Multi-scale PIC modeling of high energy density scenarios: from laboratory to astrophysics

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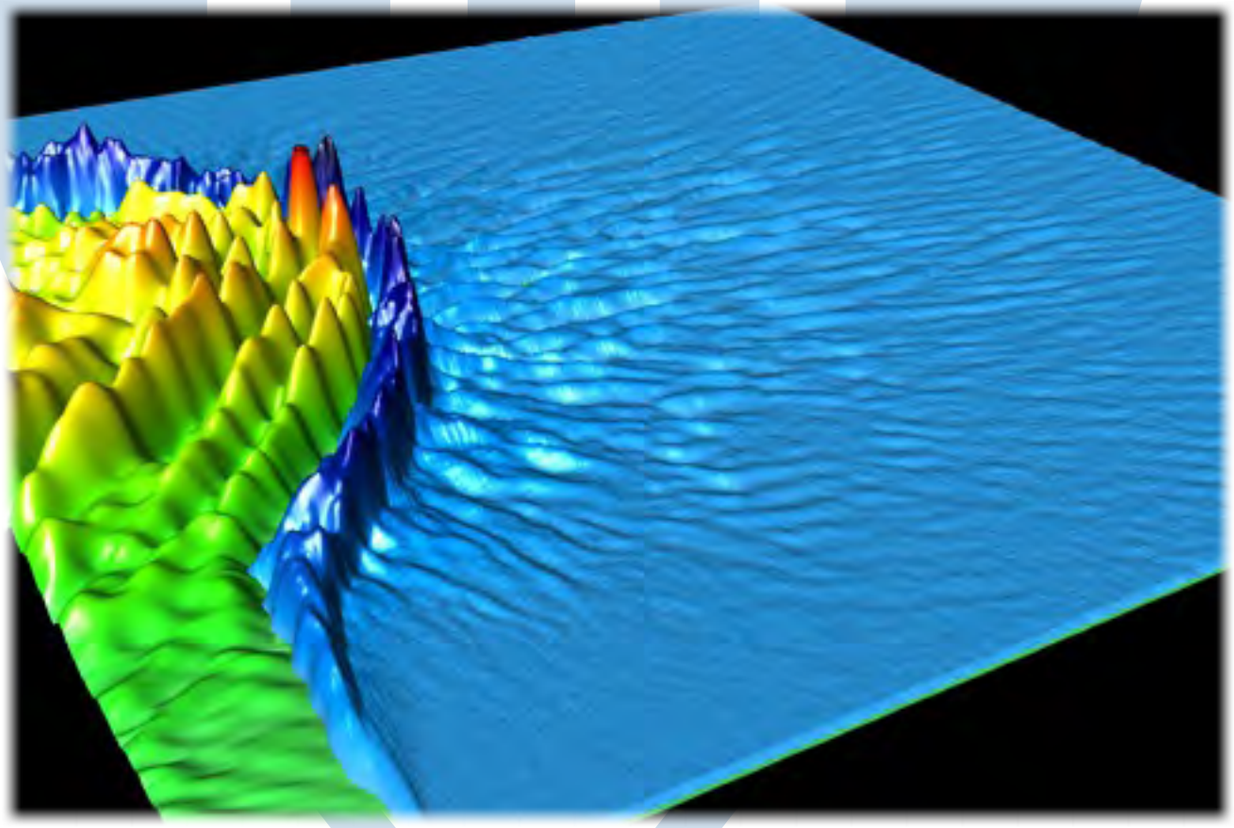

GoLP/IPFN Instituto Superior Técnico

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SEVENTH FRAMEWORK PROGRAMME

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Outline

- **Introduction/Motivation**
- **New hybrid-PIC algorithm for HED scenarios**
- **First full-scale modeling of fast ignition of ICF targets**
- **Applying new algorithm to other HED systems**
- **Conclusions and perspectives**

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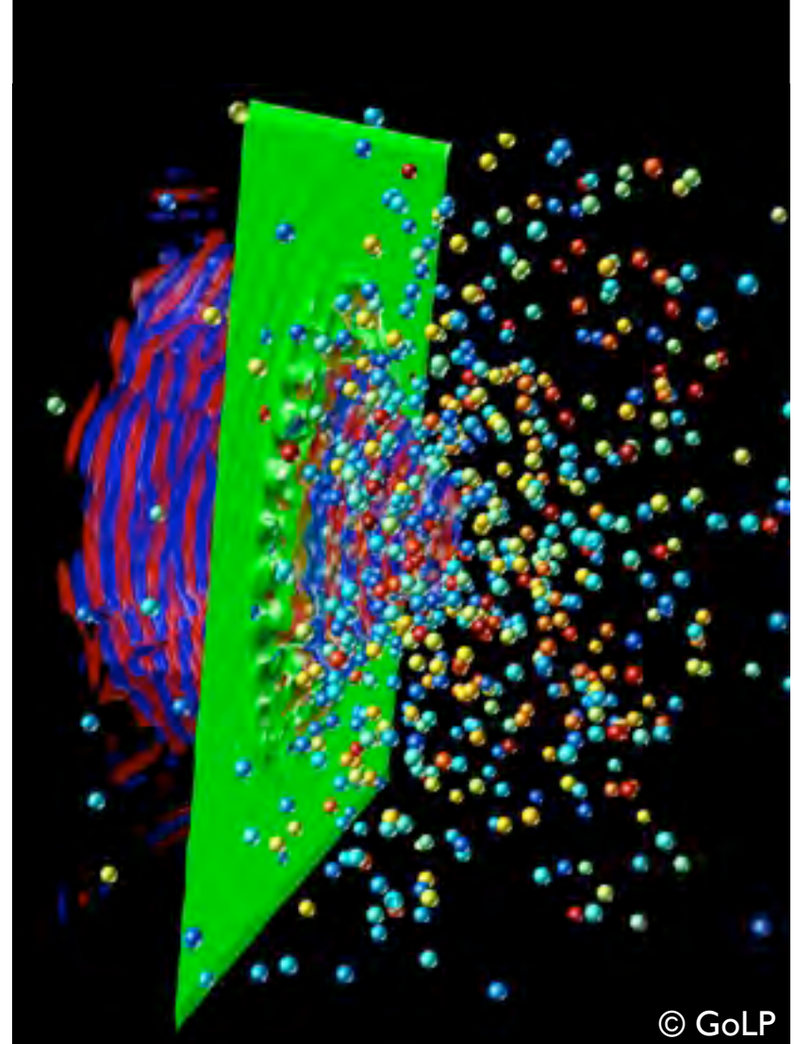
High energy density scenarios hold promising applications

