Massively parallel *ab initio* plasma simulations using the particle-in-cell method

E. Paulo Alves

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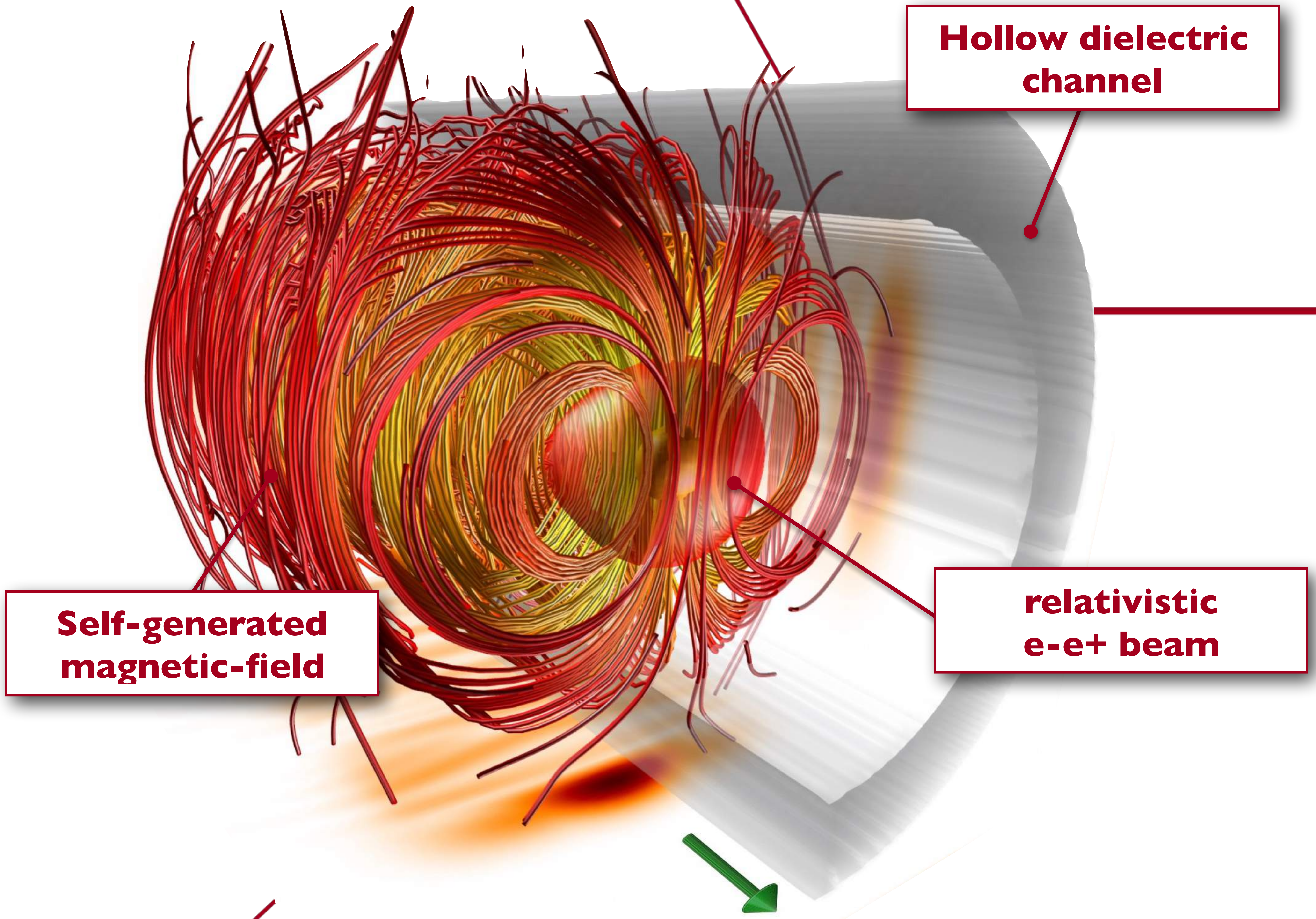

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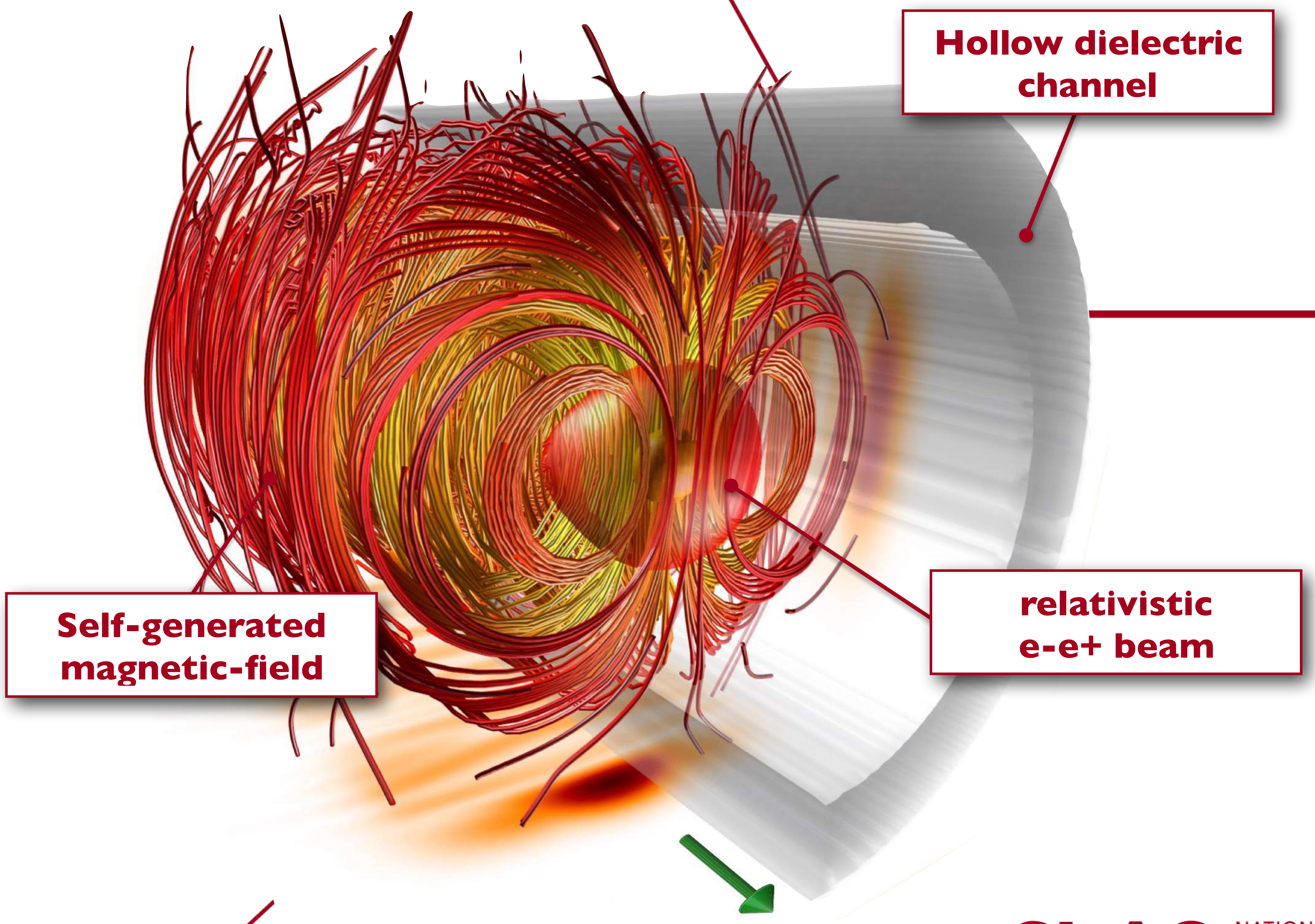

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Acknowledgements

Work in collaboration with:

- ★ **F. Fiuza**, S. Glenzer (SLAC/Stanford)
- ★ W. Mori (UCLA)
- ★ T. Grismayer, R. A. Fonseca, L. O. Silva (IST, Portugal)

HPC resources:

- ★ Juqueen, SuperMUC (PRACE)
- ★ Sequoia, Vulcan (LLNL)
- ★ Mira (ANL)

Financial support from the DOE FES and SLAC LDRD

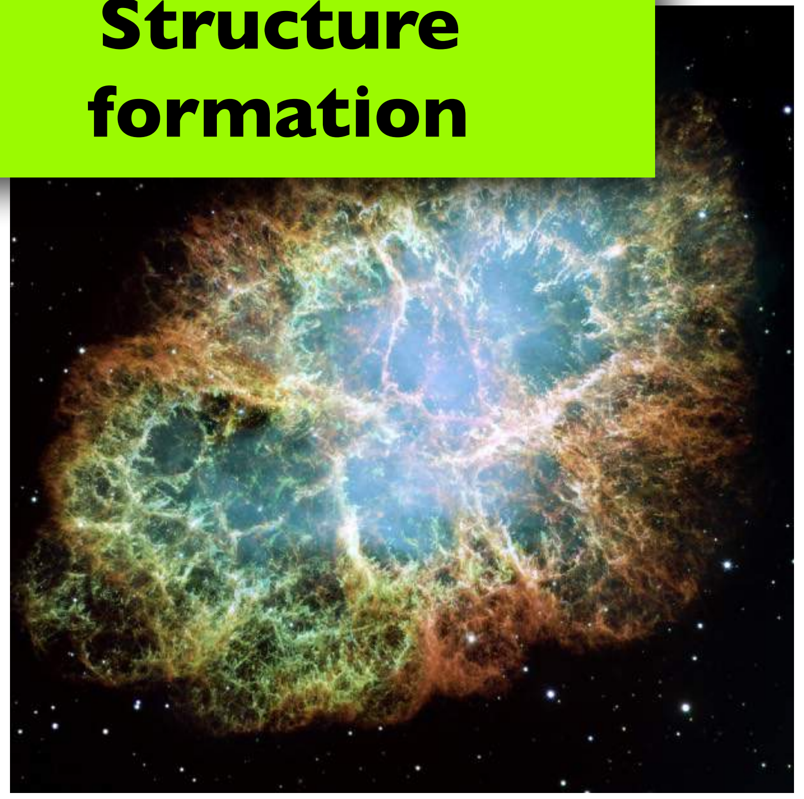
Outline

- **Rich fundamental physics and applications of astrophysical and laboratory plasmas**
- **The Particle-in-Cell (PIC) methodology to model plasmas**
- **Examples of applications in astrophysical and laboratory plasmas**
- **Conclusions and perspectives**

Plasmas in astrophysics and in the laboratory

Microscopic plasma processes underly fundamental questions in space/astrophysics

Structure formation



Hubble Space Telescope, NASA

Radiation emission

http://physicsworld.com

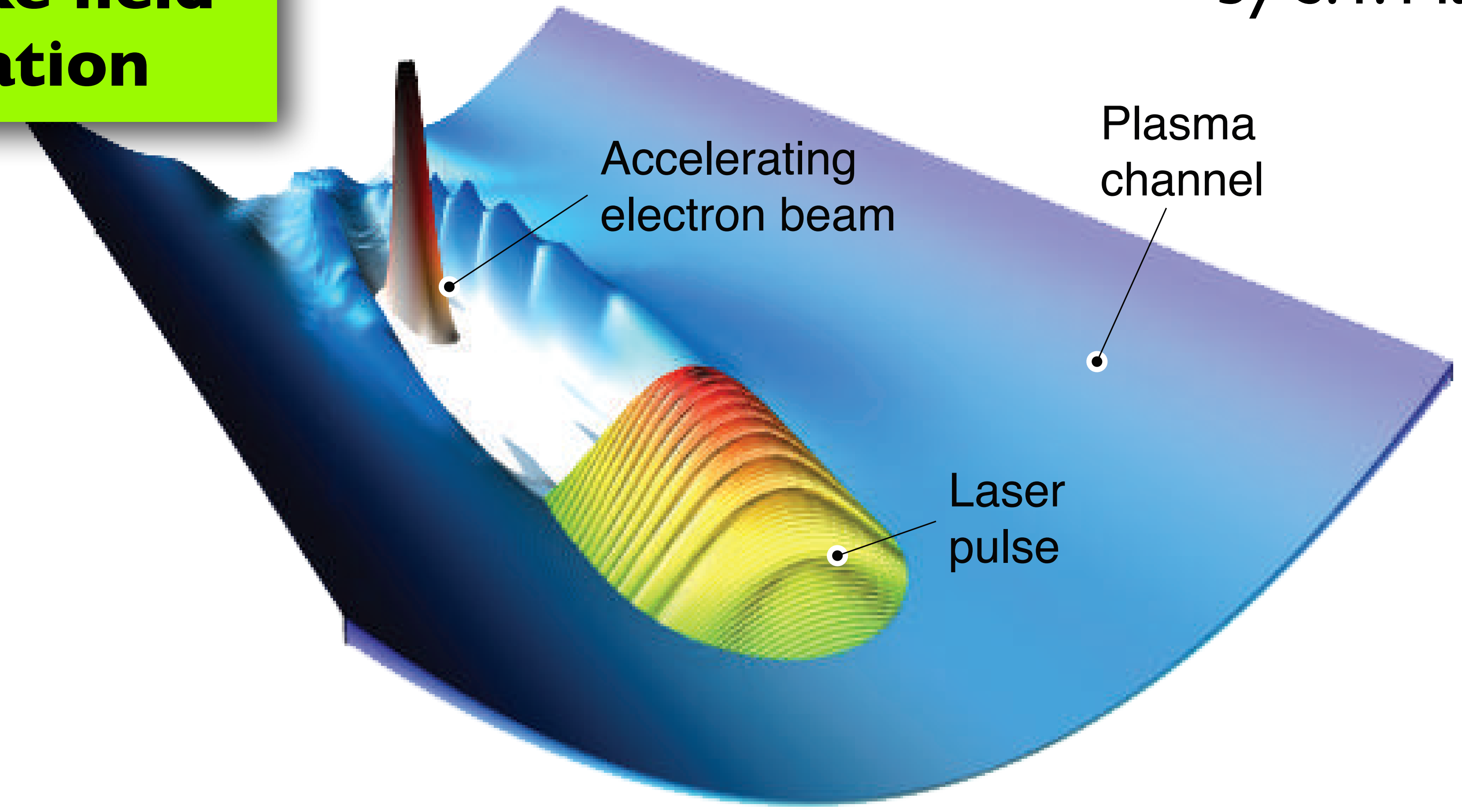
Cosmic ray acceleration

https://science.nasa.gov

Development of compact accelerators and radiation sources

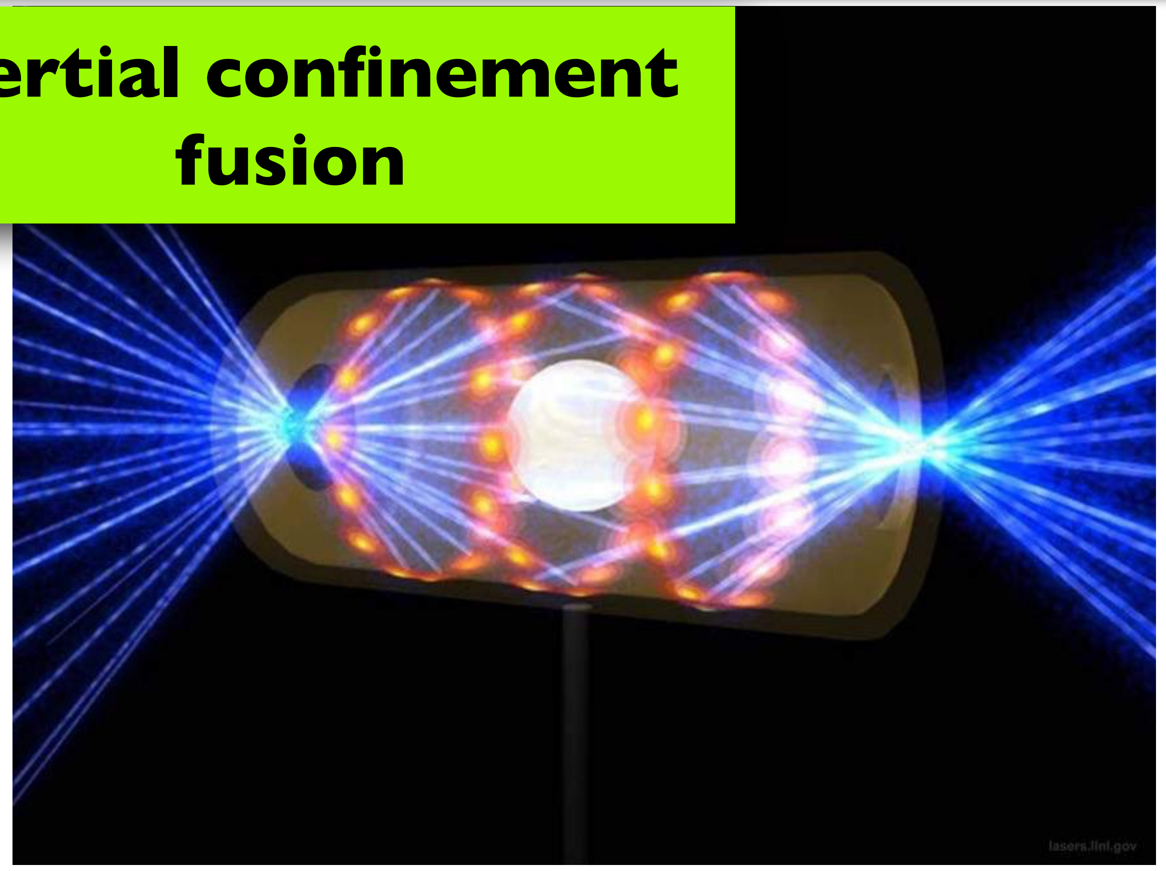
Laser wake field acceleration

by S. F. Martins



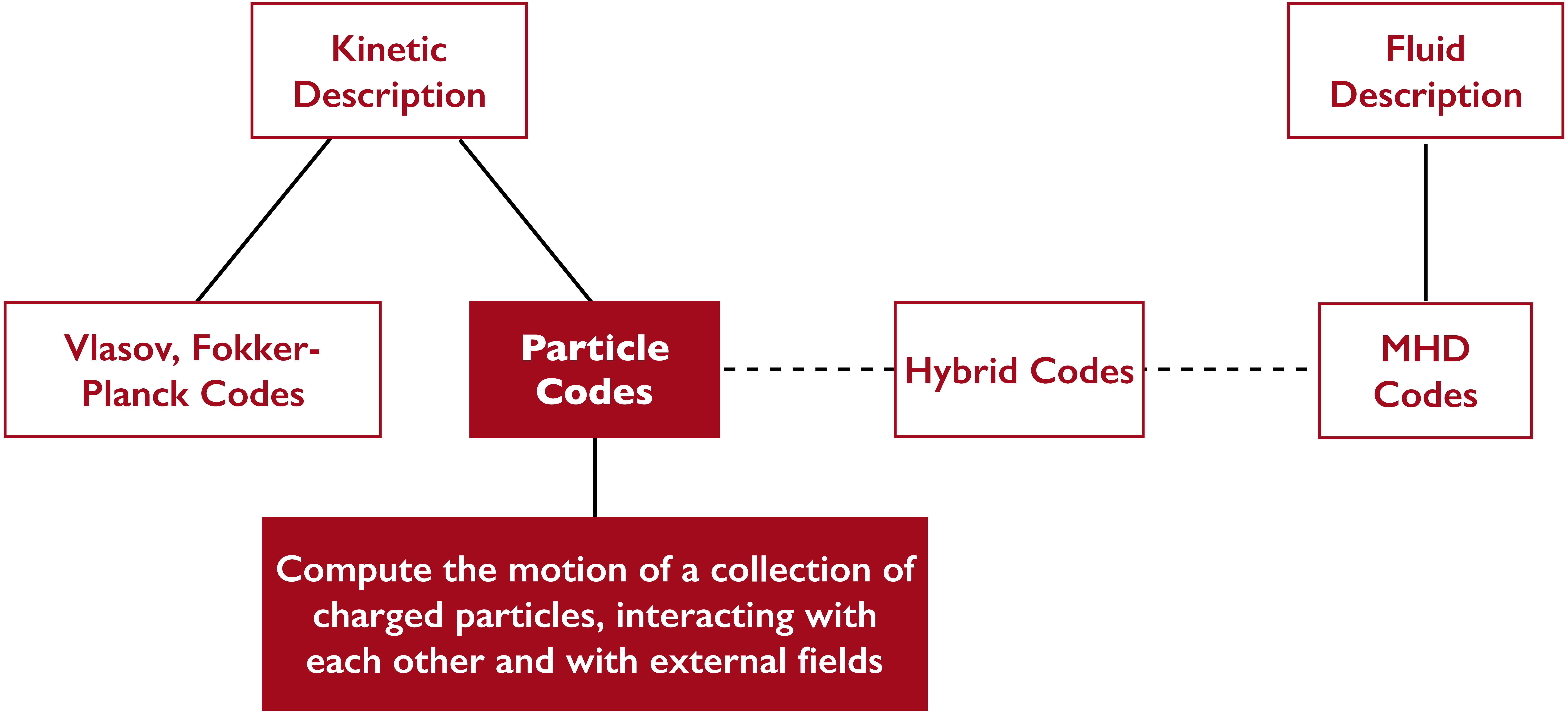
Achieving controlled fusion energy in the lab

