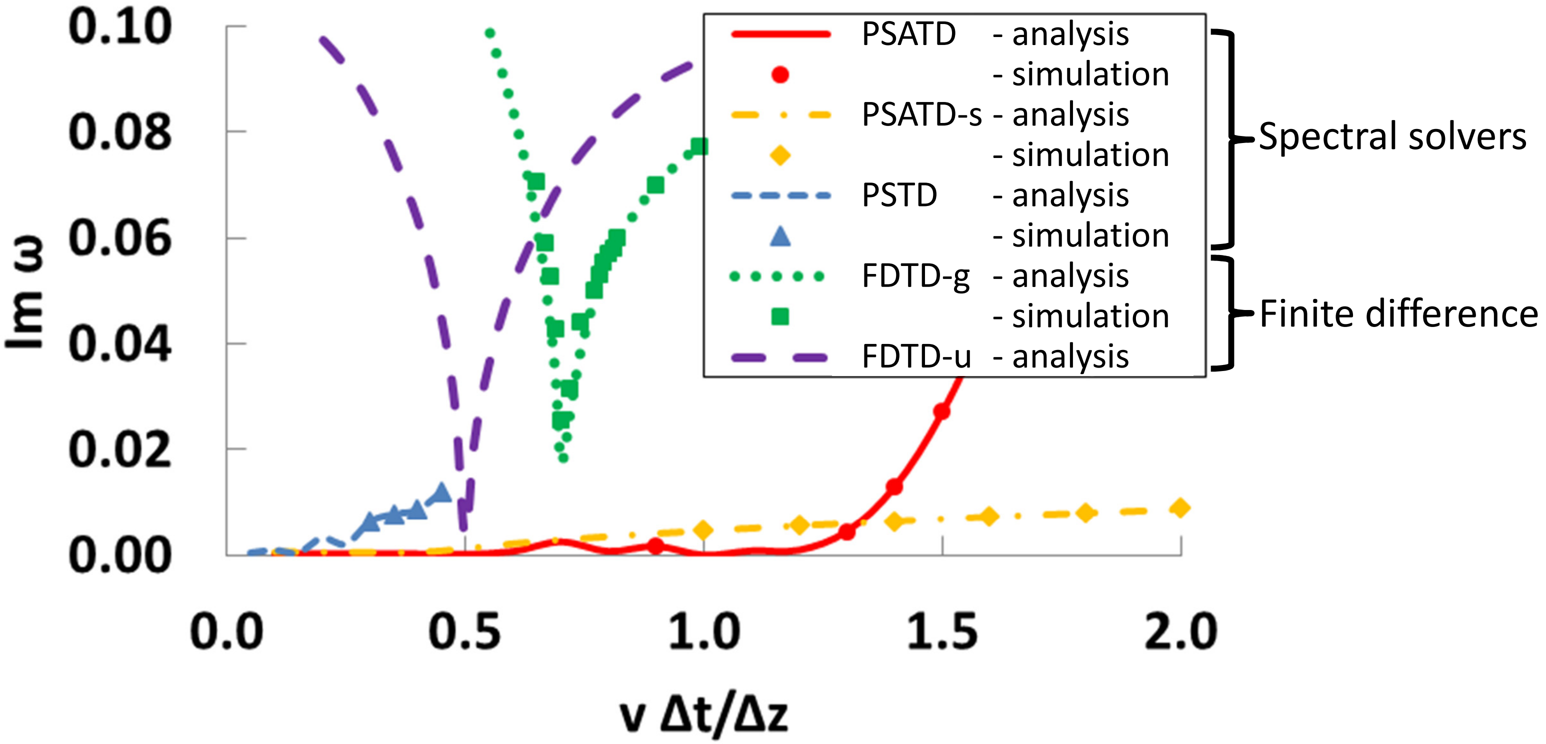



Need to consider at least first aliases $m_x$={-3…+3} to study stability.