Laser fusion

A clean and unlimited energy source

Plasma accelerators



Compact ion sources for tumor therapy

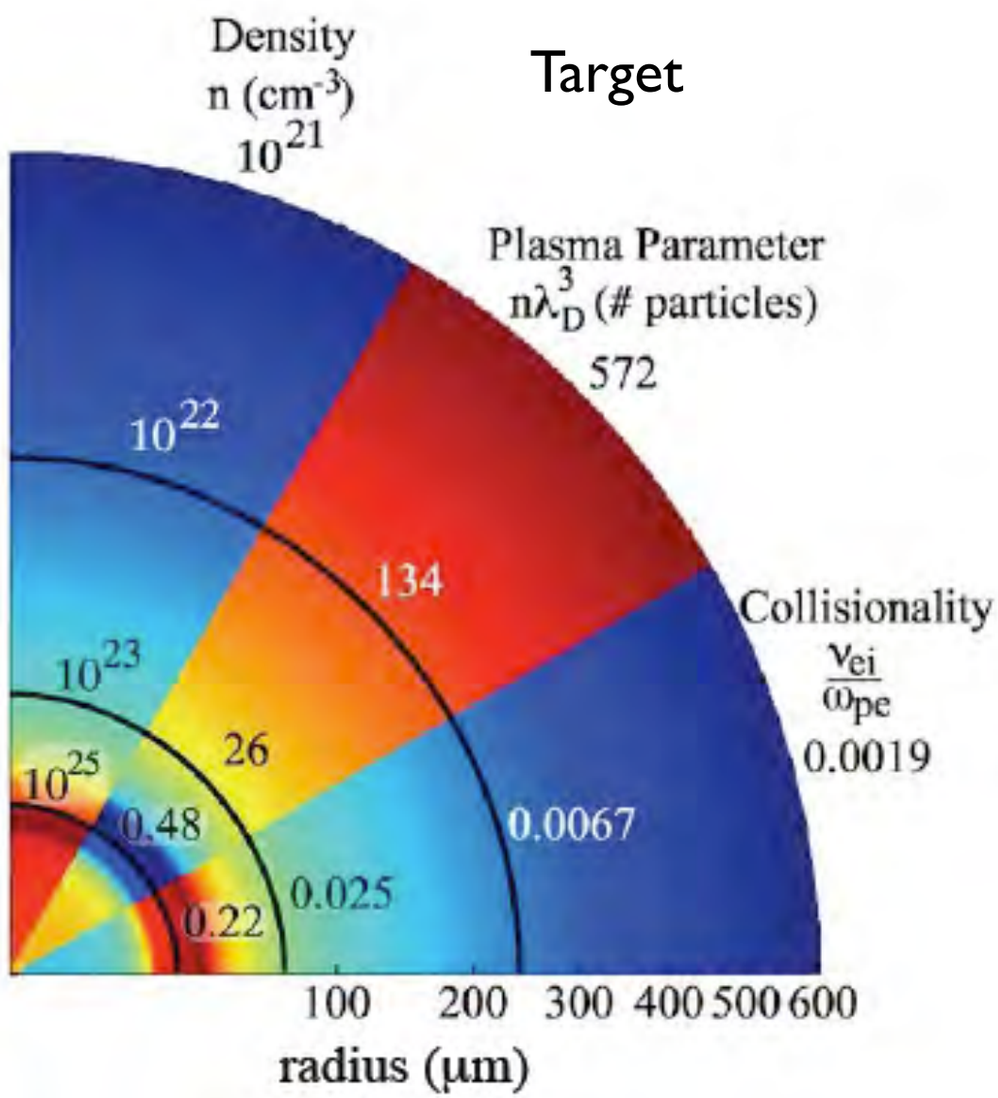
Astrophysics

Understanding origin of cosmic rays

Modeling of HED systems is demanding due to different scales involved

eg. Advanced ignition schemes (fast ignition or shock ignition)

Very different scales involved



Laser duration: 10 ps (FI) or 1 ns (SI)

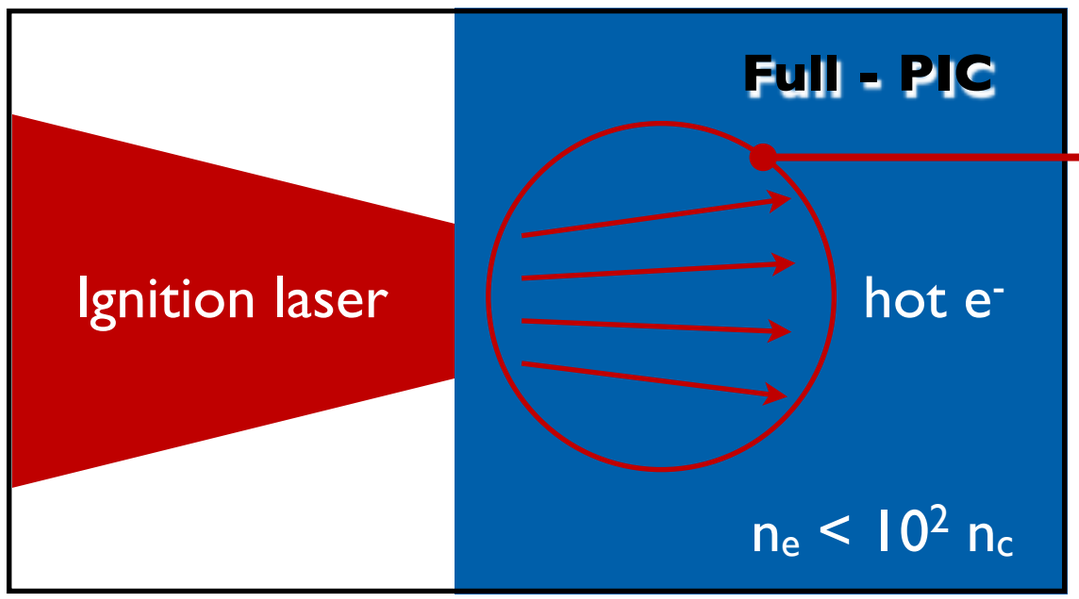
Full-scale modeling is crucial

- Ignition scale lasers are now coming online: predictive capability is required
- Several important questions need to be addressed:
  - What are the dominant laser absorption mechanisms?
  - How does laser absorption/e^- spectrum changes during 15 ps?
  - What is the beam divergence?
  - What are the stopping mechanisms?
  - How important is the modeling of spherical isolated targets?