Inertial confinement fusion



Lawrence Livermore National Laboratory

Overview of simulation methodologies in plasma physics



The particle-in-cell methodology

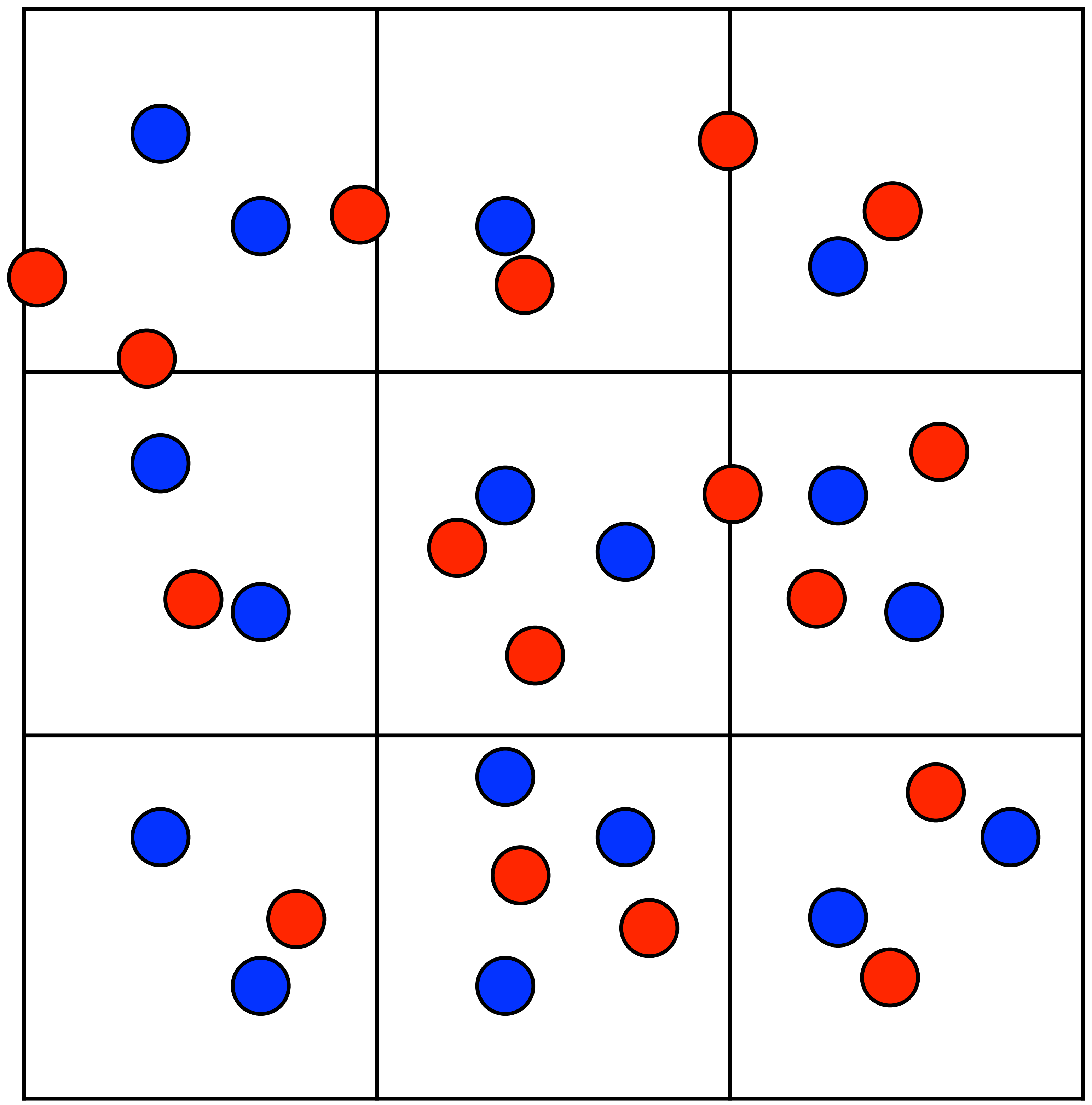
Modeling kinetic physics

- **Particle-particle simulations**
  (# operations $\propto$ N^2)

- **Particle-Mesh simulations**
  (# operations $\propto$ N)
  - Fields + densities
  - Long range interactions

- **Additional MC binary Coulomb collision module can model short range interactions**

Particle-in-cell methodology*



* Dawson, Buneman, 1960's; Birdsall and Langdon, *Plasma Phys. via Comp. Simulation* (1985)

The particle-in-cell methodology

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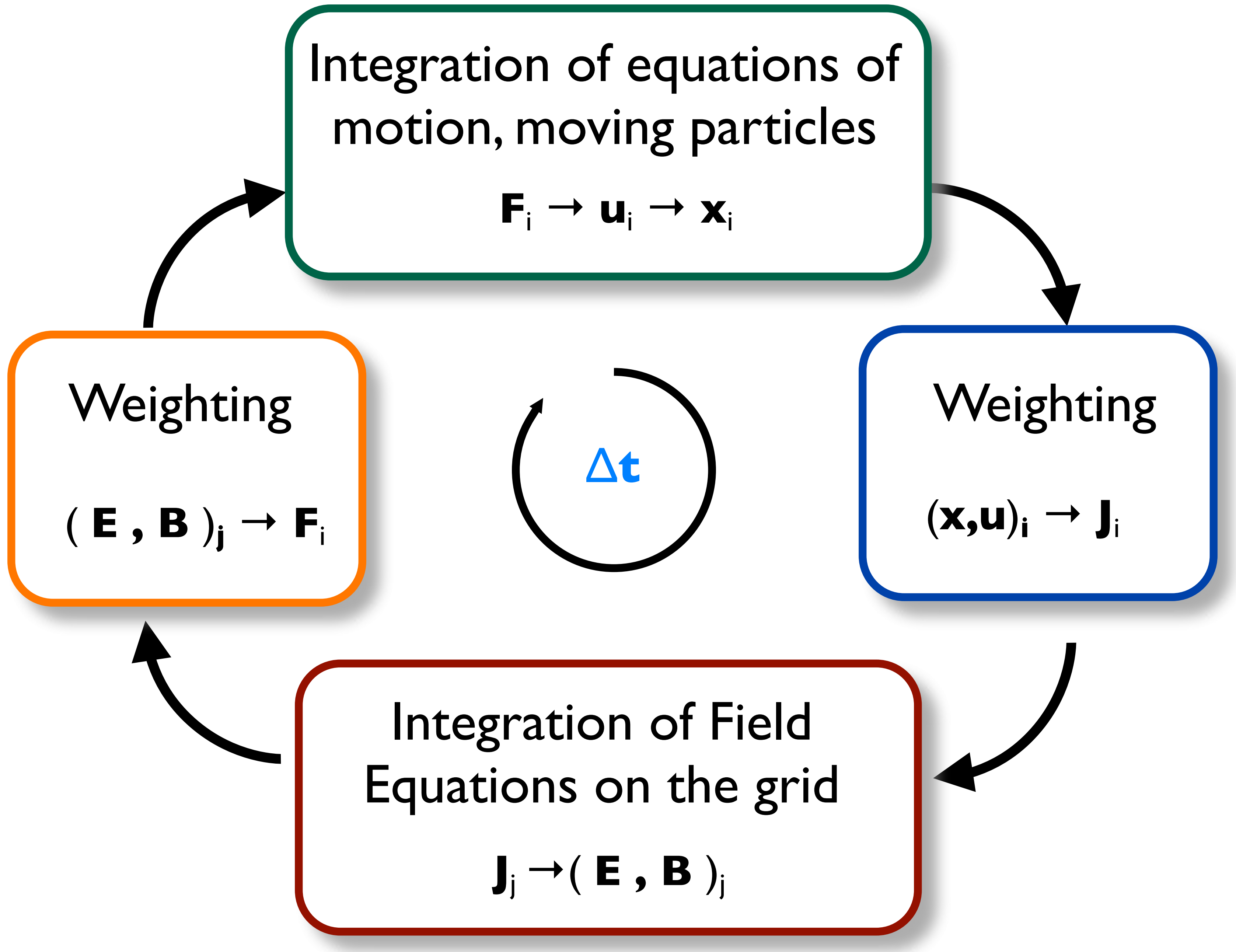
Particle-in-cell methodology*

$$\frac{d\mathbf{u}}{dt} = \frac{q}{m}\left(\mathbf{E} + \frac{1}{\gamma c}\mathbf{u} \times \mathbf{B}\right)$$



$$\frac{\partial \mathbf{E}}{\partial t} = c\vec{\nabla} \times \mathbf{B} - 4\pi \mathbf{j}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -c\vec{\nabla} \times \mathbf{E}$$

* Dawson, Buneman, 1960's; Birdsall and Langdon, *Plasma Phys. via Comp. Simulation* (1985)

The particle-in-cell methodology

Modeling kinetic physics

- **Particle-particle simulations**

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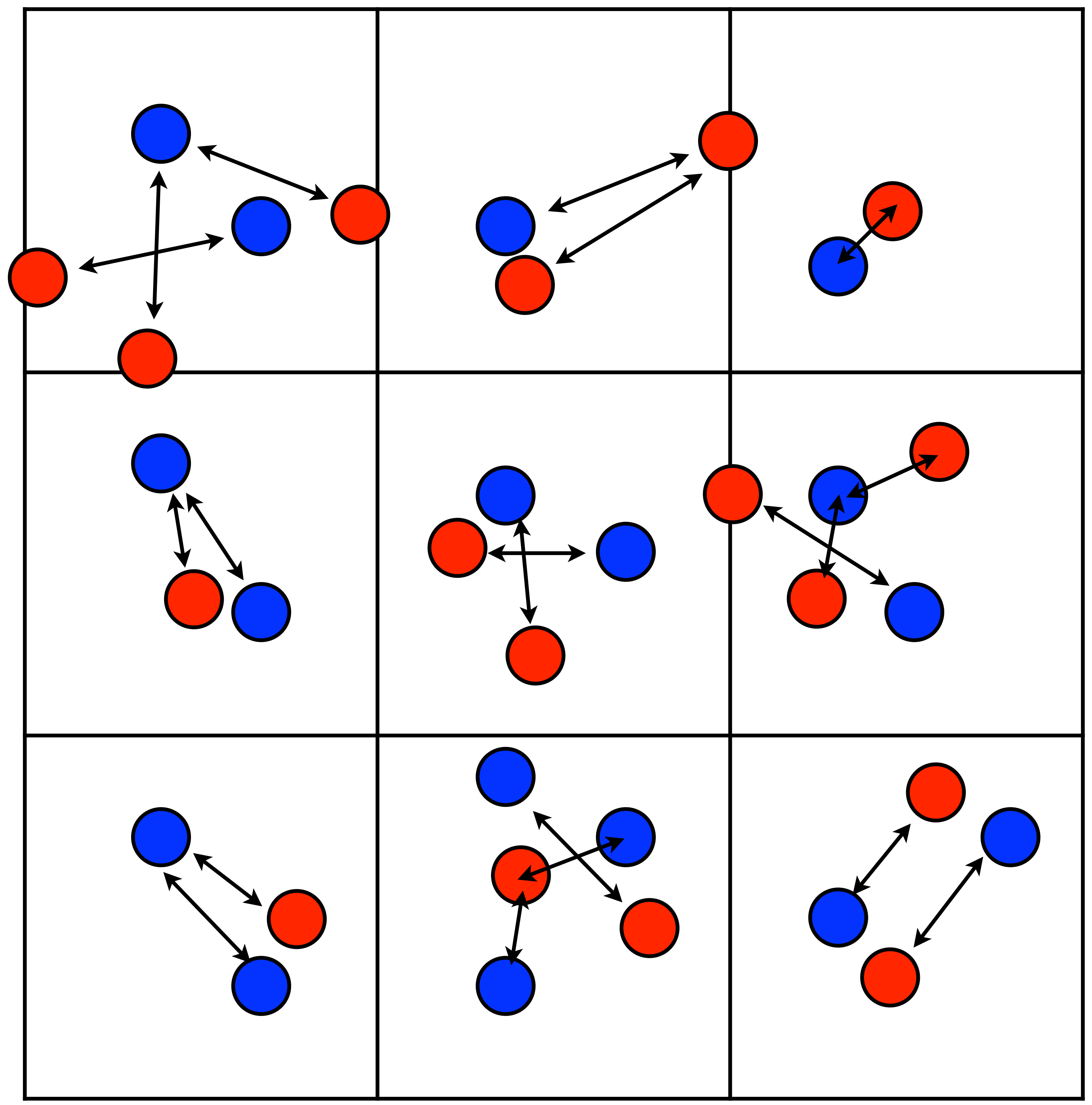
MC binary Coulomb collisions*



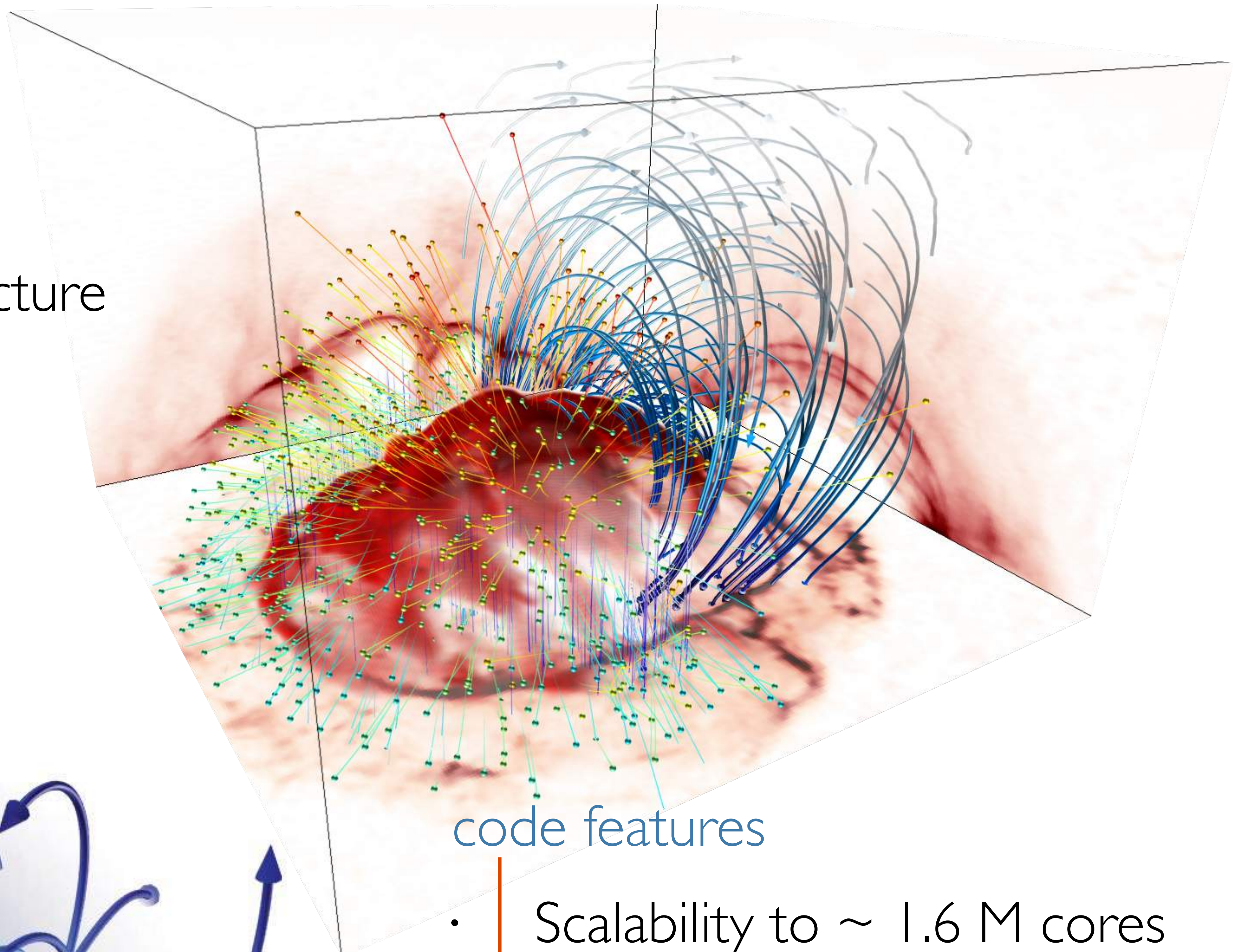
* Takizuka & Abe JCP 1977

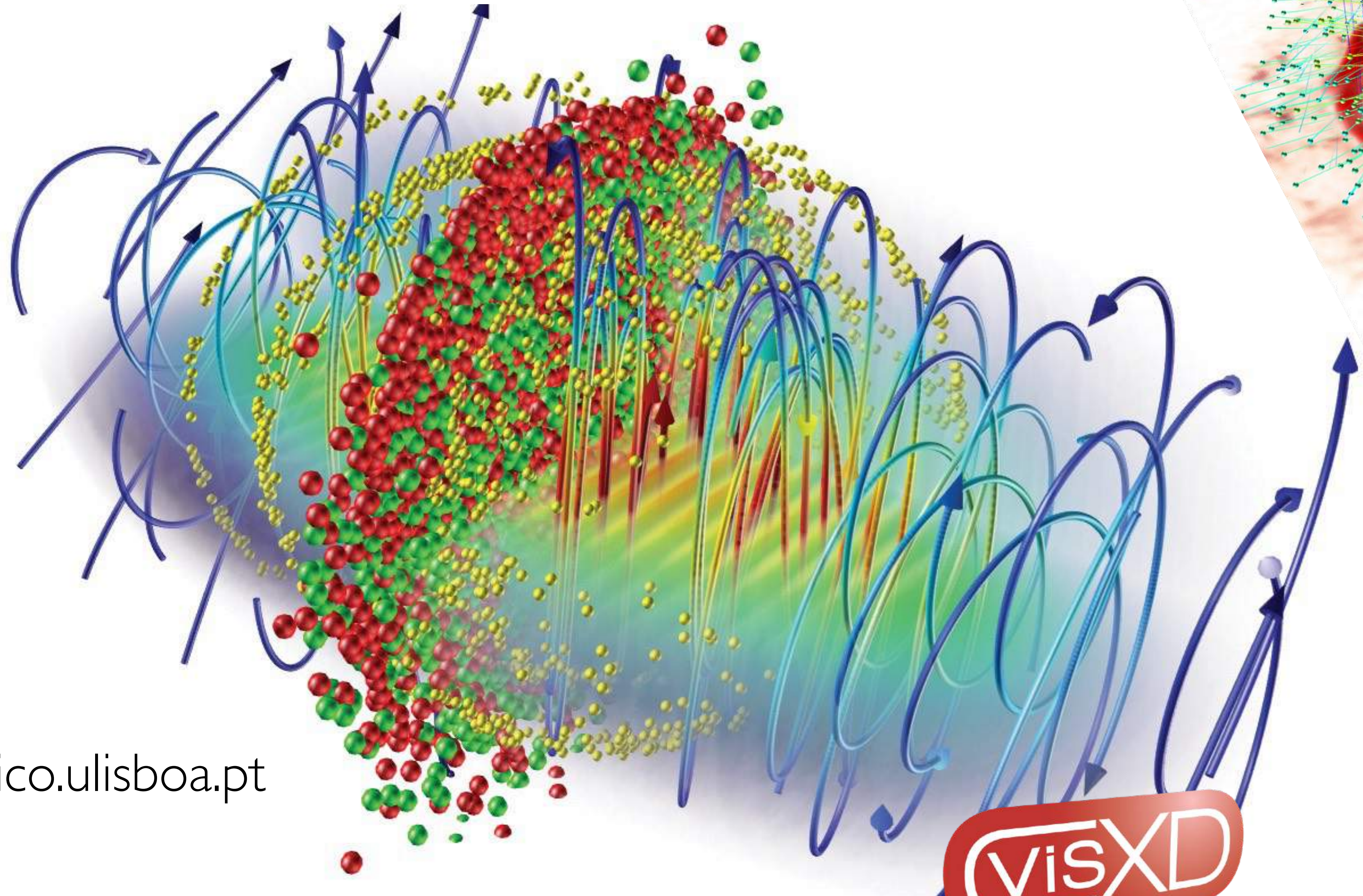
OSIRIS: a state-of-the-art PIC code for the modeling of plasmas

Osiris 3.0

osiris framework

- Massivelly Parallel, Fully Relativistic Particle-in-Cell (PIC) Code
- Visualization and Data Analysis Infrastructure
- Developed by the osiris.consortium
  ⇒ UCLA + IST





TÉCNICO LISBOA

UCLA

code features

- Scalability to ~ 1.6 M cores
- SIMD hardware optimized
- Parallel I/O
- Dynamic Load Balancing
- QED module
- Particle merging
- GPGPU support
- **Xeon Phi support**