# Spectral solvers more stable than finite difference solvers

Growth rates of numerical Cerenkov instabilities



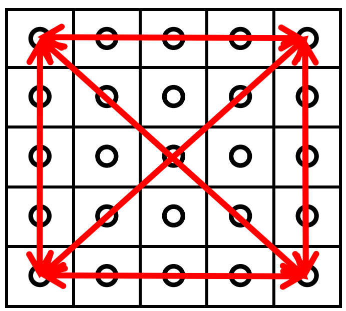

B. B. Godfrey, J.-L. Vay, "Numerical stability of relativistic beam multidimensional PIC simulations employing the Esirkepov algorithm" J. Comp. Phys. 248 (2013)

# But spectral solvers harder to scale to large # of cores

**Spectral**

global "costly"

communications



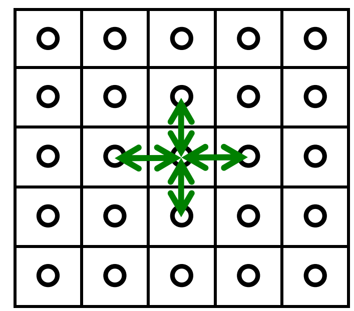
Harder to scale

vs

**Finite Difference**

local "cheap"

communications

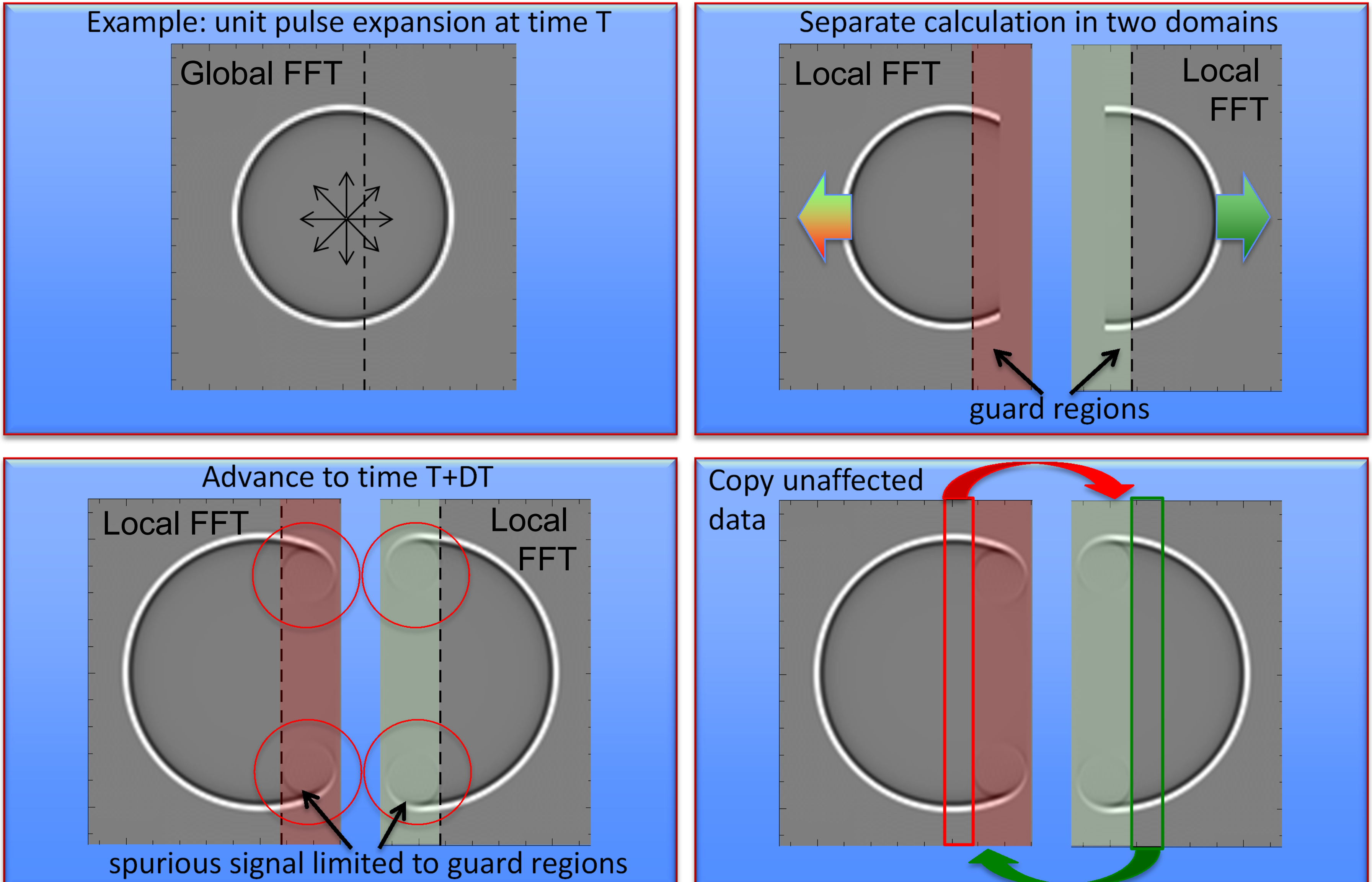


Easier to scale

**Physics insight**

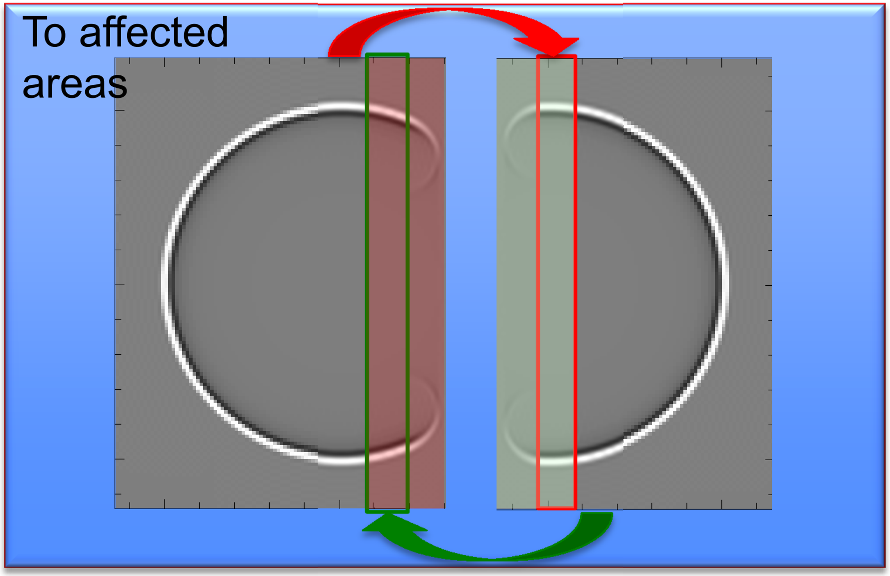
**Finite speed of light → local FFTs**

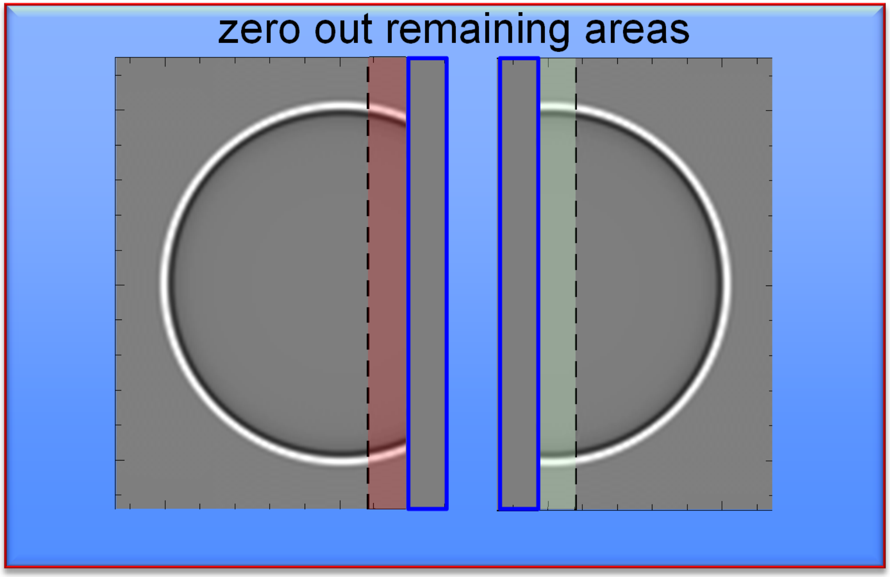
# New concept on single pulse – part 1

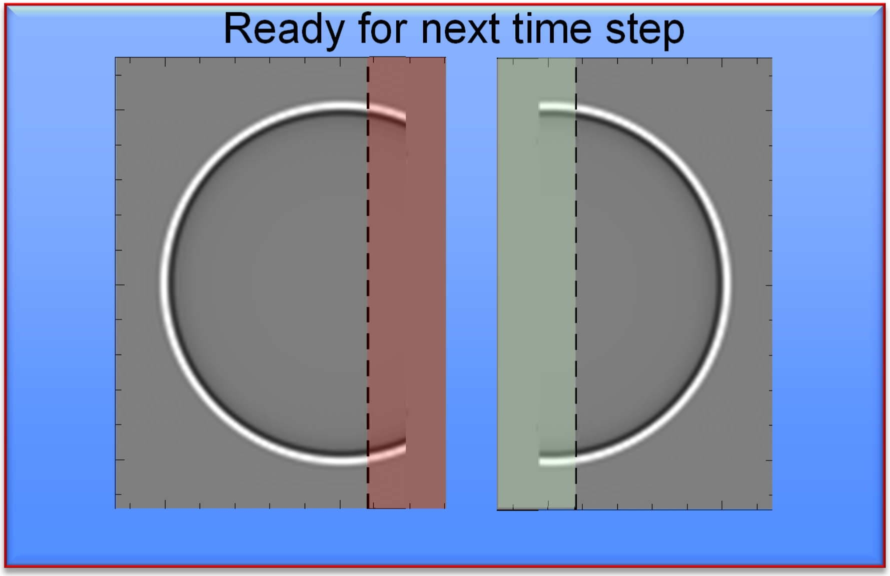