Current modeling approaches are not complete/self-consistent

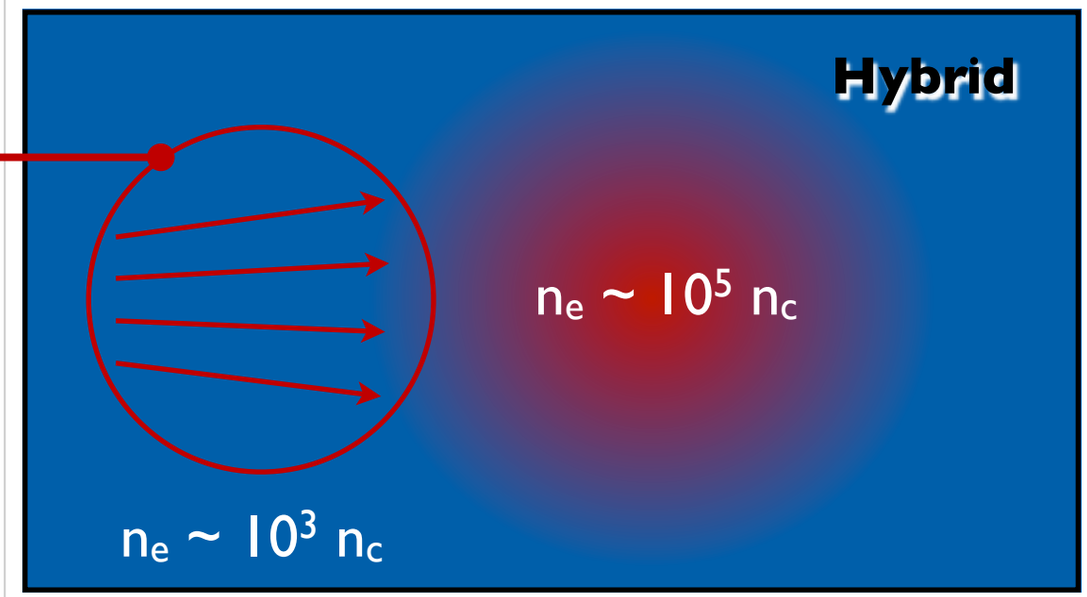
eg. Fast Ignition or Shock Igniton

Full-PIC modeling



Kinetic modeling of laser-plasma interaction and electron acceleration

Hybrid modeling



Hybrid modeling of electron transport and energy deposition

Improved algorithms are required

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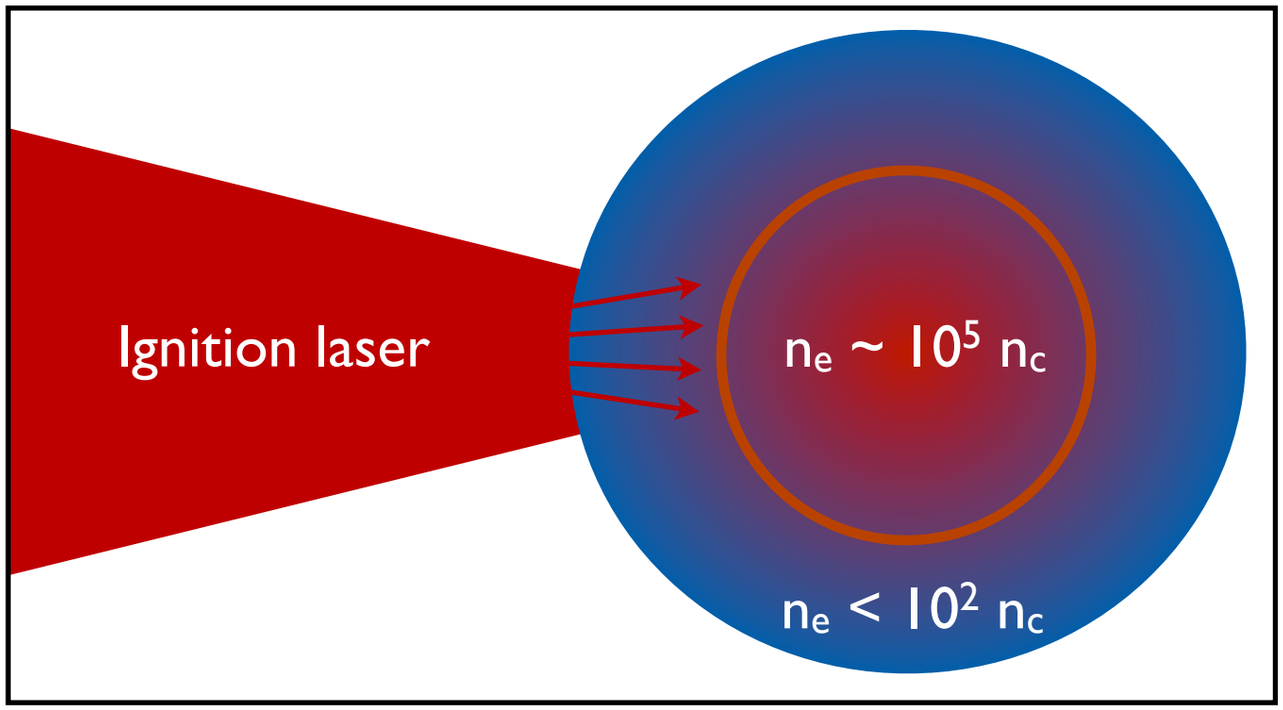
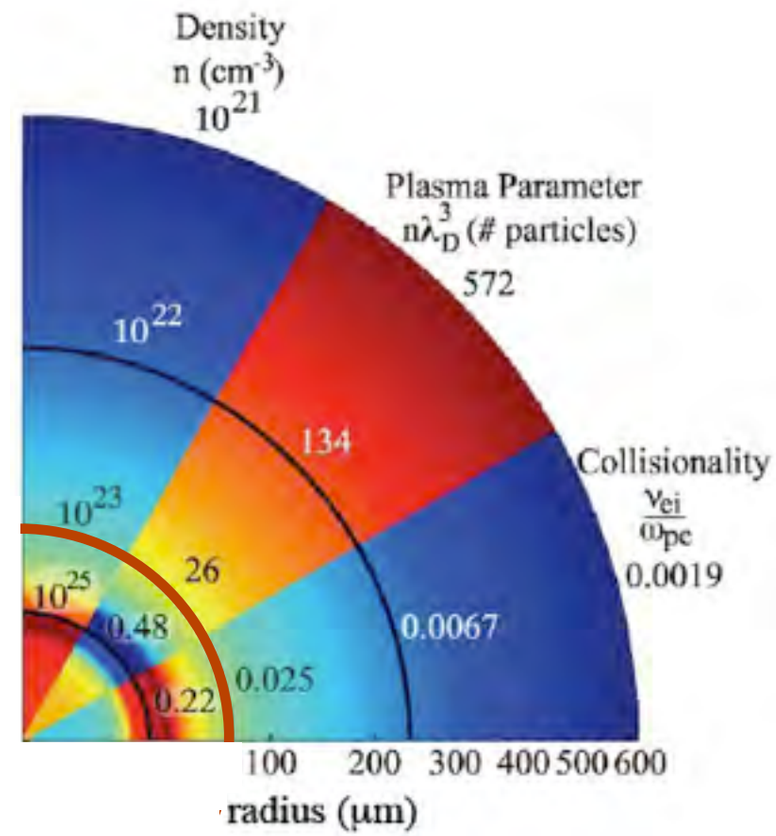
New hybrid algorithm*

* B. Cohen, A. Kemp, and L. Divol, J. Comp. Phys. 229, 4591 (2010)





Full-PIC code

- Full Maxwell's equations
- Kinetic species
- $n_0 < 10^{23}$ cm^{-3}
- $\omega_p \Delta t < O(1)$
- $\Delta x \omega_p / c < O(1)$
- $c\Delta t/\Delta x < 1$

If resistivity (Ohm's law) matches collisional model transition is natural and self-consistent

Hybrid-PIC code

- Maxwell's equations + Ohm's law (inertialess)
- Kinetic species
- $n_0 > 10^{23}$ cm^{-3}
- $\nu_{ei} \Delta t < O(1)$
- $c\Delta t/\Delta x < 1$