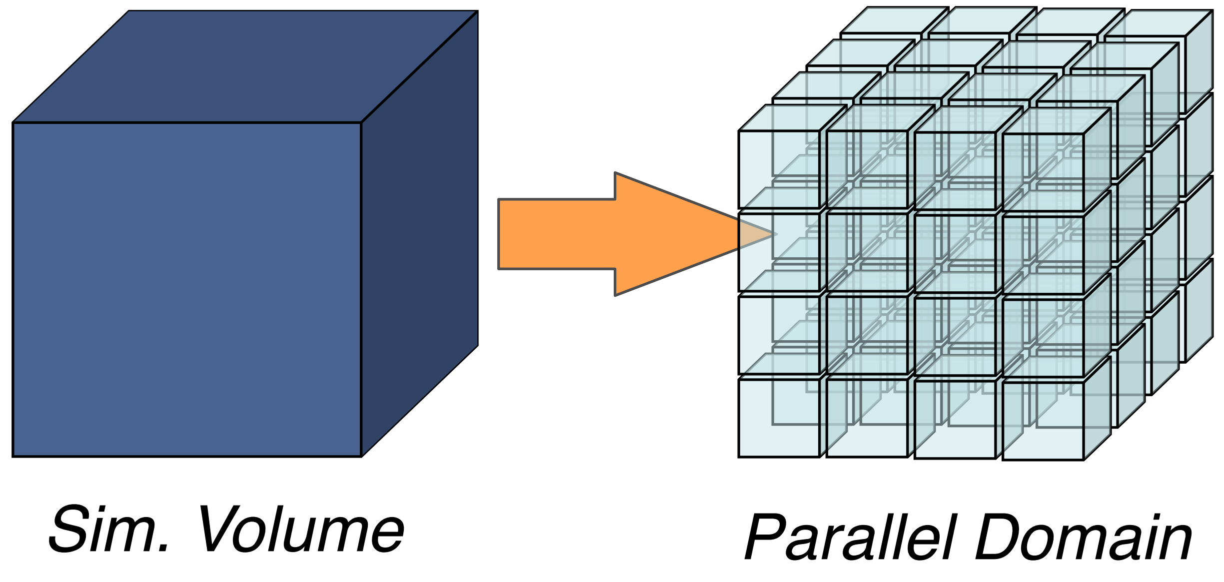
Ricardo Fonseca: ricardo.fonseca@tecnico.ulisboa.pt
Frank Tsung: tsung@physics.ucla.edu

http://epp.tecnico.ulisboa.pt/
http://plasmasim.physics.ucla.edu/

Efficient strong scaling to 1.6 million cores

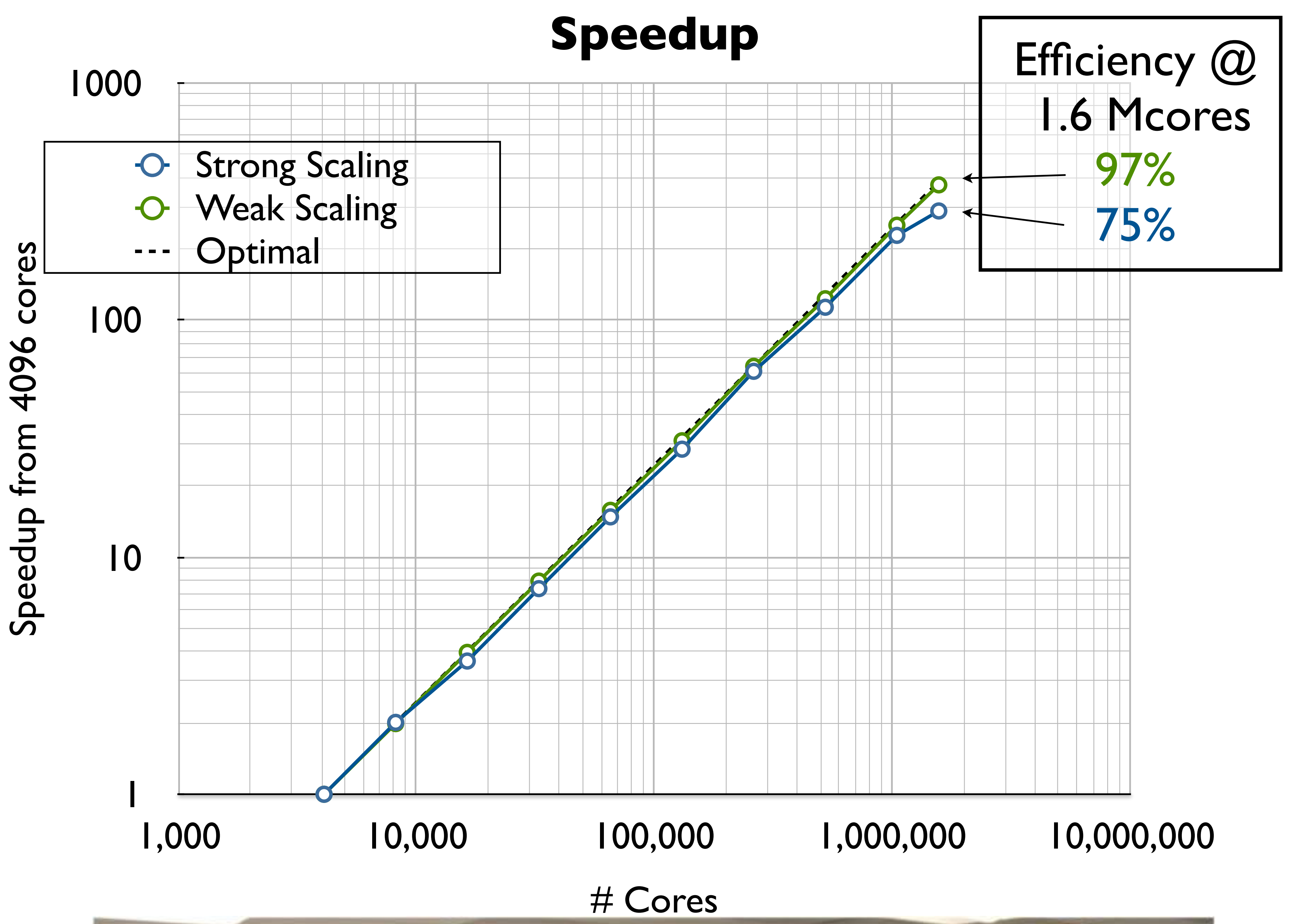
SLAC

Scaling Tests



- Scaling tests on LLNL Sequoia
  4096 → 1572864 cores (full system)
- Warm plasma tests
  Quadratic interpolation
  $u_{th} = 0.1$ c
- Weak scaling
  Grow problem size
  cells = $256^3 \times (N_{cores} / 4096)$
  2^3 particles/cell
- Strong scaling
  Fixed problem size
  cells = 2048^3
  16 particles / cell

F. Fiúza *et al.* (2013)



LLNL Sequoia
IBM BlueGene/Q
#2 - TOP500 Nov/12
1572864 cores
R_{max} 16.3 PFlop/s

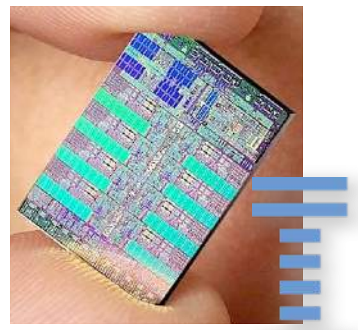
Pushing the limits of PIC simulations

Algorithm optimization

- Dynamic load-balancing
- Relativistic boosted frames
- High-order particle shapes
- Advanced field solvers
- Reduced physics algorithms for specific physical regimes

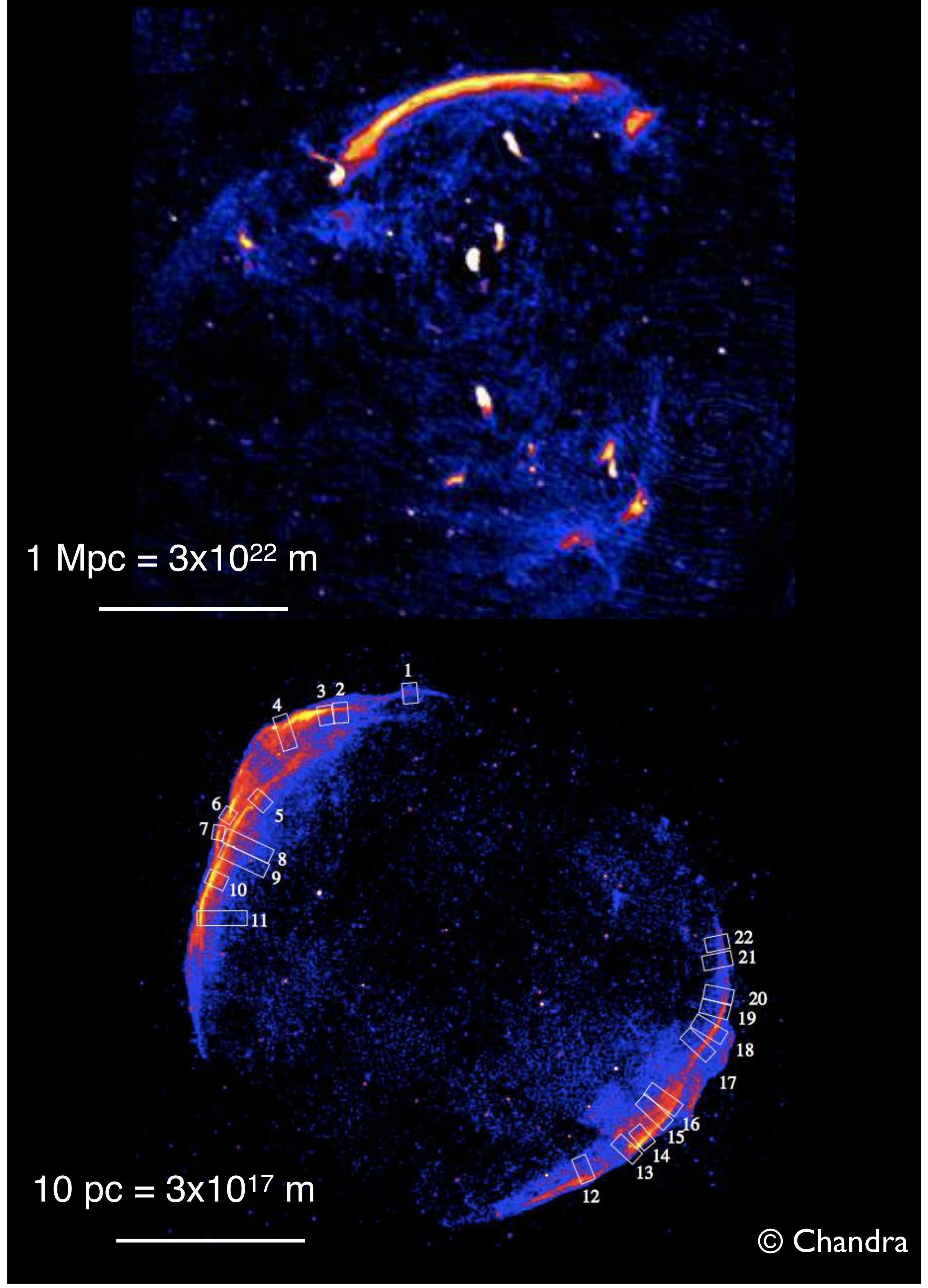
Hardware optimization via hardware-specific routines

SIMD units	Cell	GPUs
Altivec, SSE/2/3/4	PowerXCell	CUDA



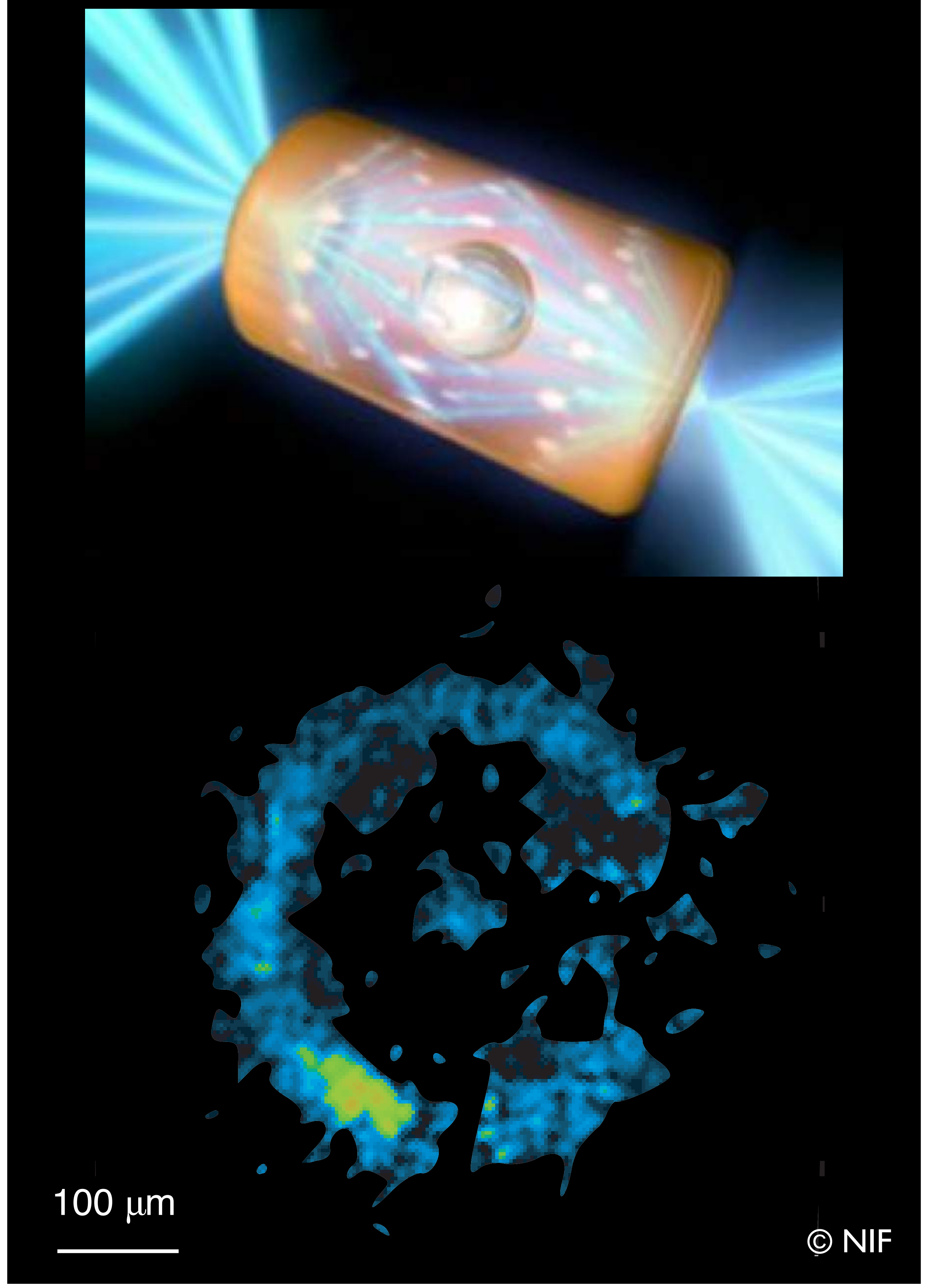
PIC codes drive plasma physics research in a broad range of areas

Astrophysics



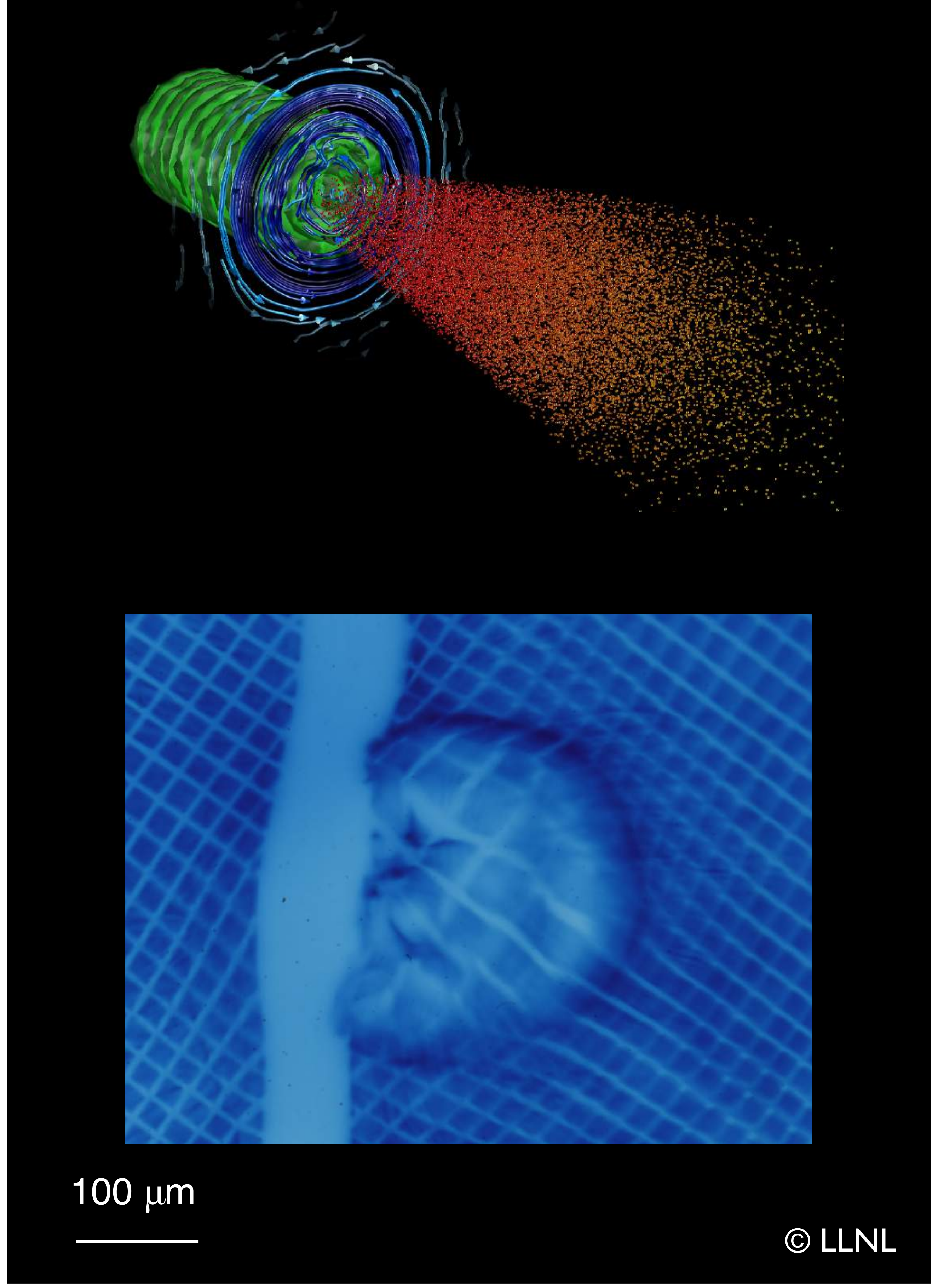
Amplify magnetic fields & accelerate cosmic rays

Laser Fusion



Compress & heat fusion fuel

Plasma Accelerators



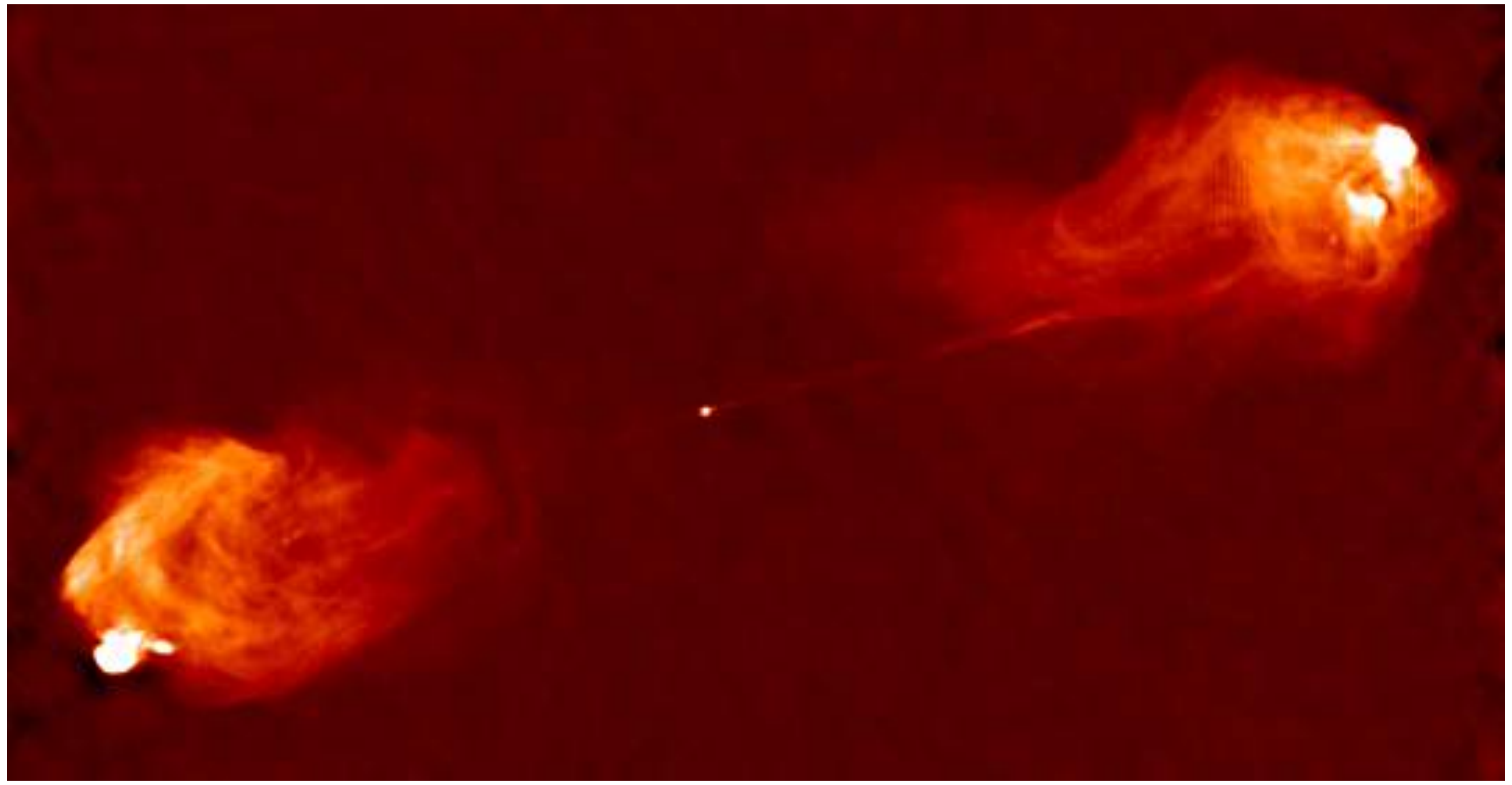
Accelerate particles in compact systems

How do extreme astrophysical systems shine?