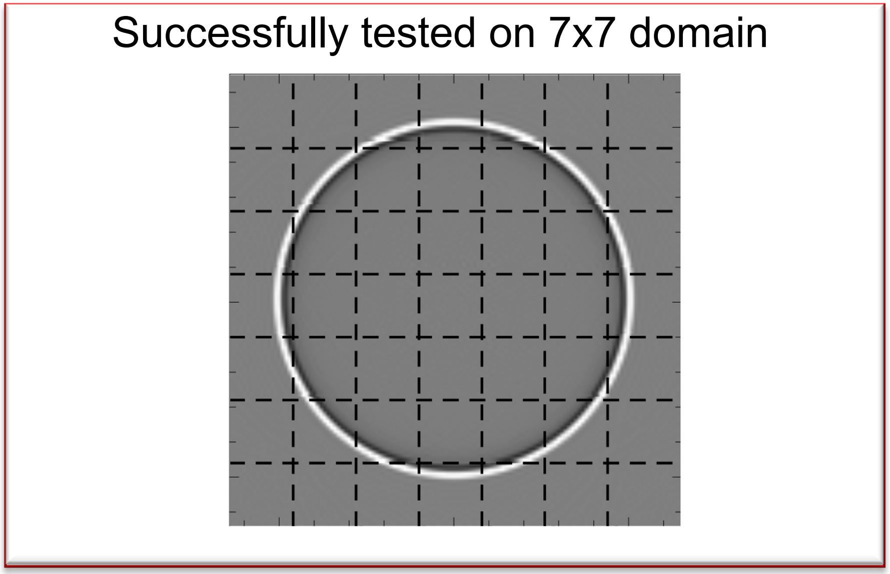

*J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

# New concept on single pulse – part 2



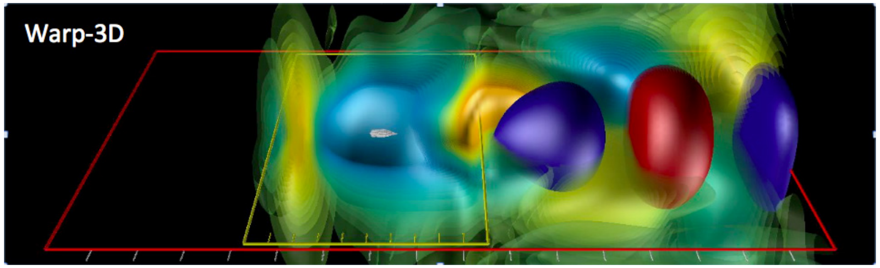



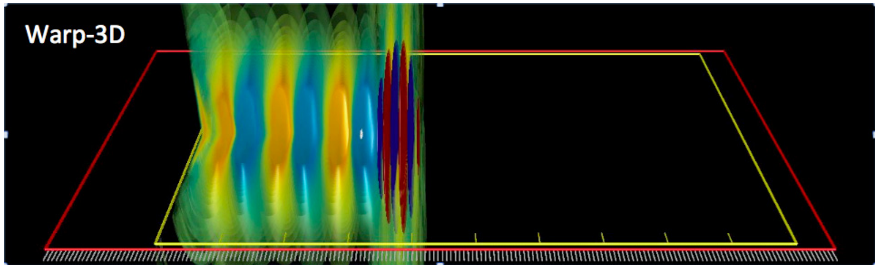

*J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

# Successfully tested on 2-D modeling of short LPA stages

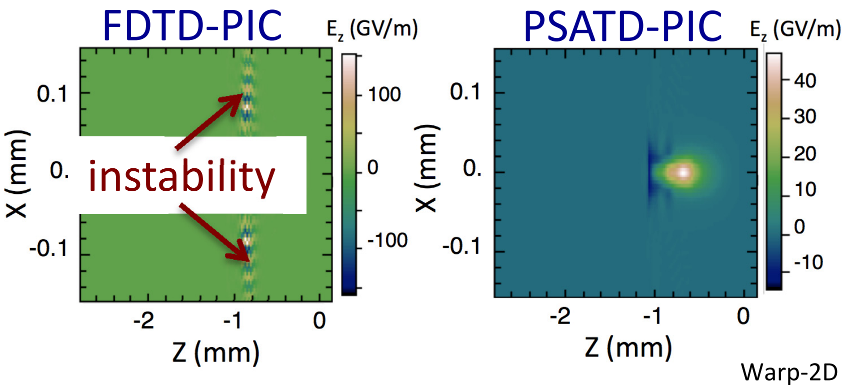
Lorentz boosted frame (wake)