Algorithm description and implementation: current deposition

Hybrid-PIC algorithm*

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

Integration of equations of motion, moving particles

$\mathbf{F}_i \rightarrow \mathbf{u}_i \rightarrow \mathbf{x}_i$

Weighting

$(\mathbf{x},\mathbf{u})_i \rightarrow \mathbf{J}_{fast}$
$(\mathbf{x},\mathbf{u})_i \rightarrow \mathbf{J}_i$

Δt

Integration of Field Equations on the grid

$\mathbf{J}_j \rightarrow (\mathbf{E}, \mathbf{B})_j$

Weighting

$(\mathbf{E}, \mathbf{B})_j \rightarrow \mathbf{F}_i$

$$0 = \mathbf{E} + \frac{\nabla p_e}{en_e} - \eta(\mathbf{J}_e + \mathbf{J}_i) - \frac{\mathbf{J}_e \times \mathbf{B}}{en_e c} + \left(\frac{d}{dt}\right)_{coll,f-e} \frac{\mathbf{P}_{e,f}}{en_e}$$

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

Weighting

deposit currents

$(\mathbf{x},\mathbf{u})_i \rightarrow \mathbf{J}_f$

$(\mathbf{x},\mathbf{u})_i \rightarrow \mathbf{J}_i$

separate fast (f) and cold (e) electrons
($v_> \alpha v_{th}$)

calculate J_e from Ampère's law
(possibility to drop displacement current)

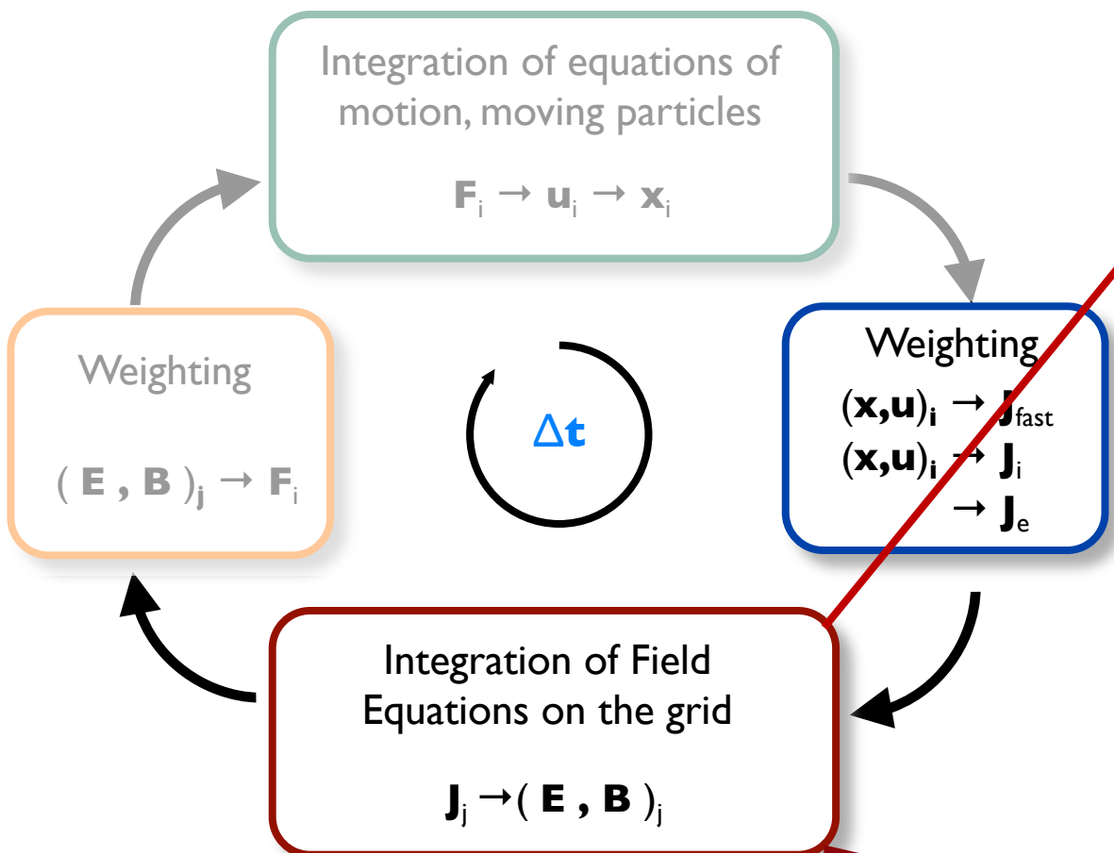
$$\cancel{\frac{\partial \mathbf{E}}{\partial t}}^{\,=0} = c\vec{\nabla}\times\mathbf{B} - 4\pi(\mathbf{J}_f + \mathbf{J}_i + \mathbf{J}_e) \rightarrow \mathbf{J}_e$$

* B. Cohen, A. Kemp, L. Divol, J. Comp. Phys. 229, 4591 (2010)

Algorithm description and implementation: field solver

Hybrid-PIC algorithm

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



$$0 = \mathbf{E} + \frac{\nabla p_e}{en_e} - \eta(\mathbf{J}_e + \mathbf{J}_i) - \frac{\mathbf{J}_e\times\mathbf{B}}{en_e c} + \left(\frac{d}{dt}\right)_{coll,f-e}\frac{\mathbf{P}_{e,f}}{en_e}$$

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

Integration of Field Equations on the grid

$$\mathbf{J}_j \rightarrow (\mathbf{E},\mathbf{B})_j$$

advance E using inertialess plasma e⁻ eq. of motion (Ohm's law)

$$0 = \mathbf{E} + \frac{\nabla p_e}{en_e} - \eta(\mathbf{J}_e + \mathbf{J}_i) - \frac{\mathbf{J}_e\times\mathbf{B}}{en_e c} + \left(\frac{d}{dt}\right)_{coll,f-e}\frac{\mathbf{P}_{e,f}}{en_e}$$

where

$$\eta = m_e\nu_{ei}/n_e e^2$$

$$\nu_{ei} =^{**} 0.51\times 4\sqrt{2\pi}e^4 Z_i^2 n_i/(3\sqrt{(m_e)}Te^{3/2})$$

$$n_e = \int f_e d^3v$$

$$\mathbf{v_e} = \int \mathbf{v} f_e d^3v$$

$$\mathbf{p_e} = \int (\mathbf{v}-\mathbf{v_e})(\mathbf{v}-\mathbf{v_e}) f_e\, d^3v$$

$$T_e = p_e/n_e$$

(possibility of spatially/temporally smooth all quantities)