Supernovae explosion

http://physicsworld.com

Relativistic plasma jets



web.ct.astro.it

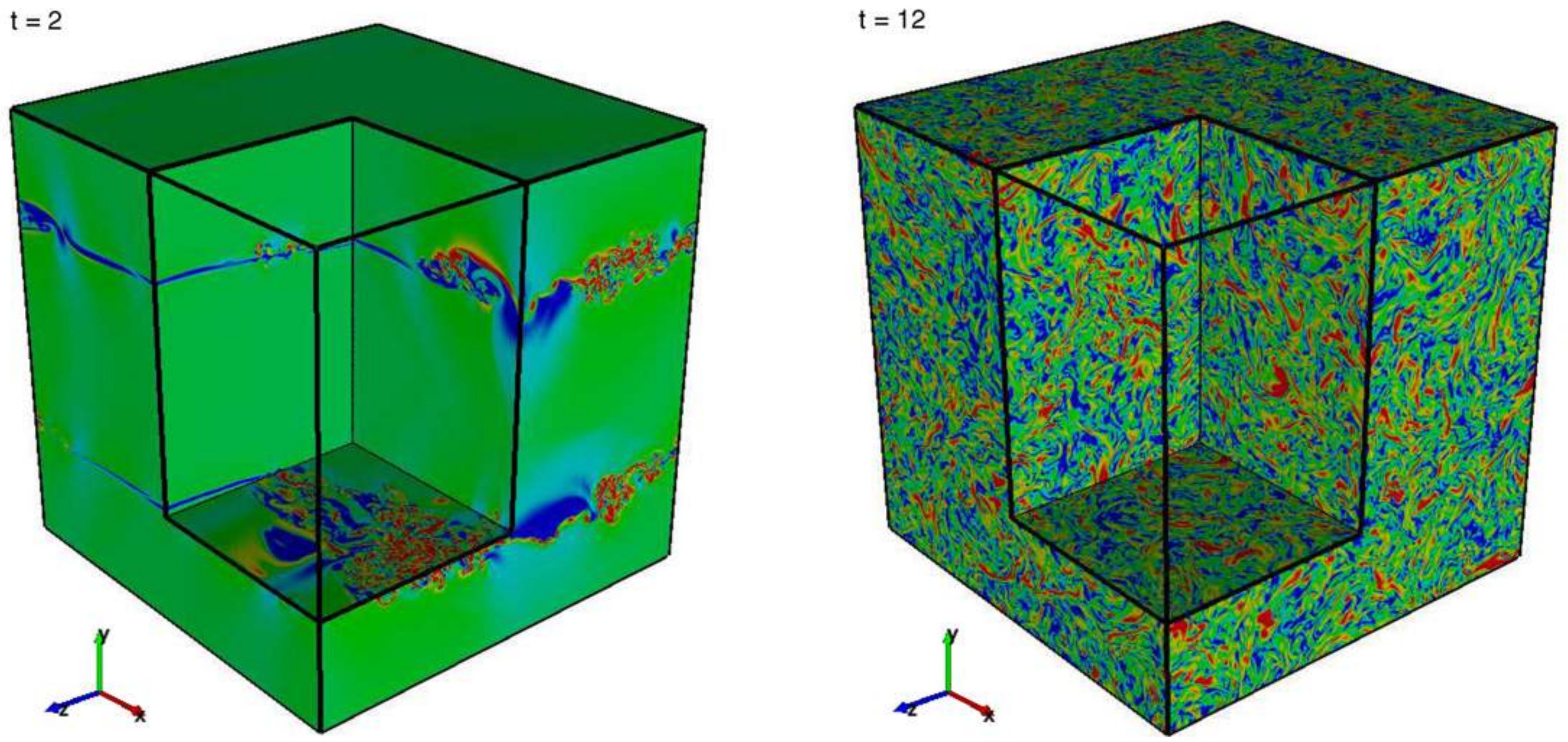
Plasma instabilities can convert the enormous kinetic energy of these plasma outflows into E/B-fields, energetic particles and radiation

Shear flow configurations are pervasive in nature

Hydrodynamic shear flows

http://wikipedia.org

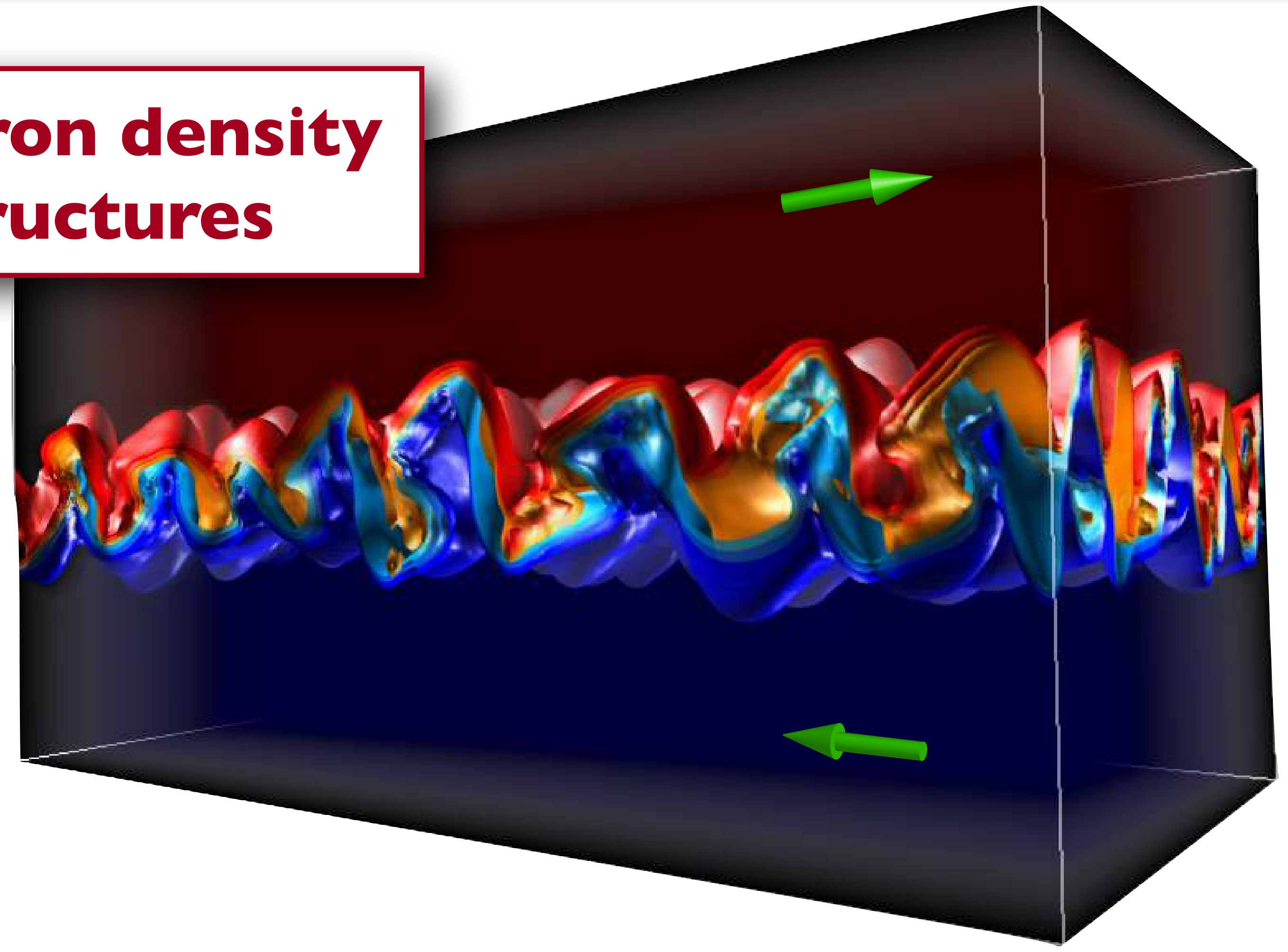
Magnetohydrodynamic (MHD) shear flows



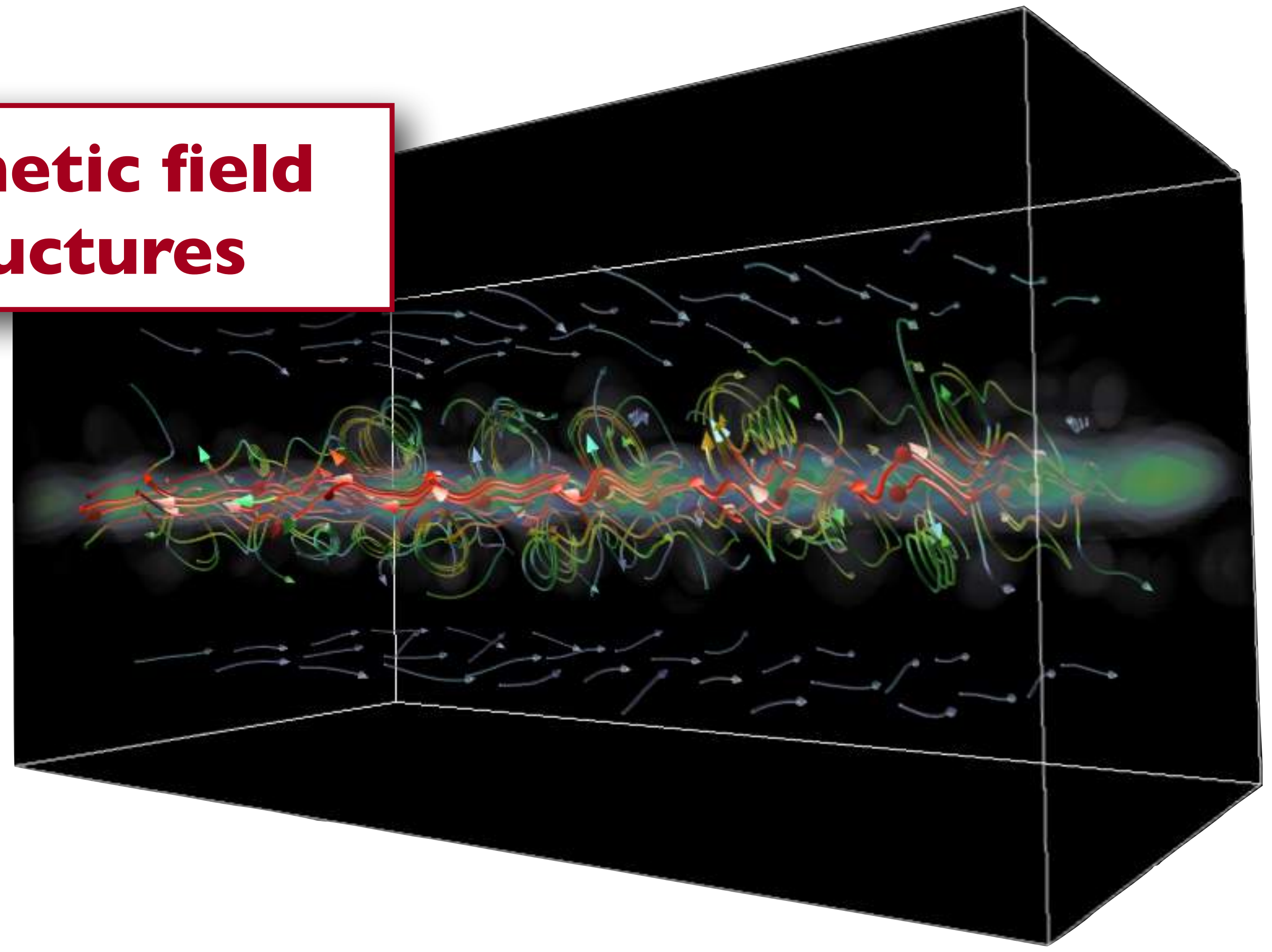
W. Zhang et al., ApJL (2009)

Unmagnetized collisionless shear flows

Electron density structures



Magnetic field structures

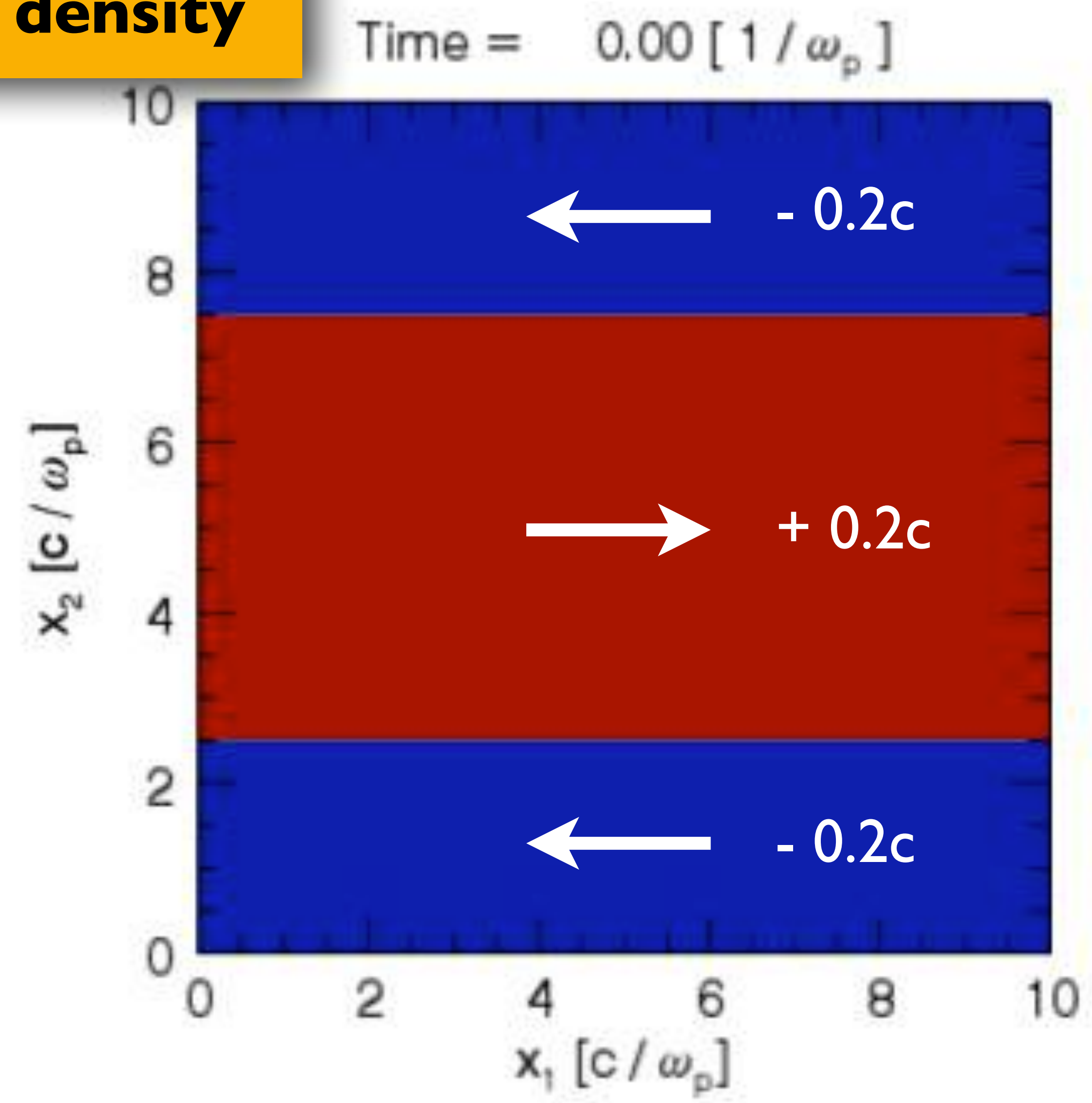


E. P. Alves et al., ApJL (2012)

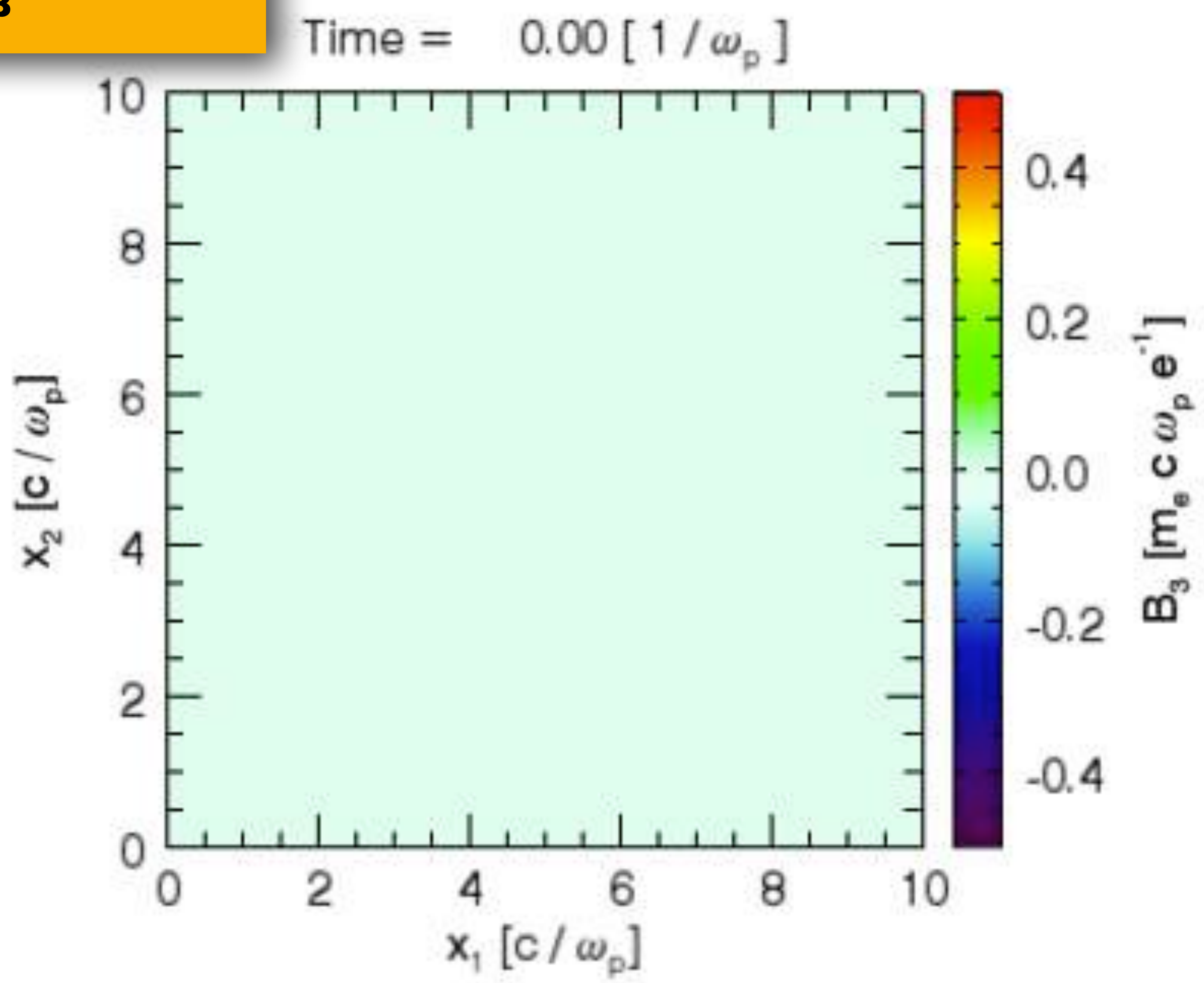
Self-generation of electric & magnetic fields via the ESKHI