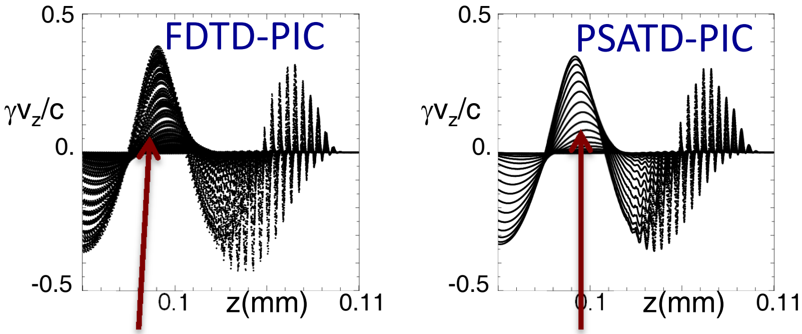

Lab frame




Improved stability




Improved phase space accuracy




spurious heating

➔ Artificial trapping

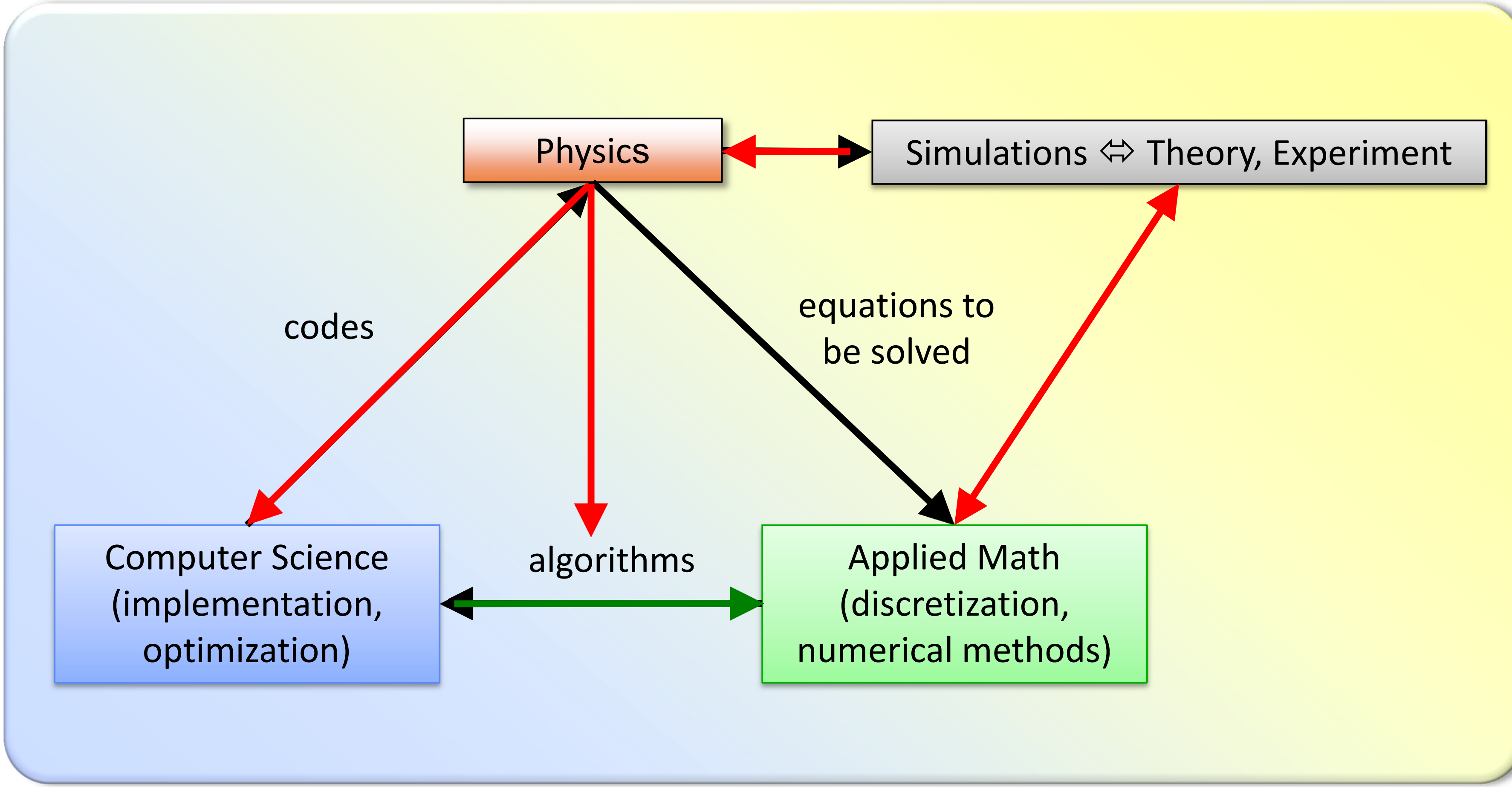
correct behavior

Warp-2D

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

# Modeling of beams and accelerators is complex

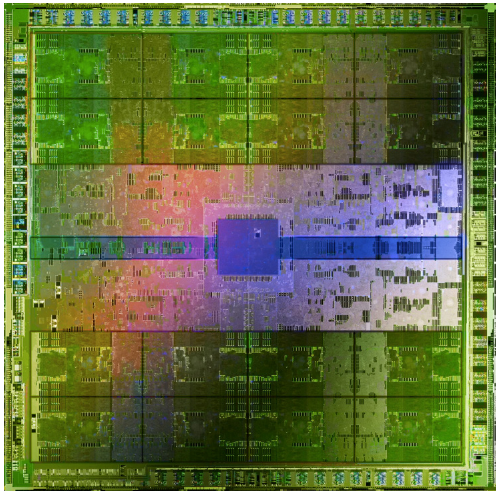
Physics impacts all aspects of modeling of beams and accelerators.



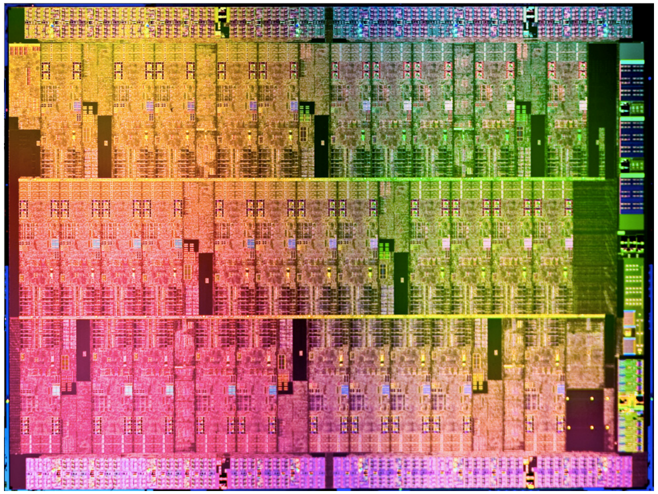
# Summary & Outlook

- **Importance** of computer modeling is **on the rise**.
- Modeling of B&A are **very complex** and **specialized tasks.**
- Expect to see emergence of **local** and **global (virtual) centers**:
  - teams of **physicists** + **applied math** + **computer scientists,**
  - **dedicated** to the **science** and **technology** of **B&A modeling,**
  - develop codes **w/ more physics** on **more complex** machines.

NVIDIA GPU Fermi



Intel MIC



# Thanks!

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- LOASIS/BELLA: W. Leemans, C. Geddes, E. Cormier (now Tech-X).
- Center for Beam Physics: W. Fawley, M. Furman.
- Heavy Ion Fusion Virtual National Lab : Alex Friedman & Dave Grote for Warp.