advance B using Faraday's law

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

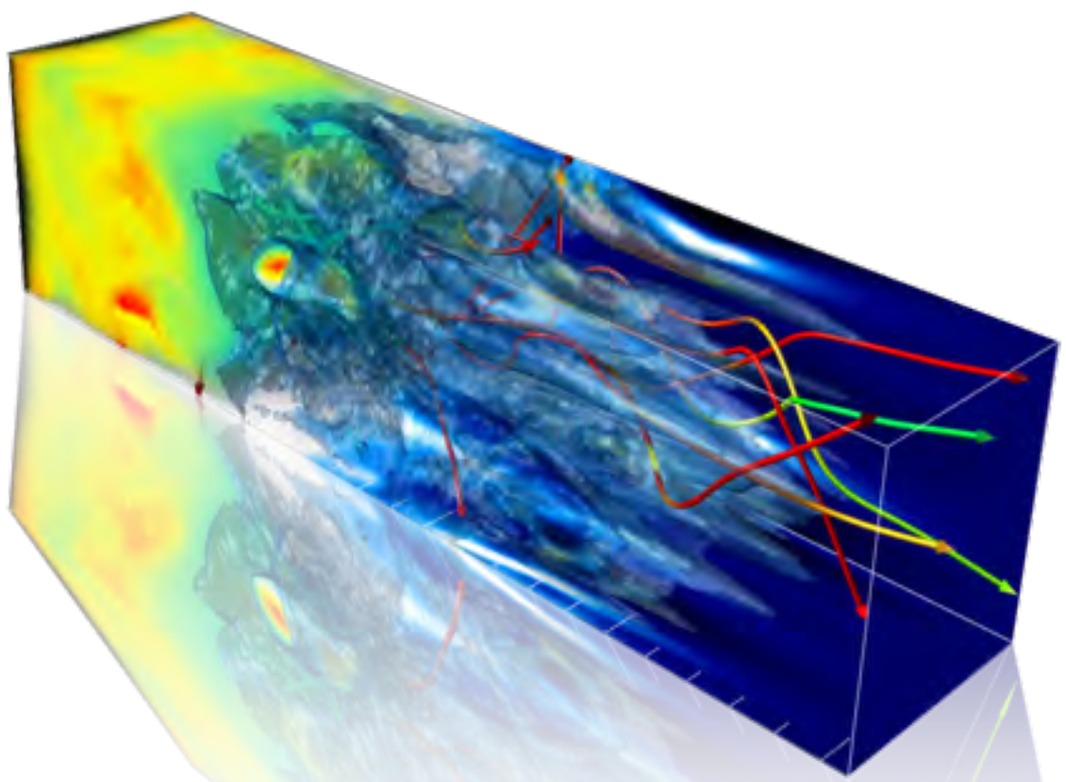
** S.I. Braginskii, Rev. Plasm. Phys. 1, 205 (1965)

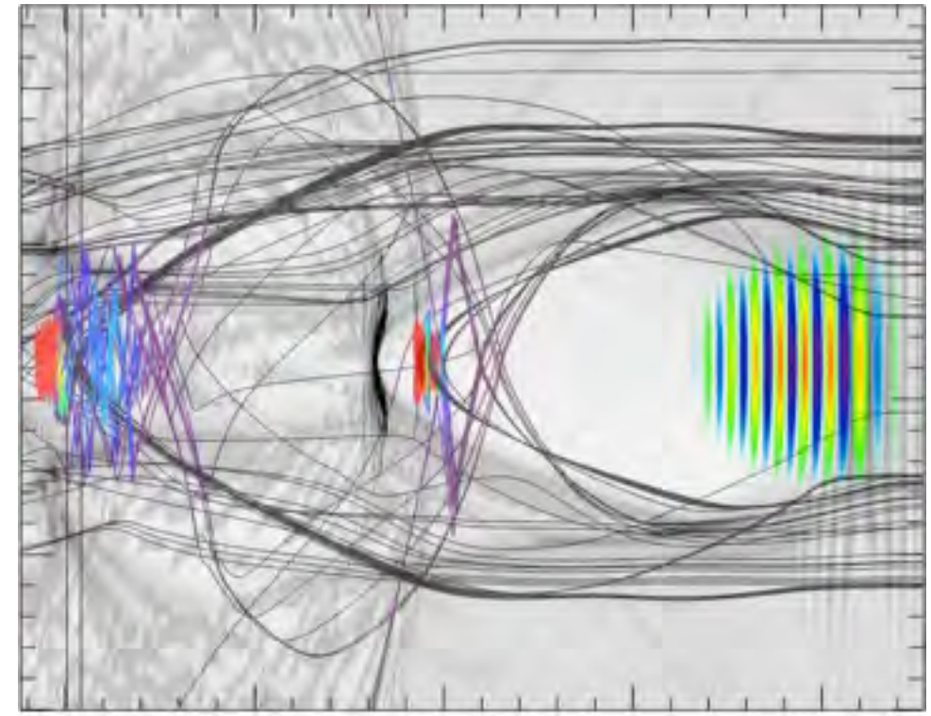
OSIRIS 2.0

osiris v2.0

osiris framework

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





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New Features in v2.0

- High-order splines
- Binary Collision Module
- PML absorbing BC
- Tunnel (ADK) and Impact Ionization
- Dynamic Load Balancing
- Parallel I/O

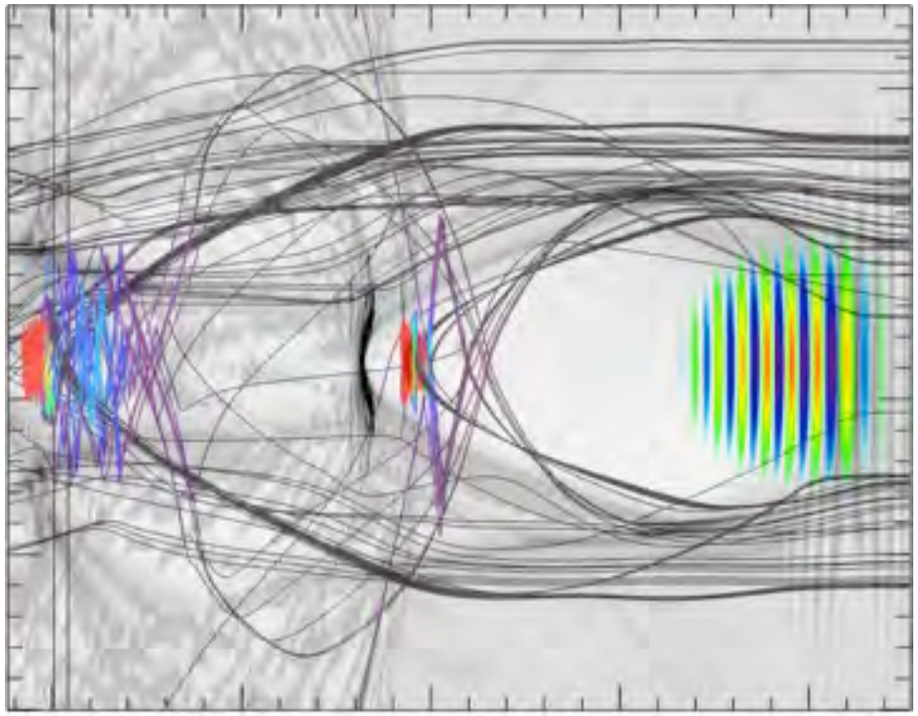
OSIRIS 2.0

UCLA

Numerics are crucial for accurate transition

- **High-order splines**
  - **control grid heating for >10^5 time steps**
  - **ensure equivalent heating between PIC and hybrid**
- **MC binary Coulomb collision module**
  - **statistically correct**
  - **fully relativistic**
- **Advanced smoothing**
  - **spatial and temporal smoothing for fluid quantities and fields near transition**
- **PML absorbing boundary conditions**
  - **efficiently absorb radiation at all boundaries (model isolated targets)**