SLAC

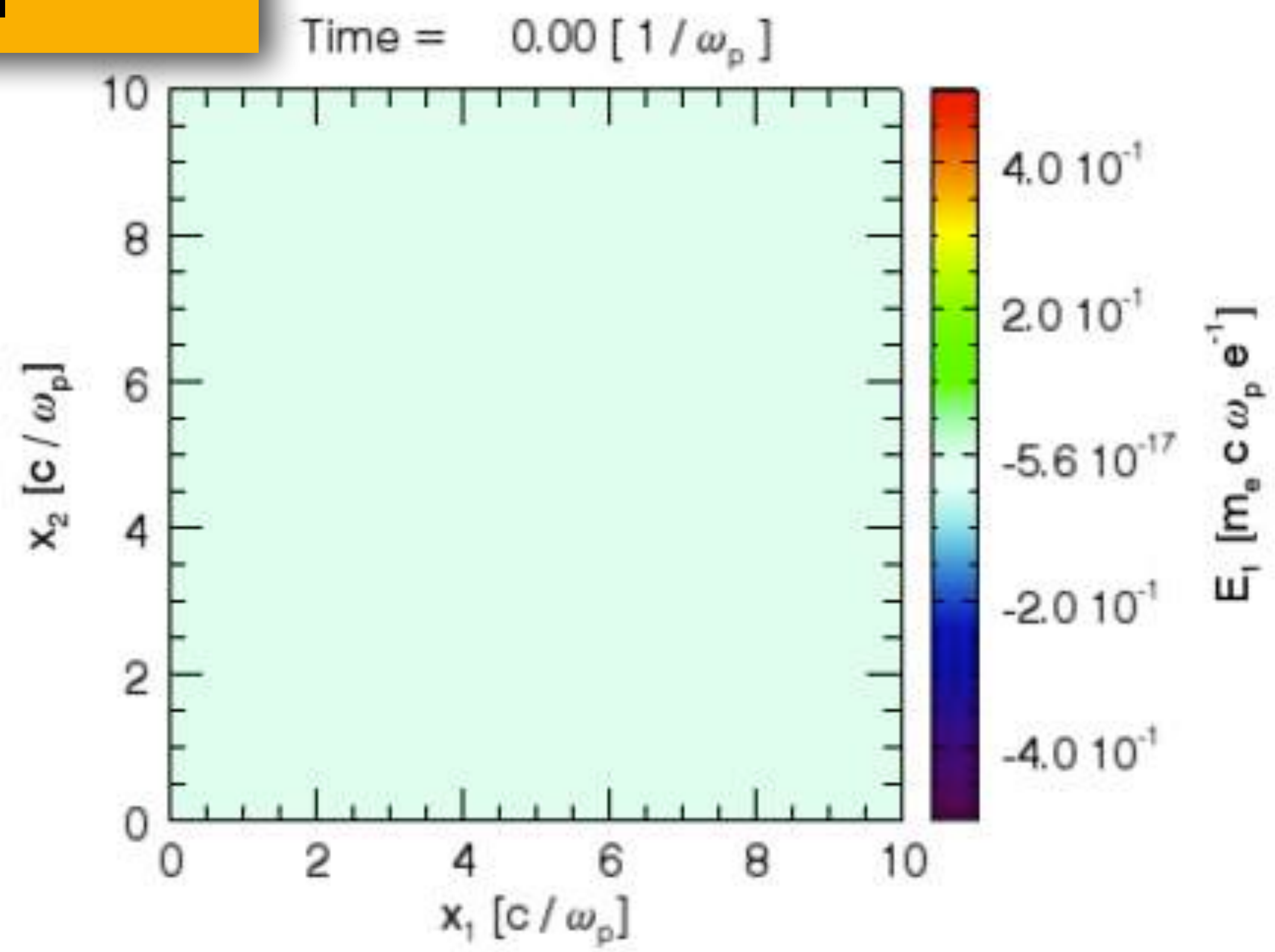
Electron density



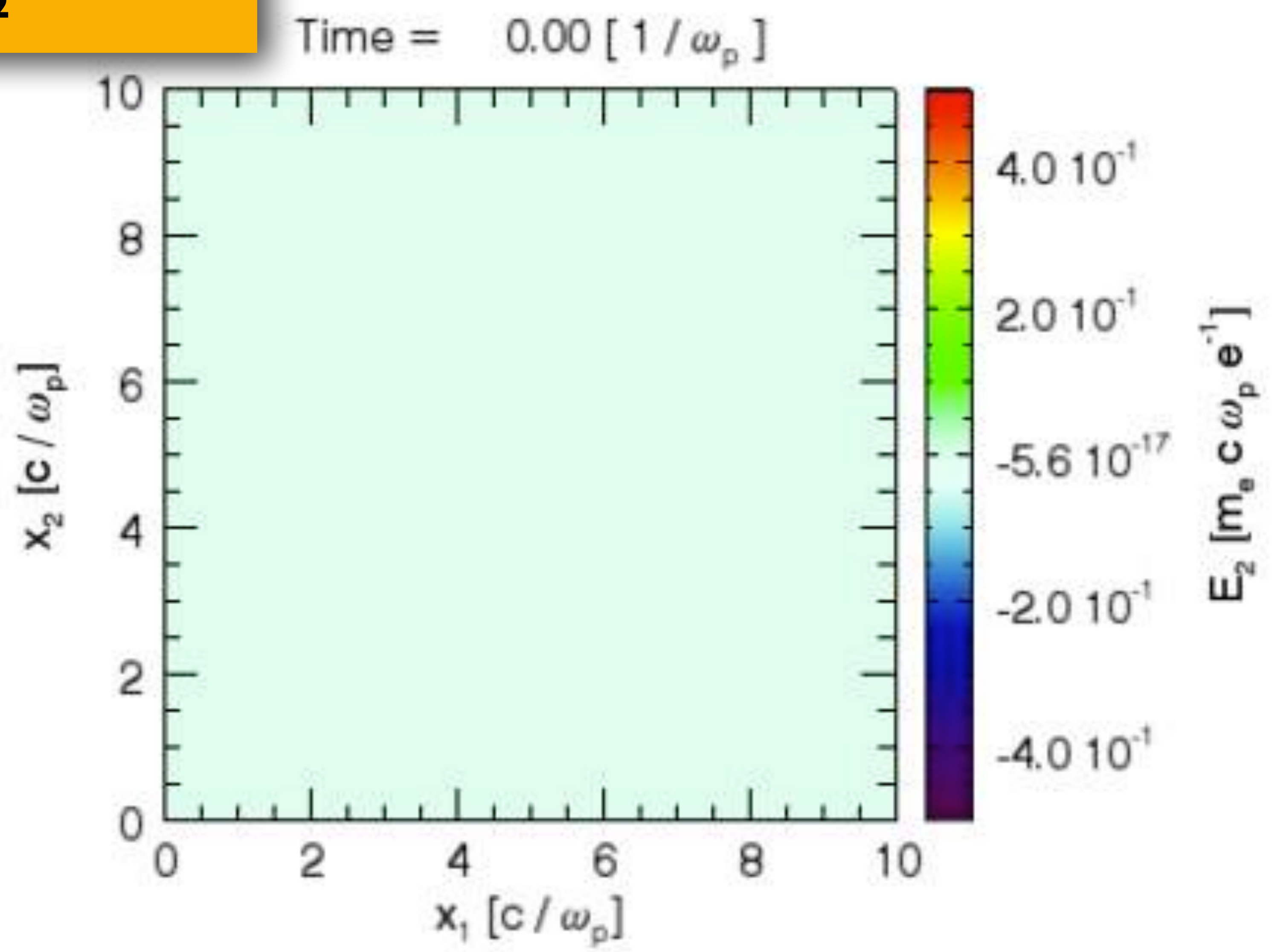
B₃



E₁



E₂



Self-generation of electric & magnetic fields via the ESKHI

SLAC

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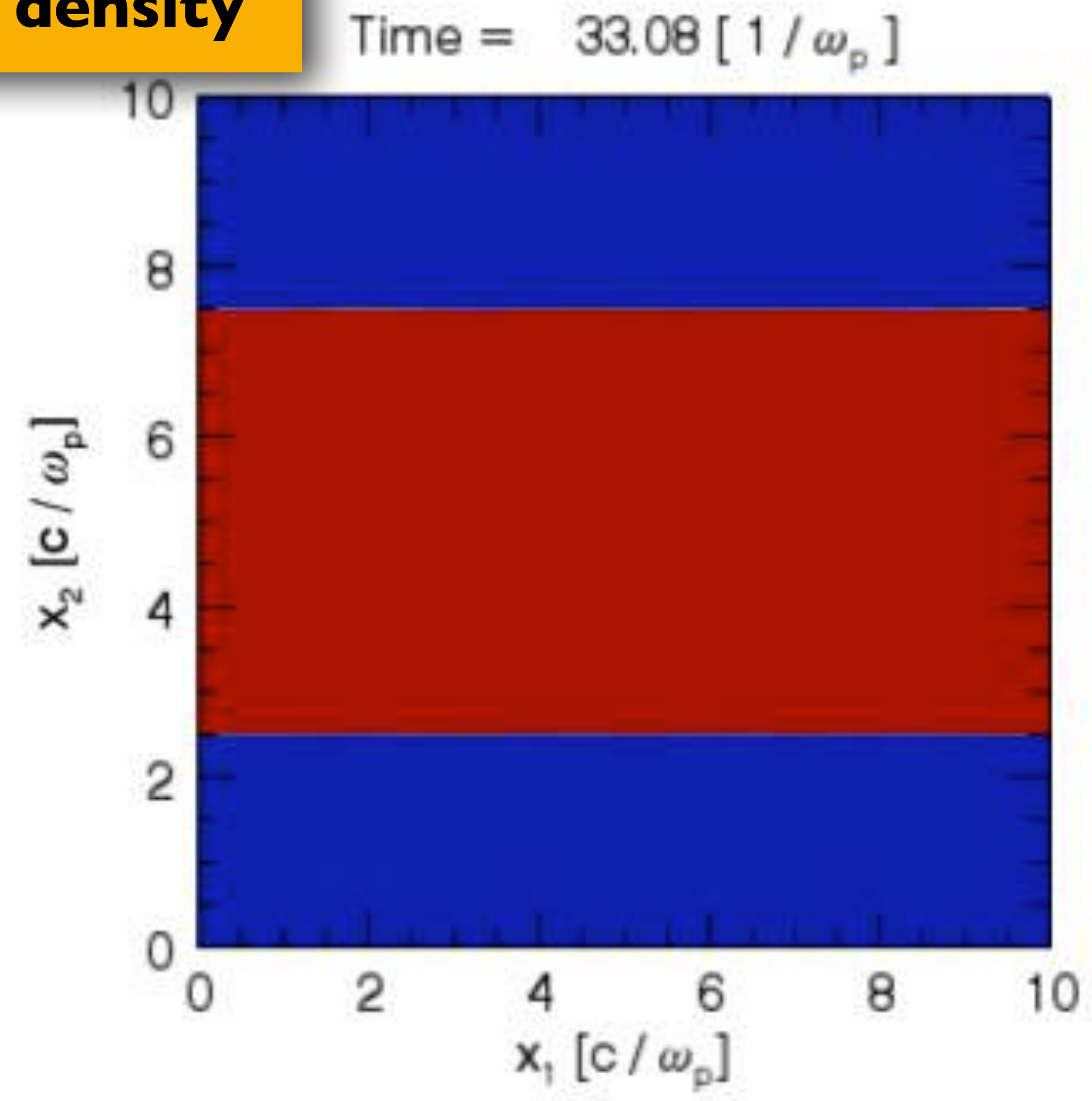
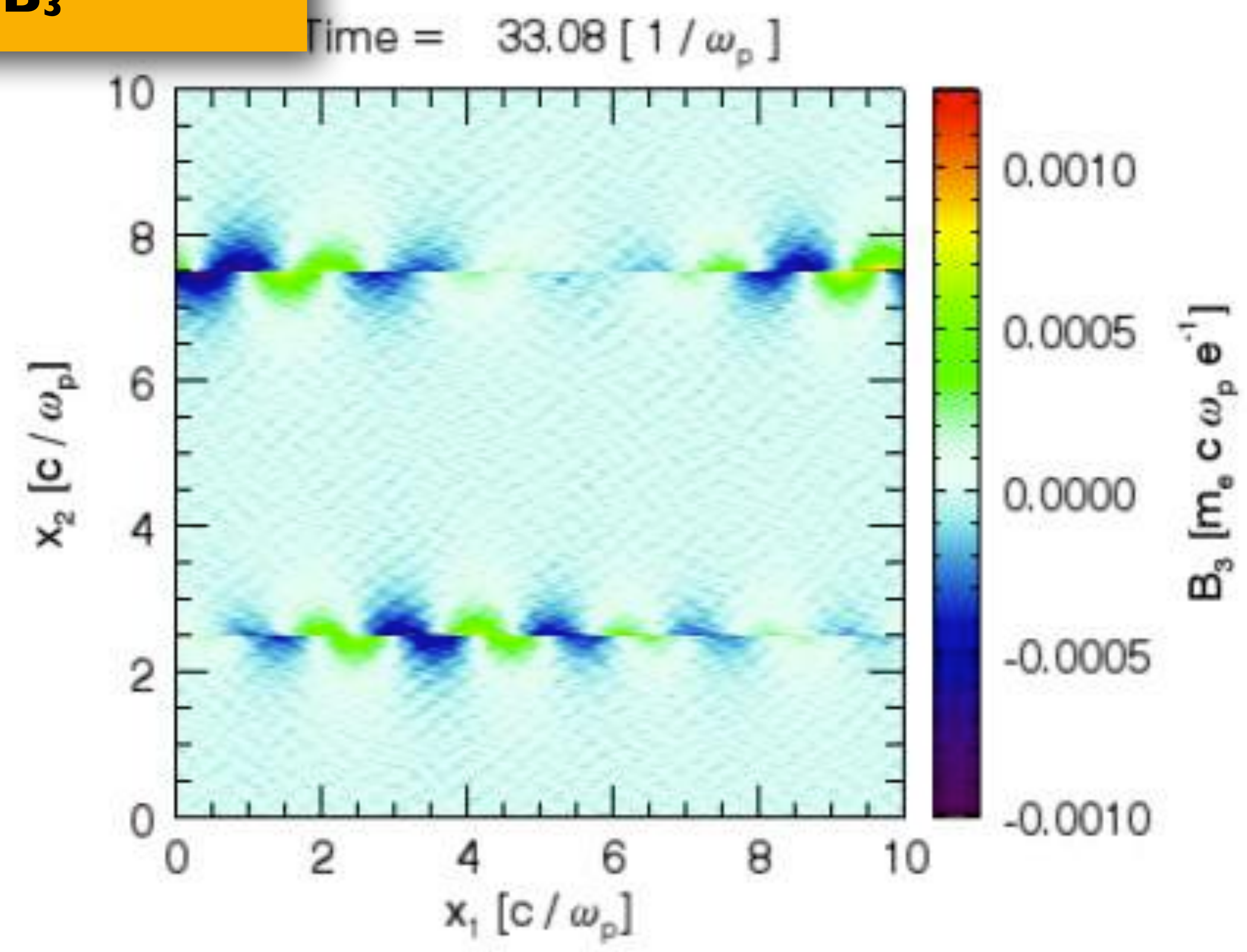
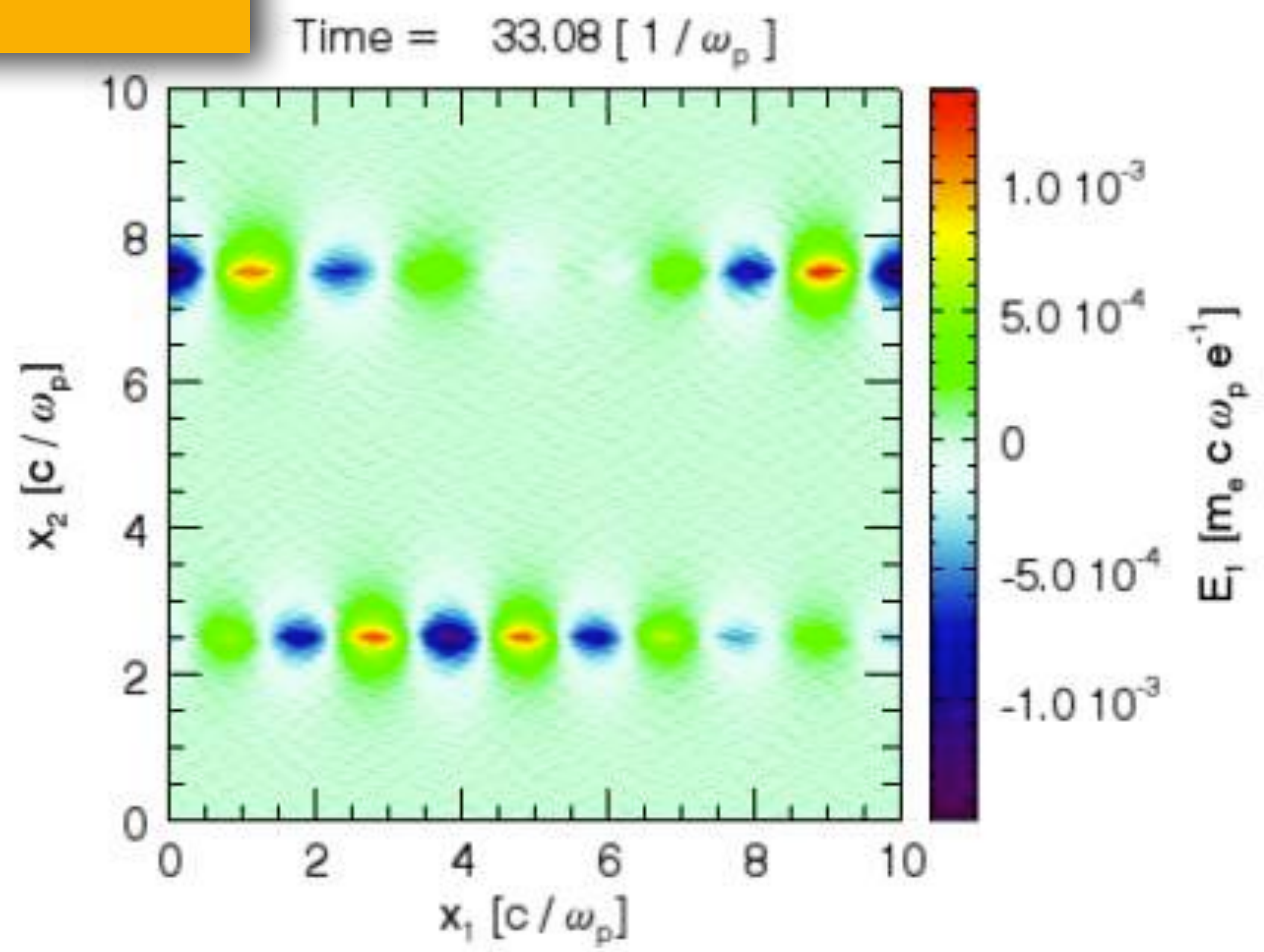