F. Fiuza et al. PPCF 53, 074004 (2011)



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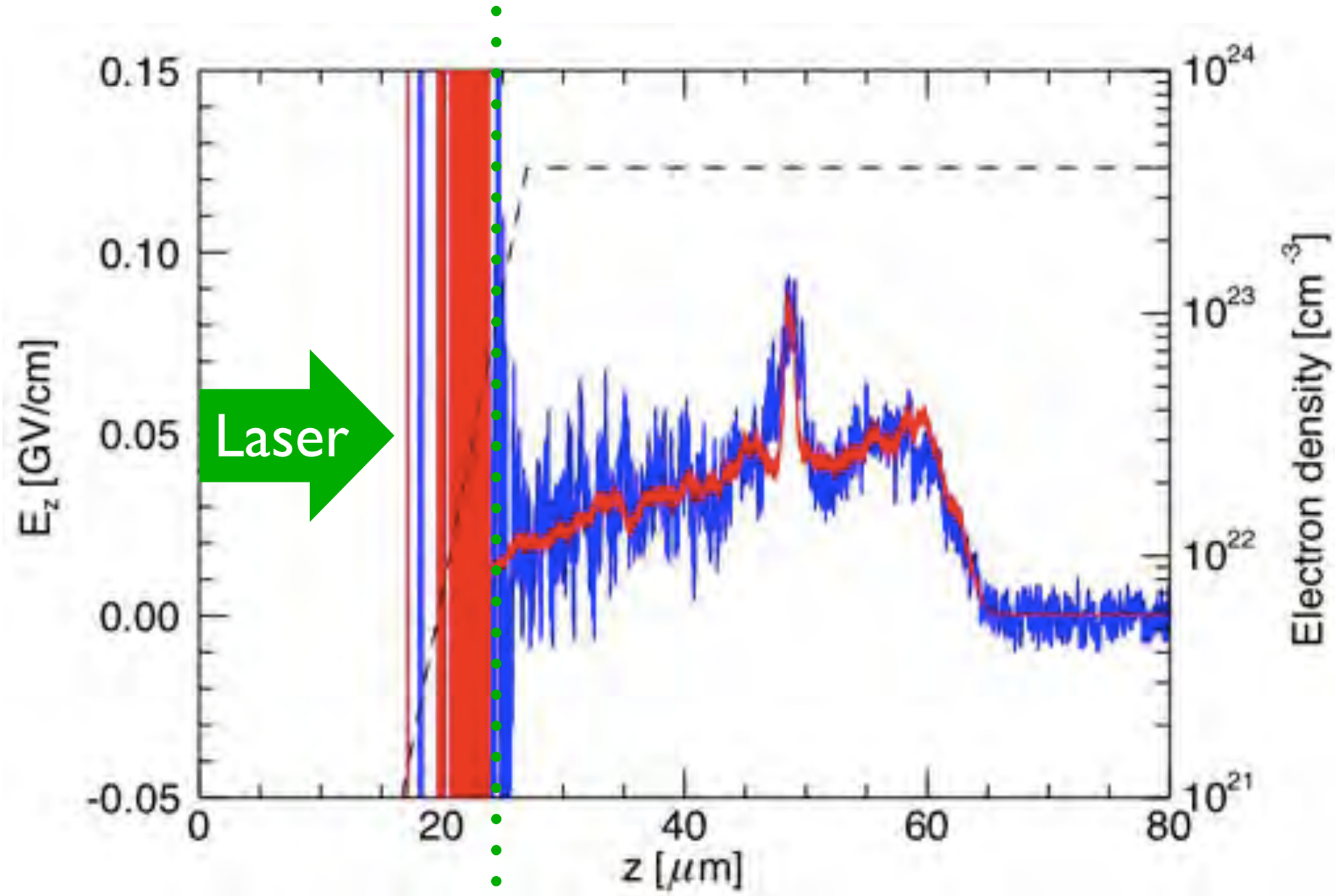
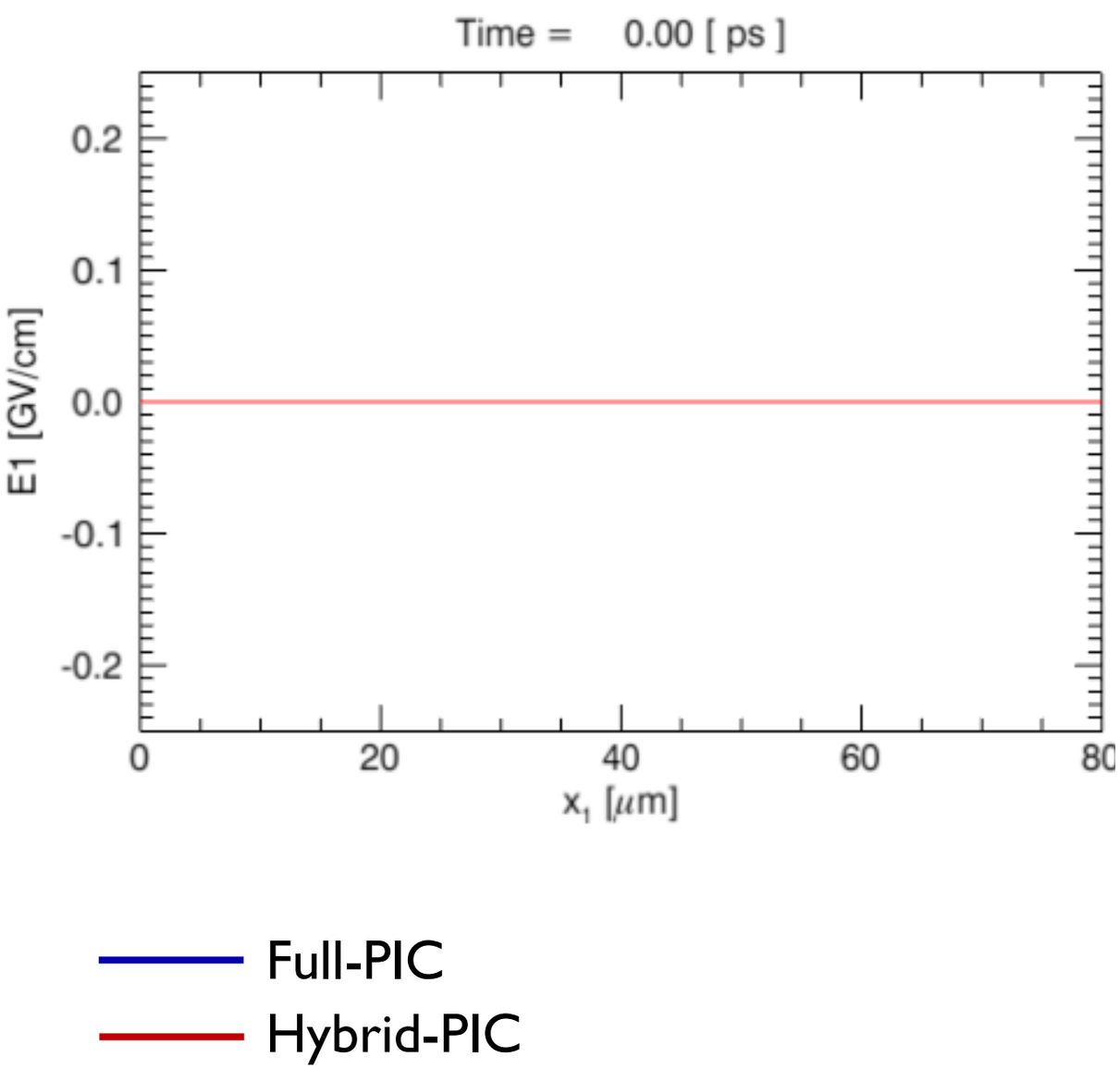
E-field is continuous w/ appropriate numerics & collisional model



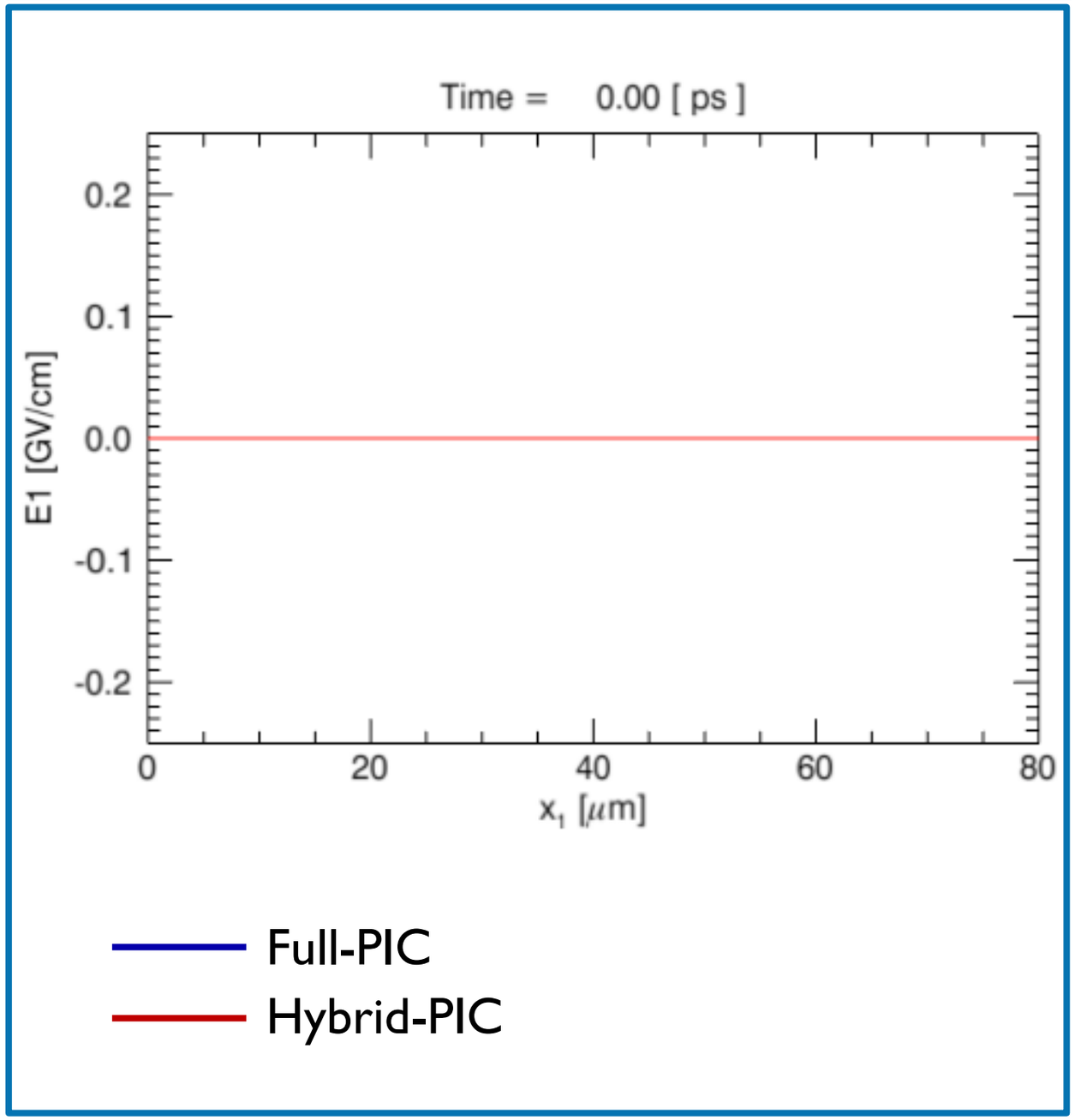
hybrid-PIC transition
@ 100 n_c

E-field is continuous w/ appropriate numerics & collisional model

No smooth



Smoothed fields in full-PIC

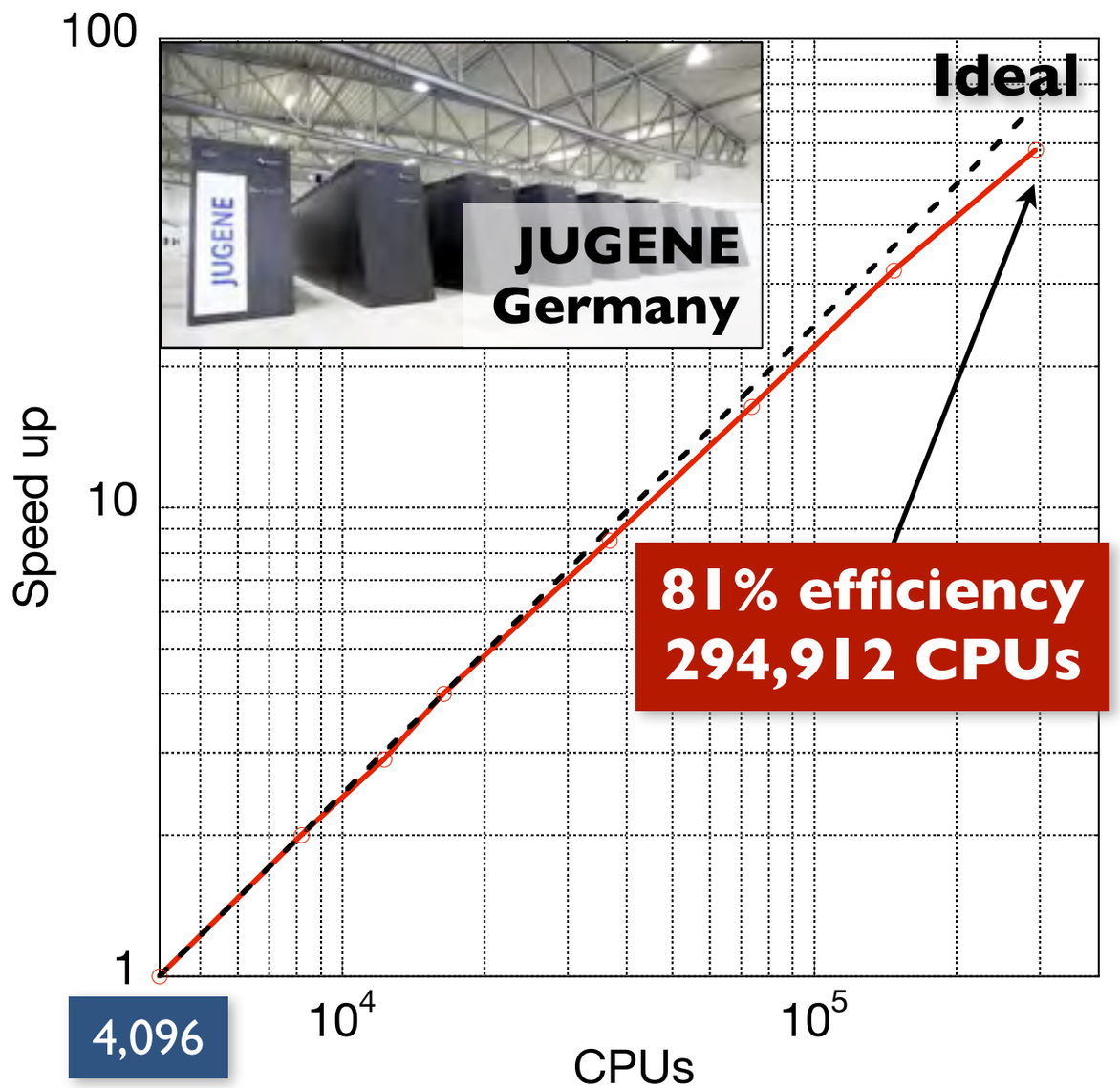


Towards full-scale modeling of fast ignition

	2D full-scale	3D scaled down	3D full-scale
Laser			
a_0	6-12	6-12	6-12
Spot [μm]	20-30	7-10	20-30
Duration [ps]	15	15	15
Target			
Density [n_c]	$1\text{-}2\times10^5$	$1\text{-}2\times10^5$	$1\text{-}2\times10^5$
Size [$\mu m^{2(3)}$]	400x400	100x100x100	400x400x400
Simulation time [CPU hours*]			
PIC	2×10^{11}	4×10^{13}	1×10^{15}
Hybrid-PIC	1×10^6	7×10^6	2×10^8

OSIRIS is highly optimized for modeling at very large scales

OSIRIS strong scaling up to ~300k CPUs