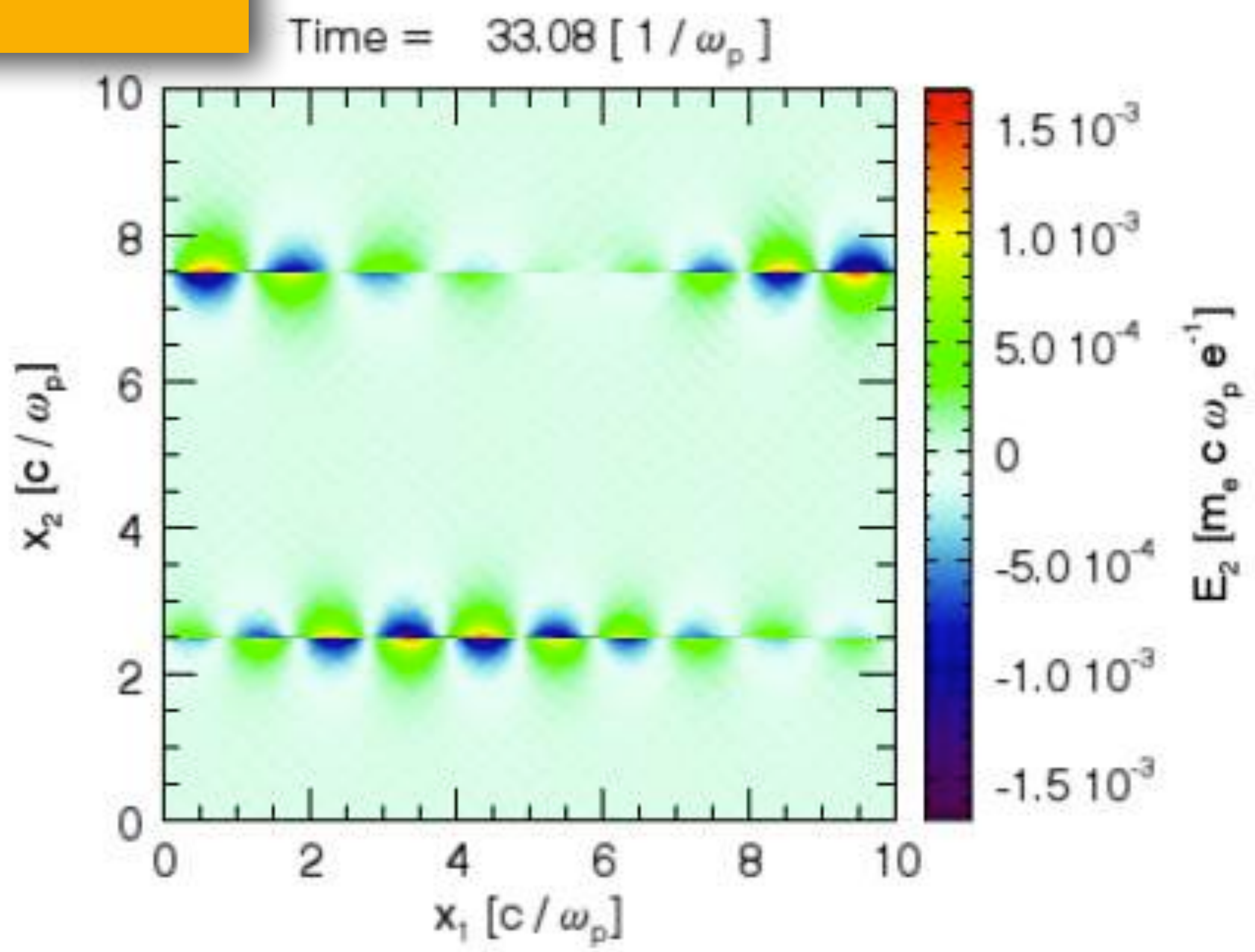
B_3



E_1

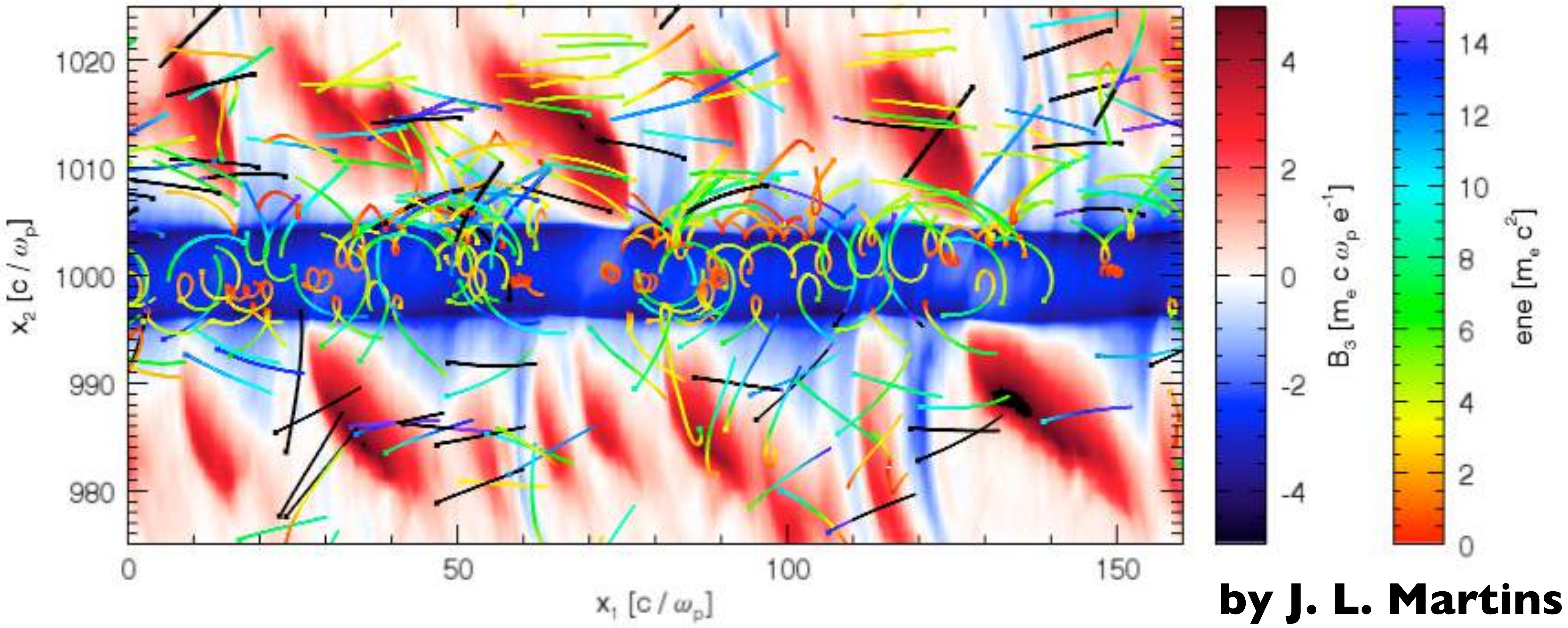


E_2



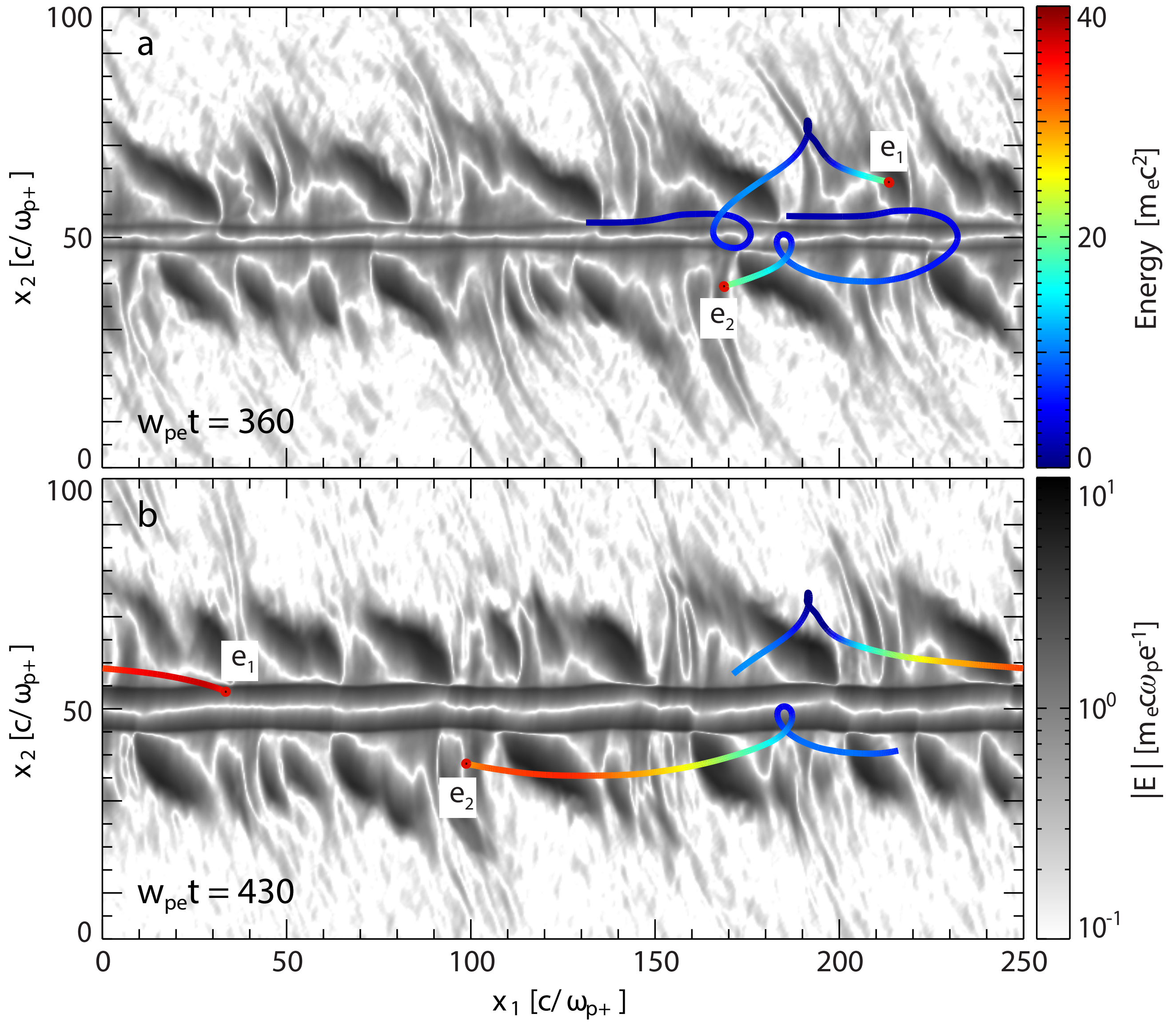
Radiation emission & particle acceleration in instability-generated fields

Nonthermal radiation emission

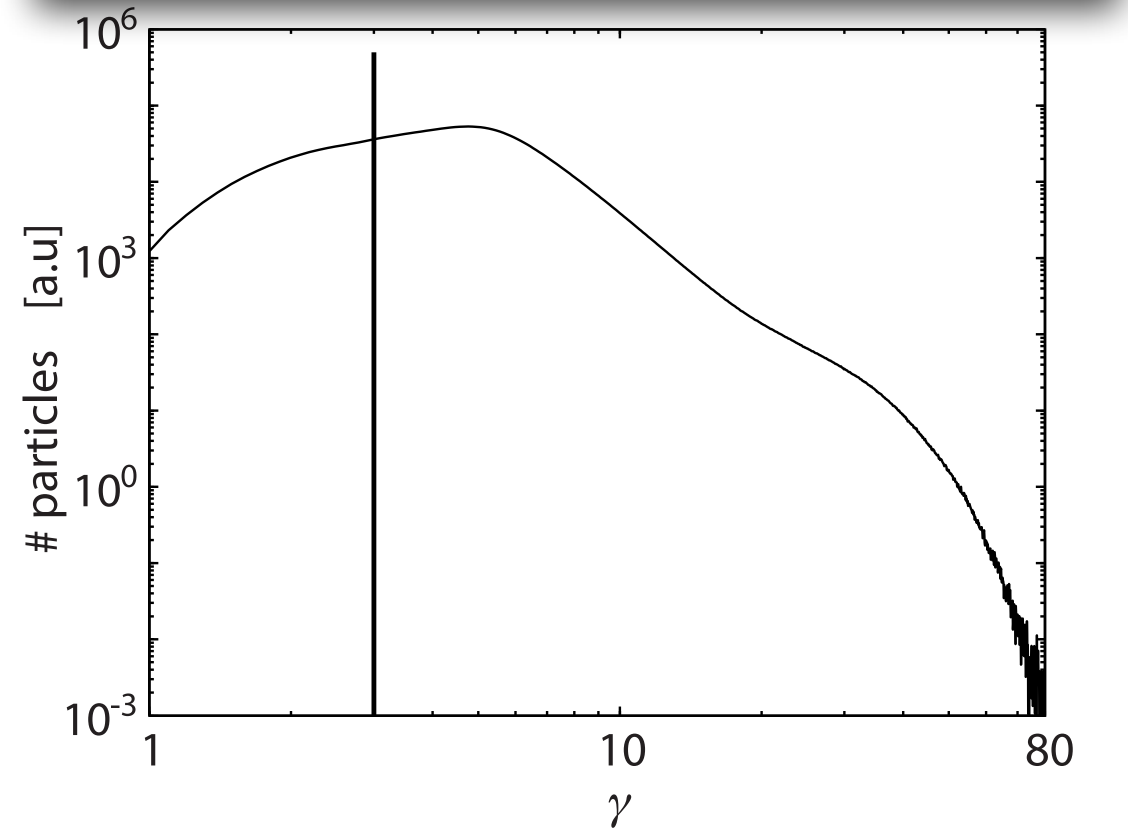


by J. L. Martins

Particle acceleration



Electron energy spectrum

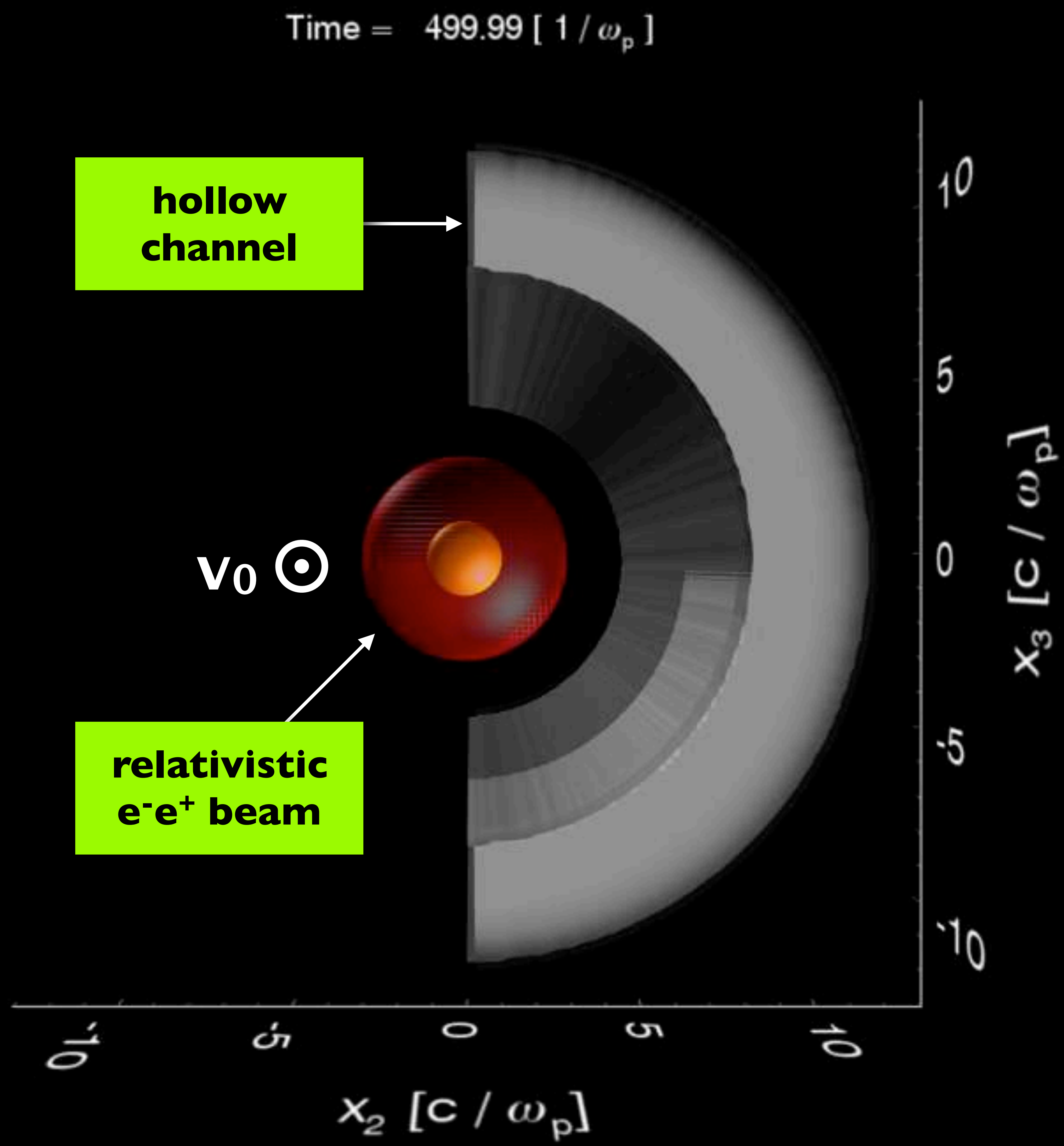


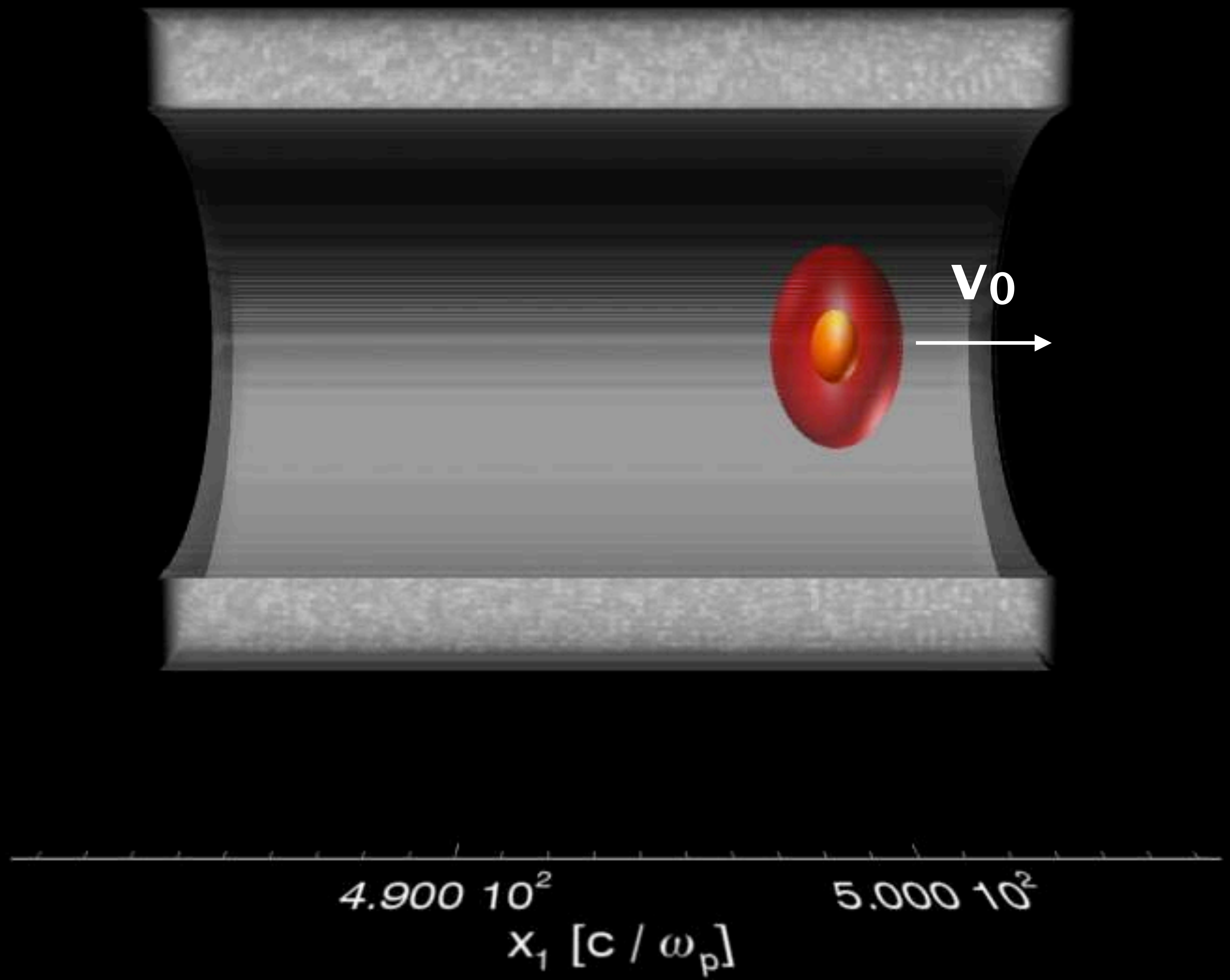
$$\Delta E_{\max} \sim \gamma_0^4 \; m_e c^2$$

M. Bussmann et al., ICHPCNSA (2013), E.P. Alves et al., NJP 16, 035007 (2014)

Exploring microphysics of relativistic collisionless shear flows in the laboratory

~10^6 particles
~10^6 time steps
1M core hours





Parameters

$\gamma_{e-e+} = 10^4$

$\sigma_\perp = 2\,\sigma_\parallel = 2c/\omega_{pe}$

$R_{channel} = 4\,\sigma_\perp$

SI

$n_{e-e+} = 10^{17}\ \mathrm{cm}^{-3}$

Propagation ≃ 50 cm

E. P. Alves et al. PPCF 58, 014025 (2015)

Intense lasers drive lab exploration of extreme plasma phenomena

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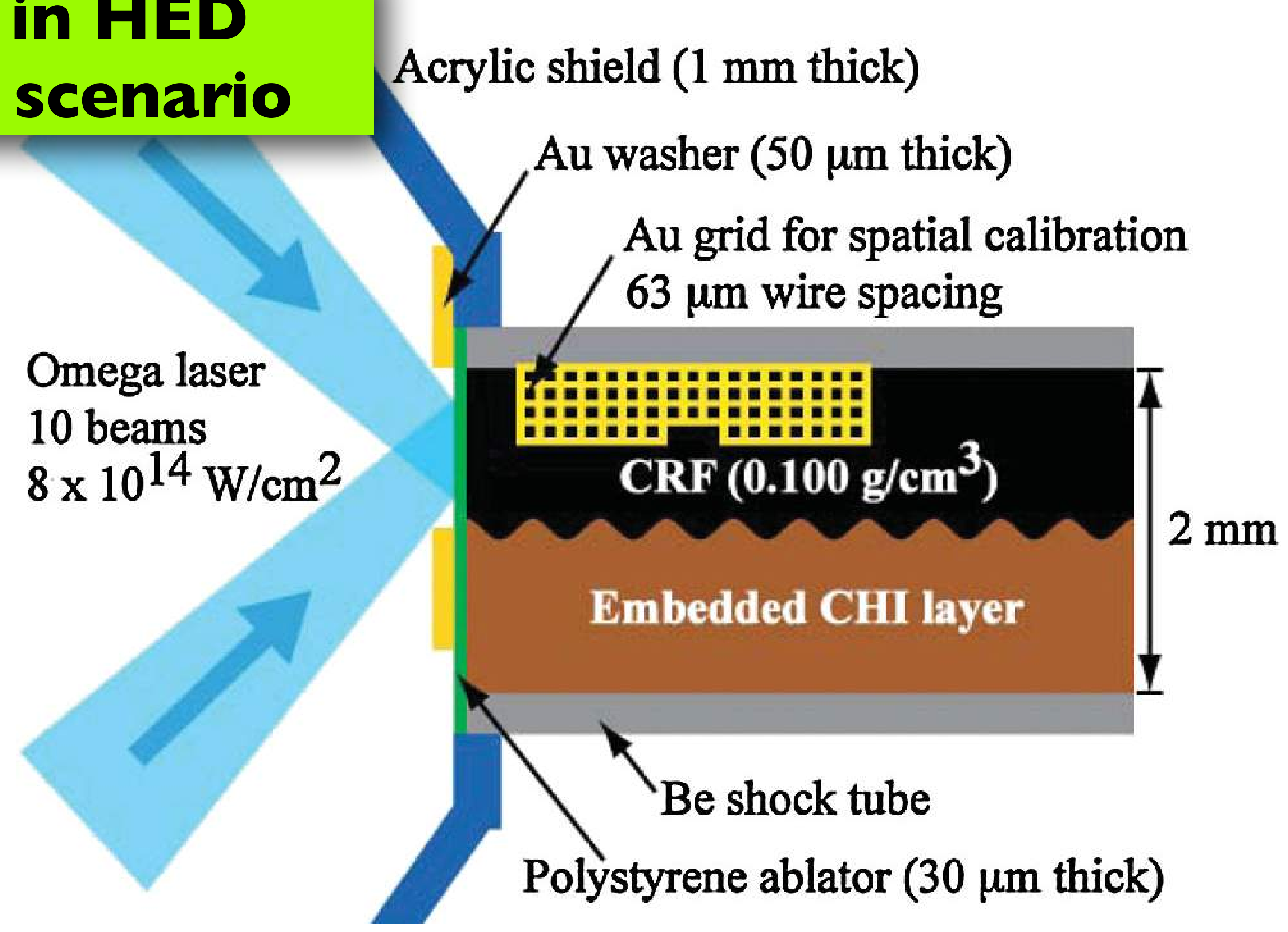
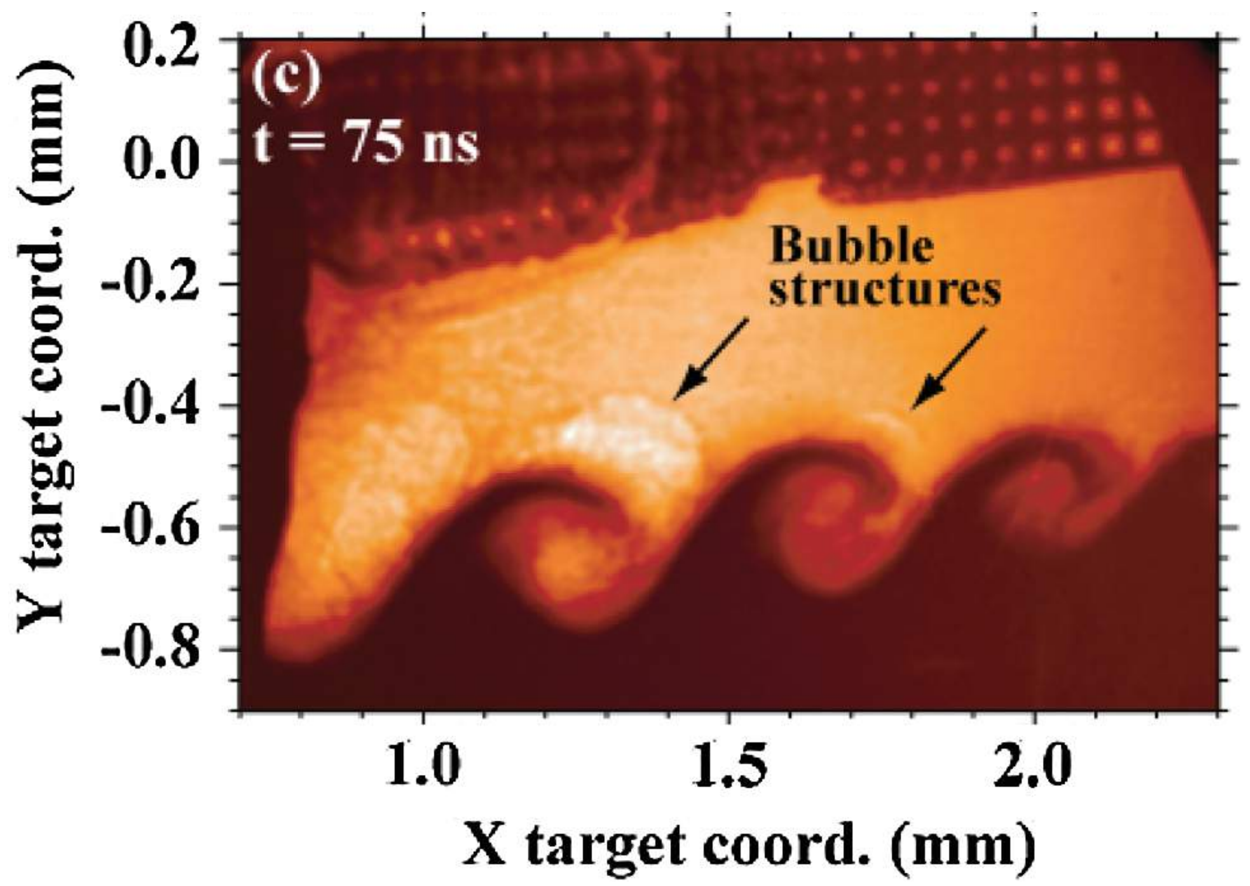
Mimicking extreme space/astrophysical scenarios via intense laser-matter interactions

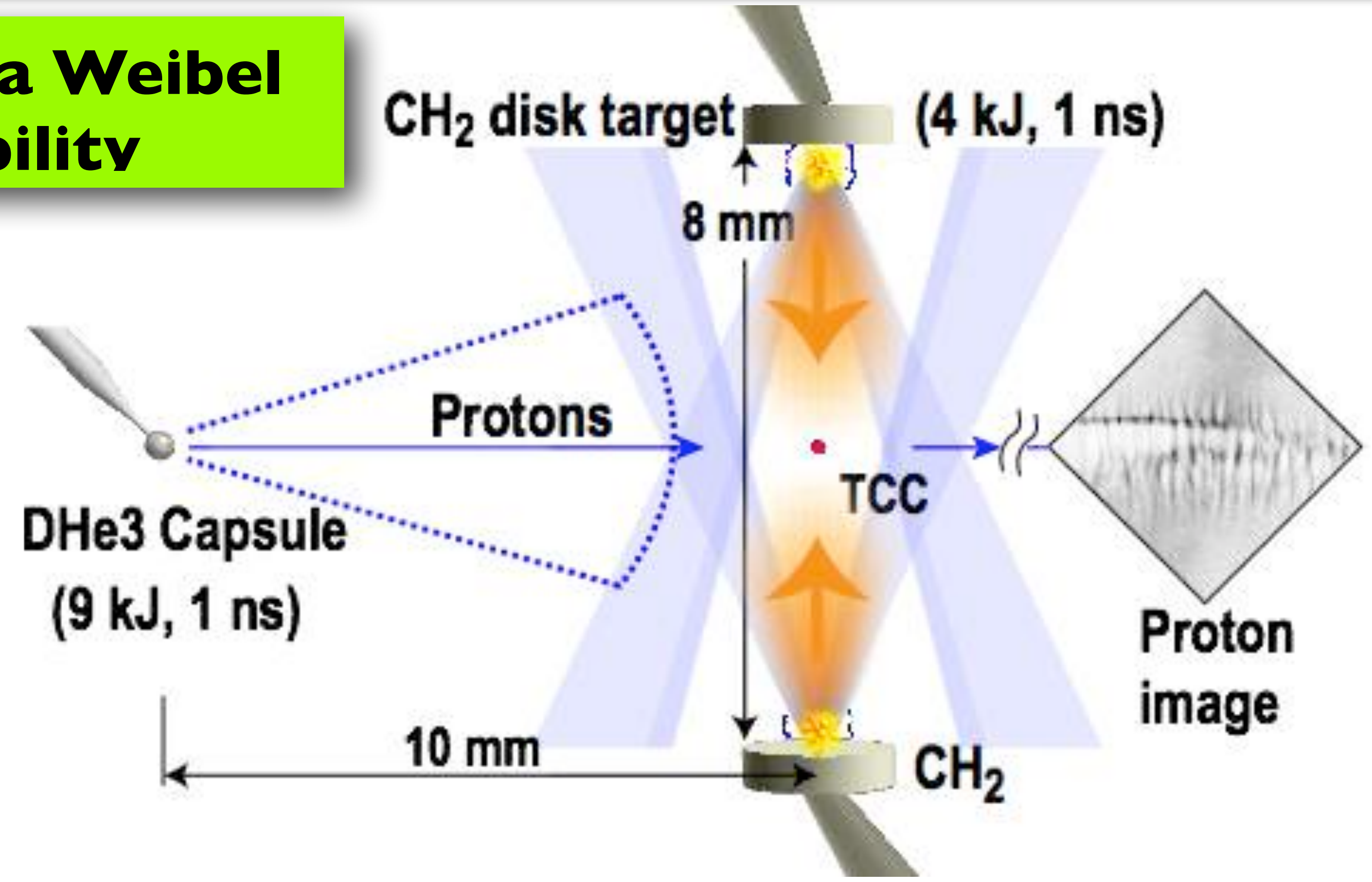
KHI in HED shear scenario

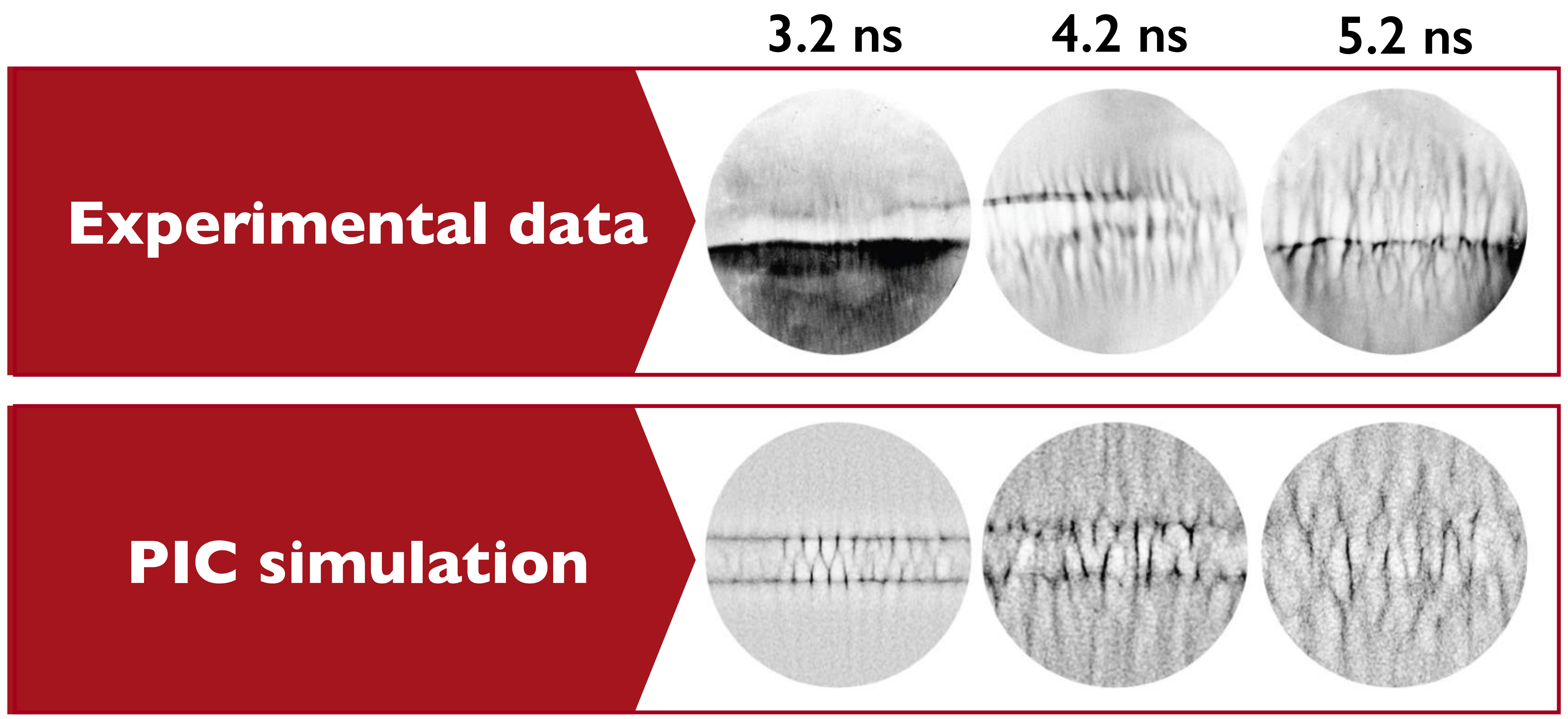




E.C. Harding et al., Phys. Rev. Lett. (2009)

B-fields via Weibel instability





C. Huntington, F. Fiuza, S. Ross et al. Nat. Phys. (2015)

Plasma-based laser amplifiers promise next-generation laser energy-densities

SLAC

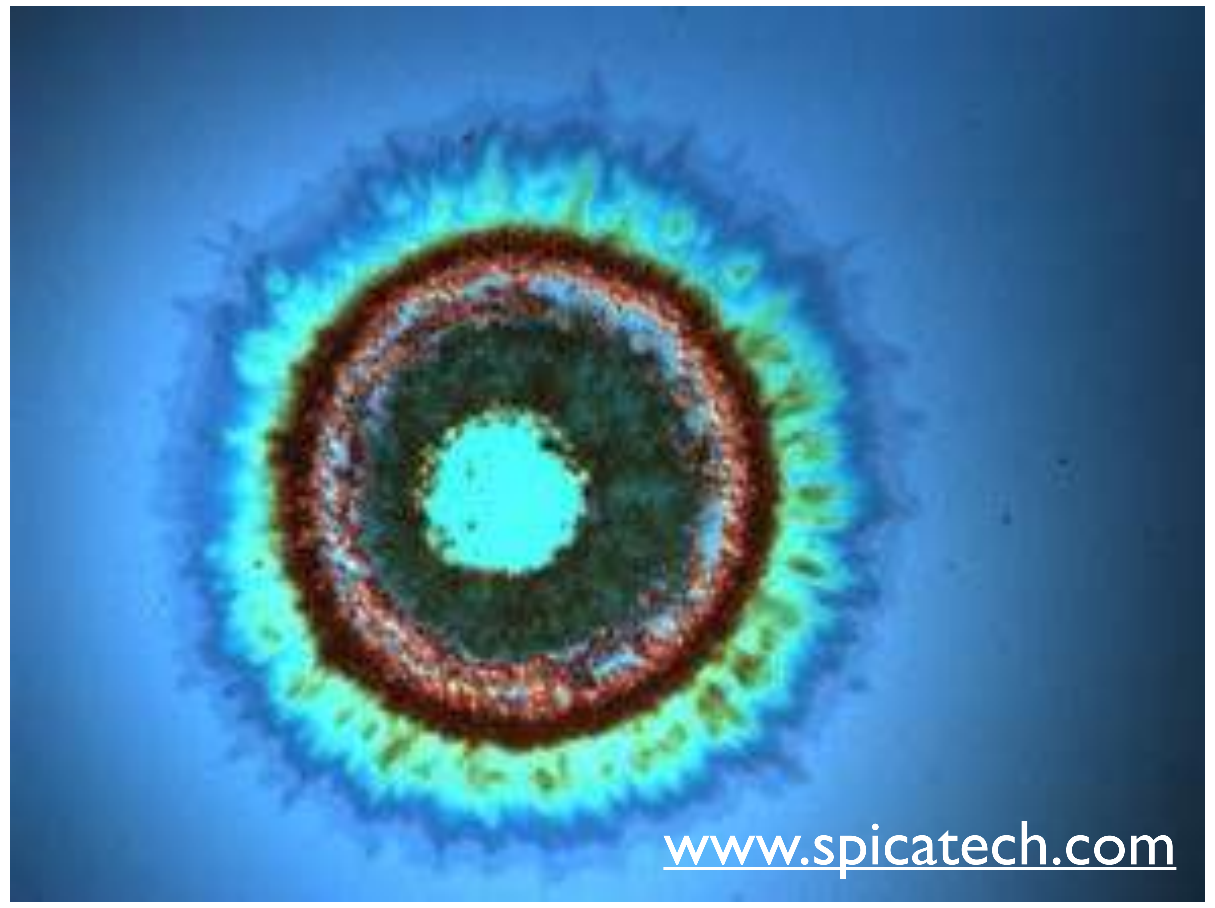
High damage threshold in plasmas

Solid state optics

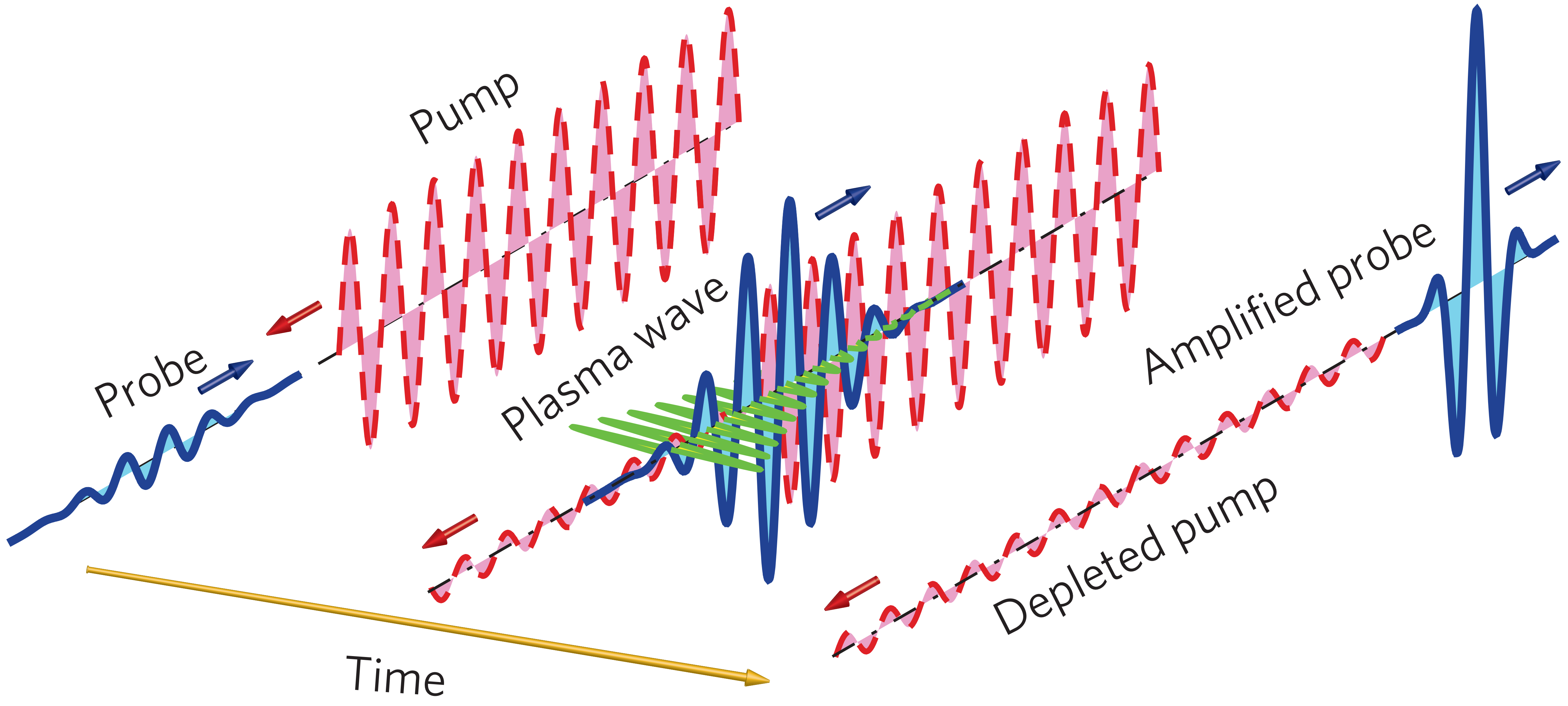
$$I_{\text{damage}} = 10^{12}\text{W/cm}^2$$

Plasmas

$$I_{\text{damage}} = 10^{17}\text{W/cm}^2$$

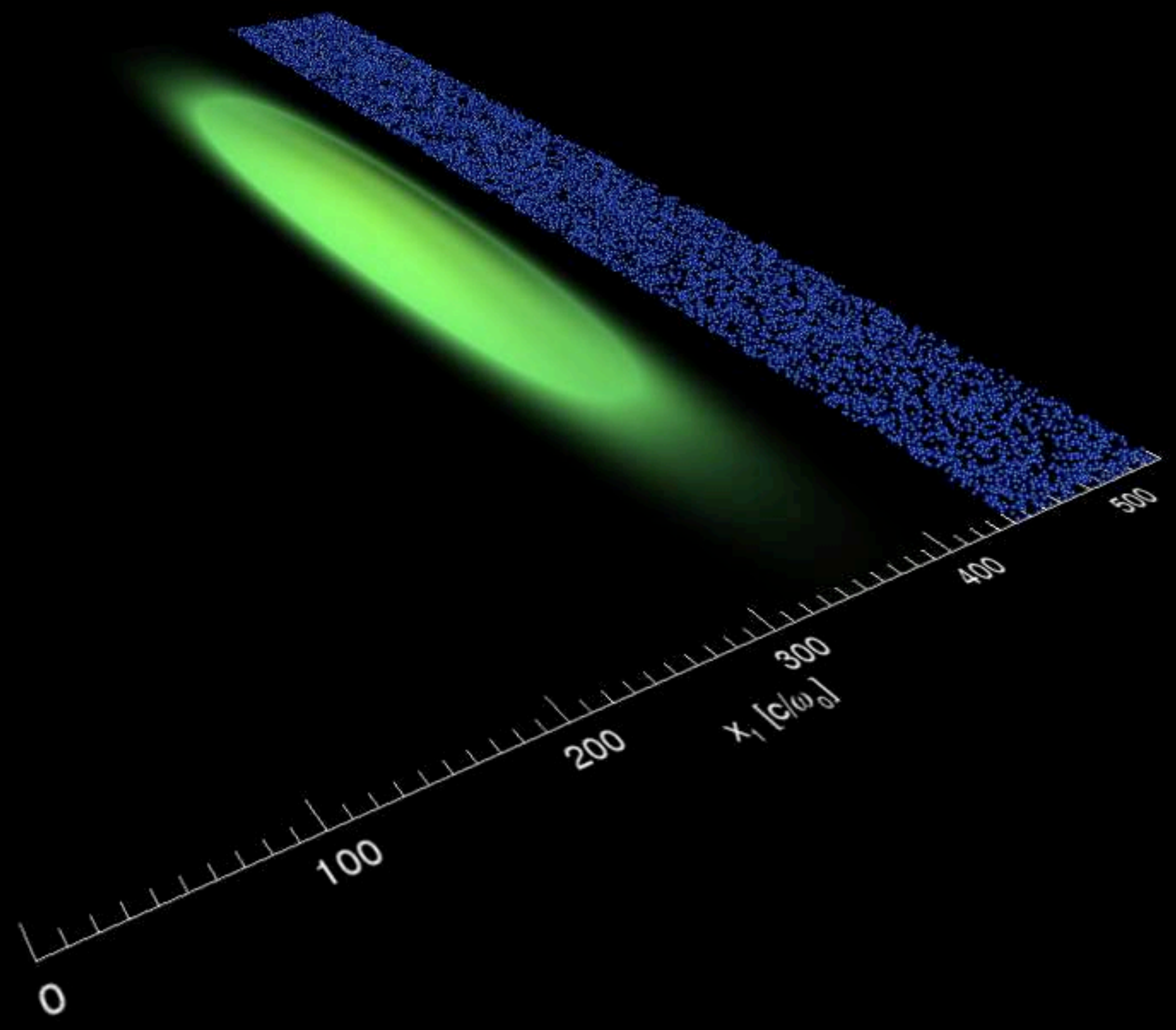


Plasmas as laser-amplifying media



Multidimensional dynamics of Brillouin-amplification

$I_{seed} = I_{pump} = 10^{16}W/cm^2$
$n_0 = 0.3n_{cr}$



~10^8 particles
~10^4 time steps
3M core hours

E.P.Alves et al., arXiv:1311.2034 (2014)

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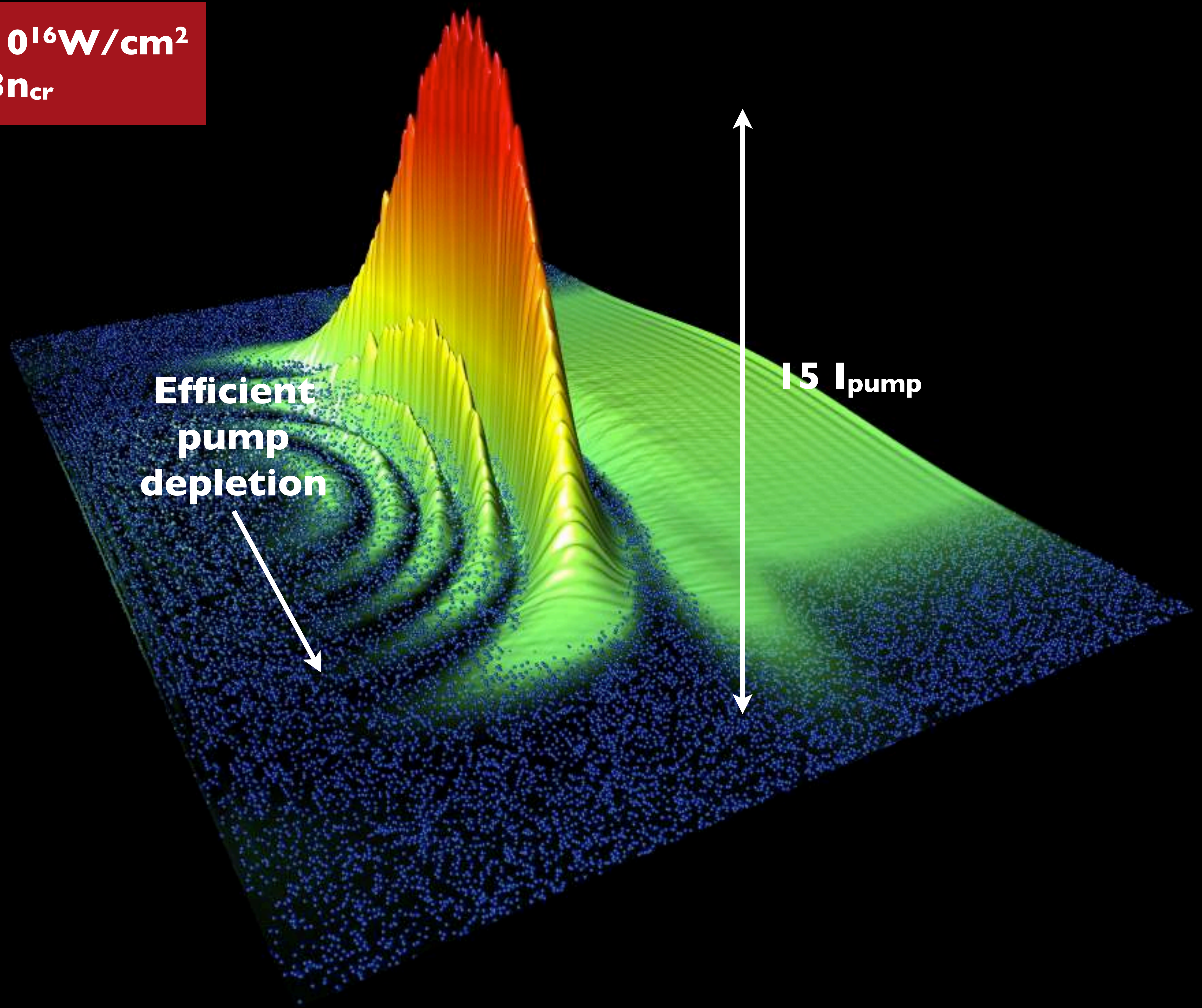

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E.P.Alves et al., arXiv:1311.2034 (2014)

Multidimensional dynamics of Brillouin-amplification

SLAC

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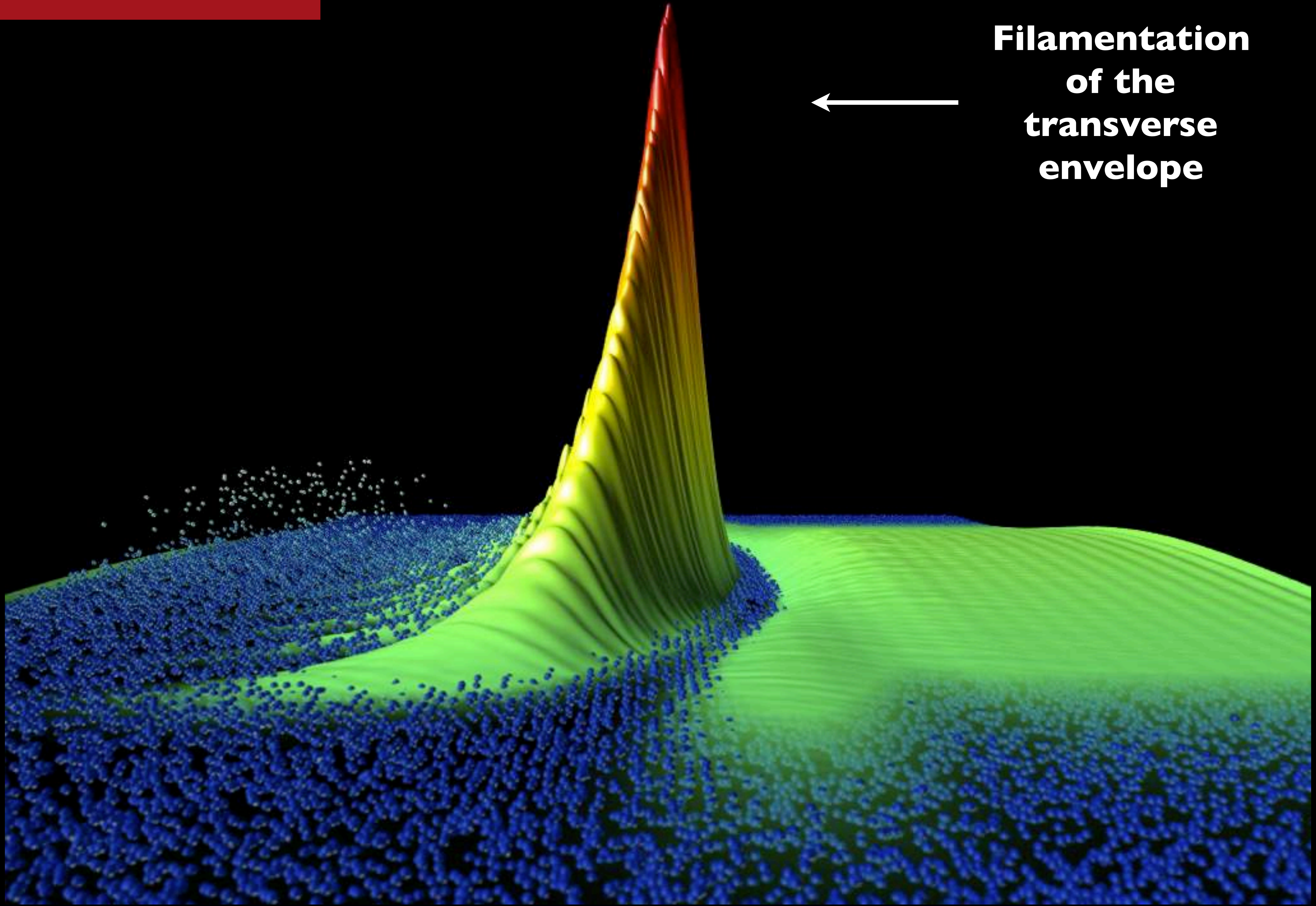


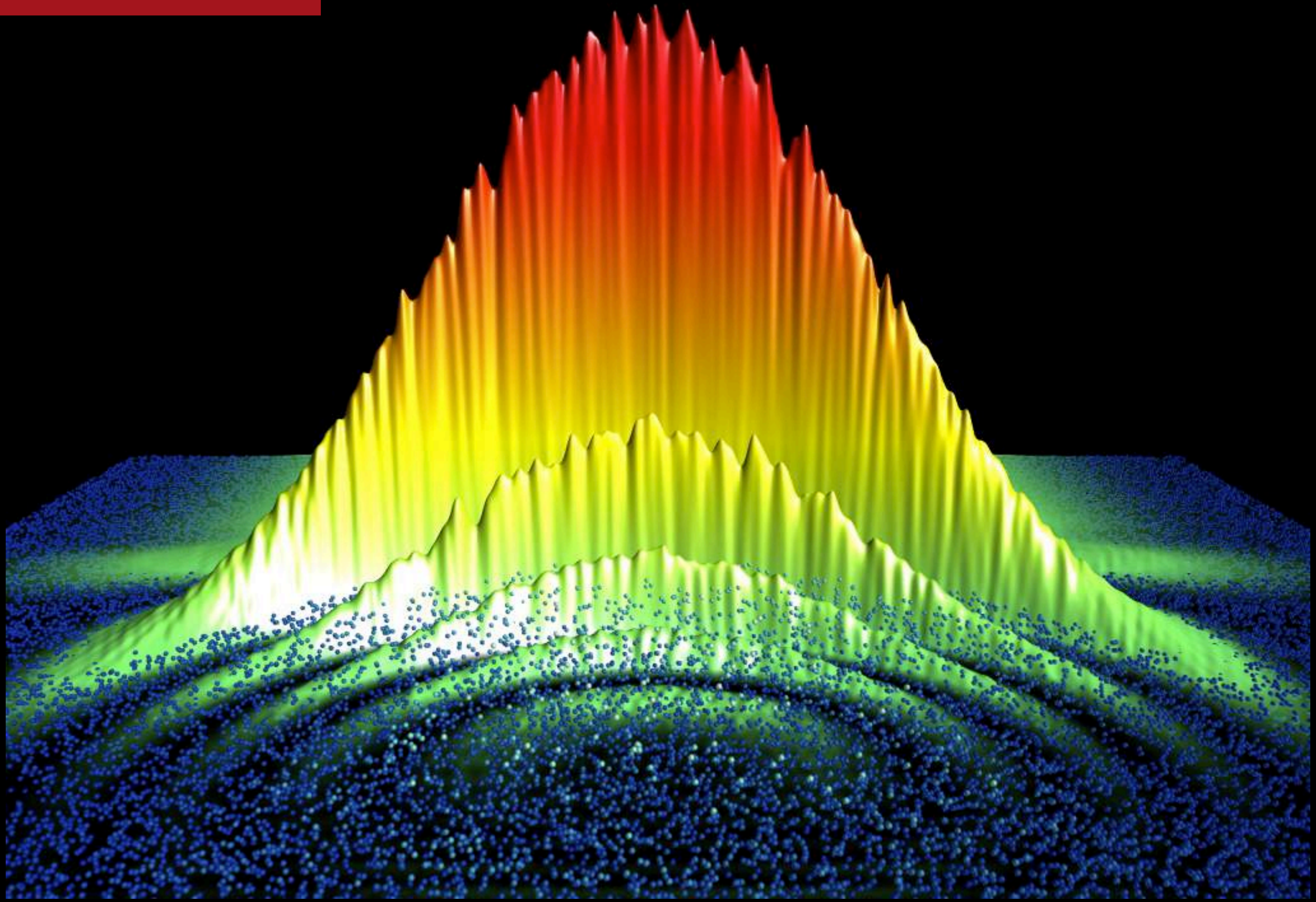
Filamentation of the transverse envelope

~10^8 particles
~10^4 time steps
3M core hours

E.P.Alves et al., arXiv:1311.2034 (2014)

Multidimensional dynamics of Brillouin-amplification

$I_{seed} = I_{pump} = 10^{16} W/cm^2$
$n_0 = 0.3 n_{cr}$



$\sim 10^8$ particles
$\sim 10^4$ time steps
3M core hours

E.P. Alves et al., arXiv:1311.2034 (2014)

Multidimensional dynamics of Brillouin-amplification

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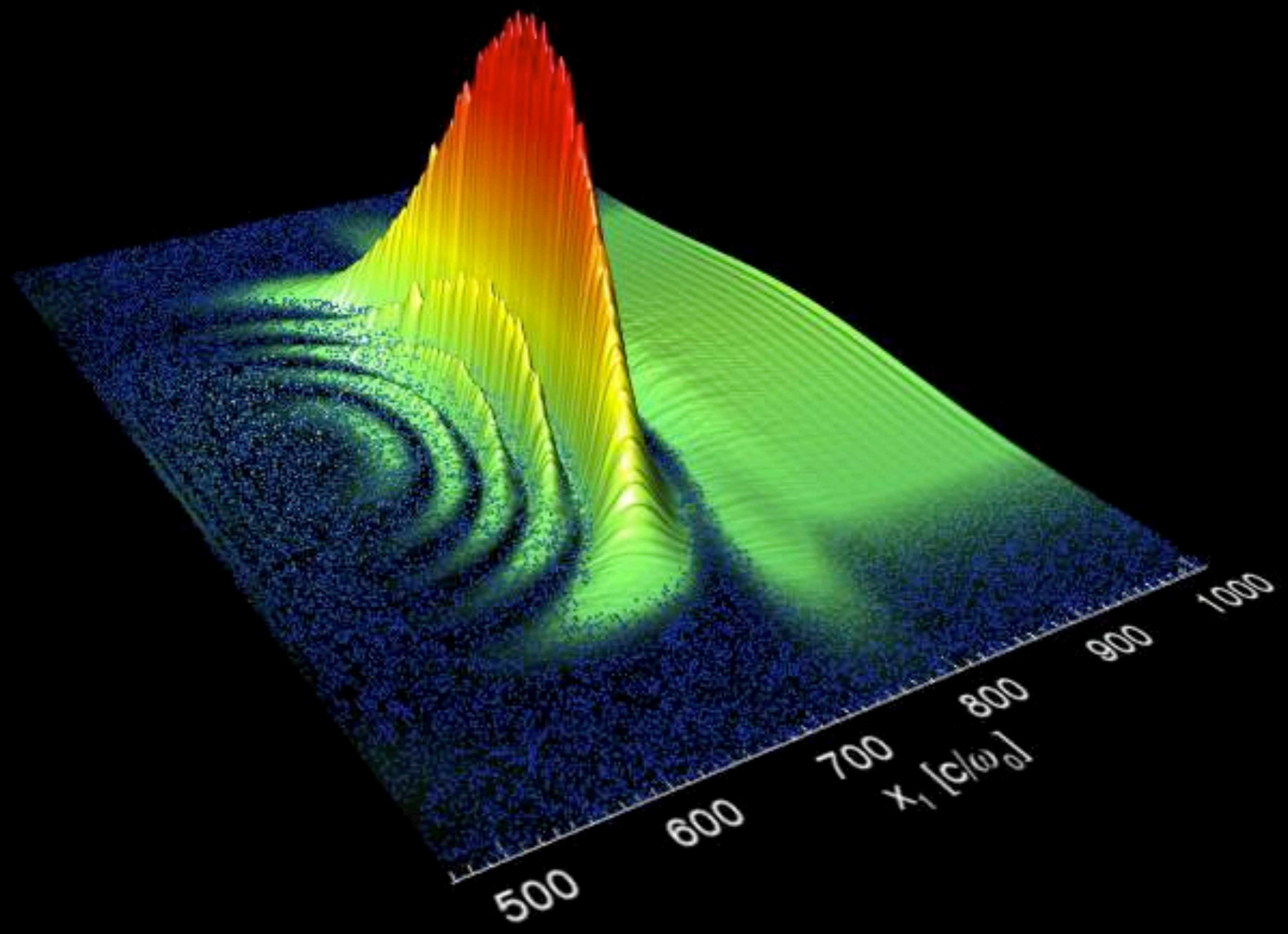

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SLAC

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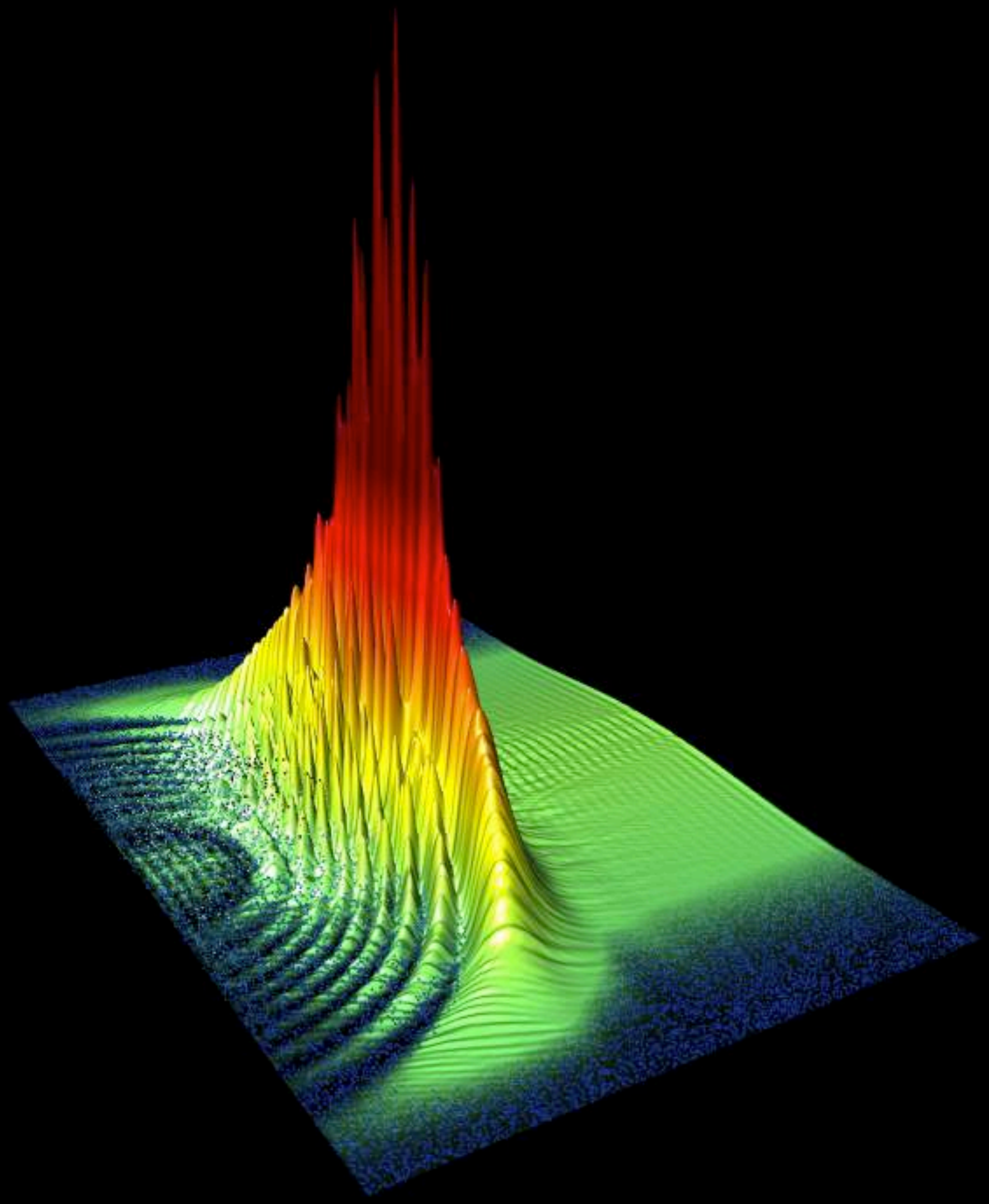

~10^8 particles
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3M core hours

E.P.Alves et al., arXiv:1311.2034 (2014)

Conclusions

- **PIC codes are a powerful tool to model kinetic physics (microphysics) of plasmas**
- **Current HPC resources enable PIC simulations of large-scale domains, revealing self-consistent interplay between plasma microphysics and global evolution**
- **PIC codes are successfully being used to guide and interpret laser-plasma experiments**
- **Combination of improved PIC algorithms + HPC is revolutionizing plasma science across different applications**