- Spatial domain decomposition
- Local field solver
- Minimal communication
- Dynamic Load Balancing

New hardware features

SIMD units

tailored code already in production

GPUs

CUDA development (test PIC code)

OSIRIS is highly optimized for modeling at very large scales

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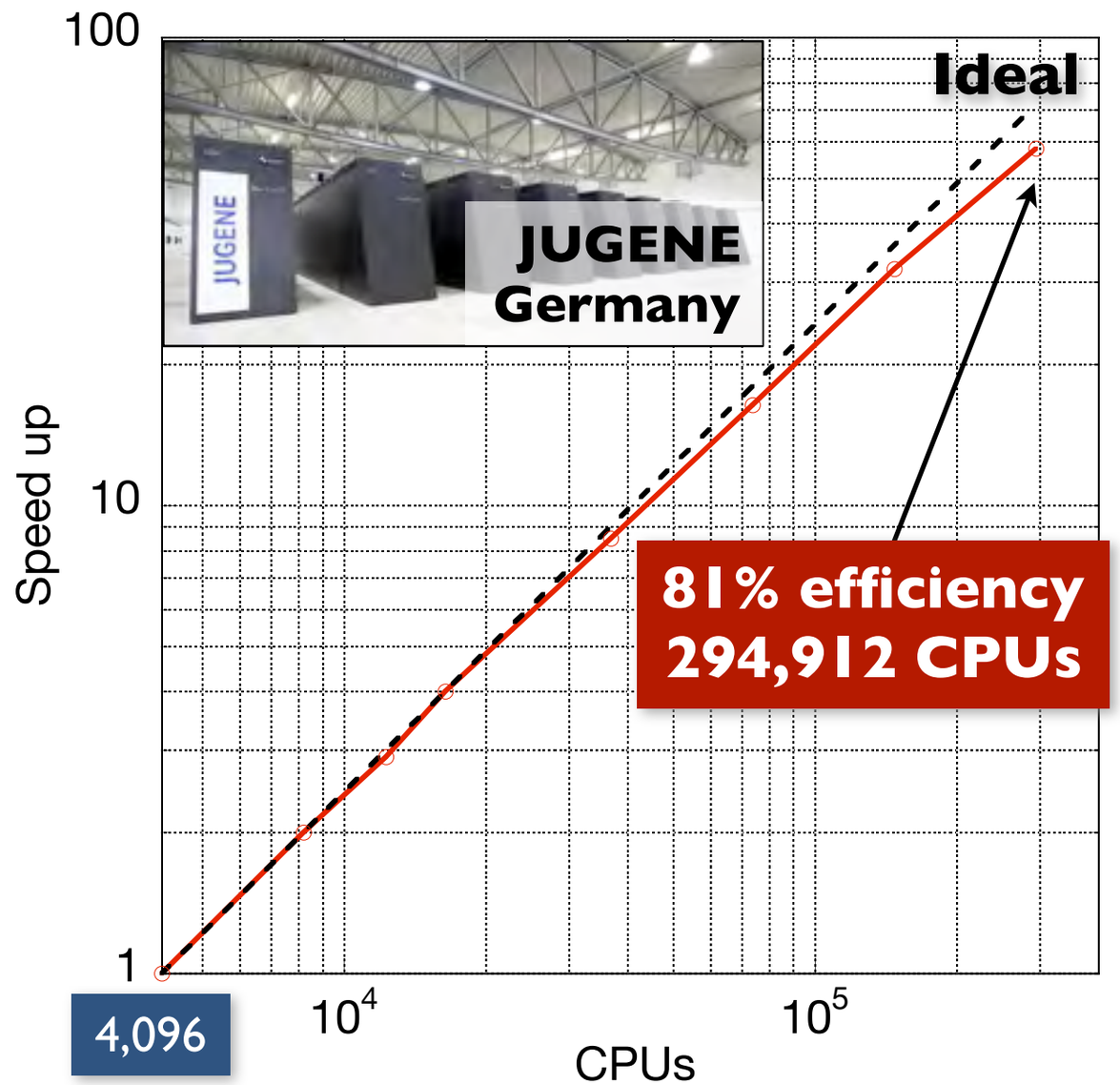

- Spatial domain decomposition
- Local field solver
- Minimal communication
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New hardware features

SIMD units

tailored code already in production

2D full-scale simulation in 2.5h 128k cpus on Jaguar

GPUs

CUDA development (test PIC code)

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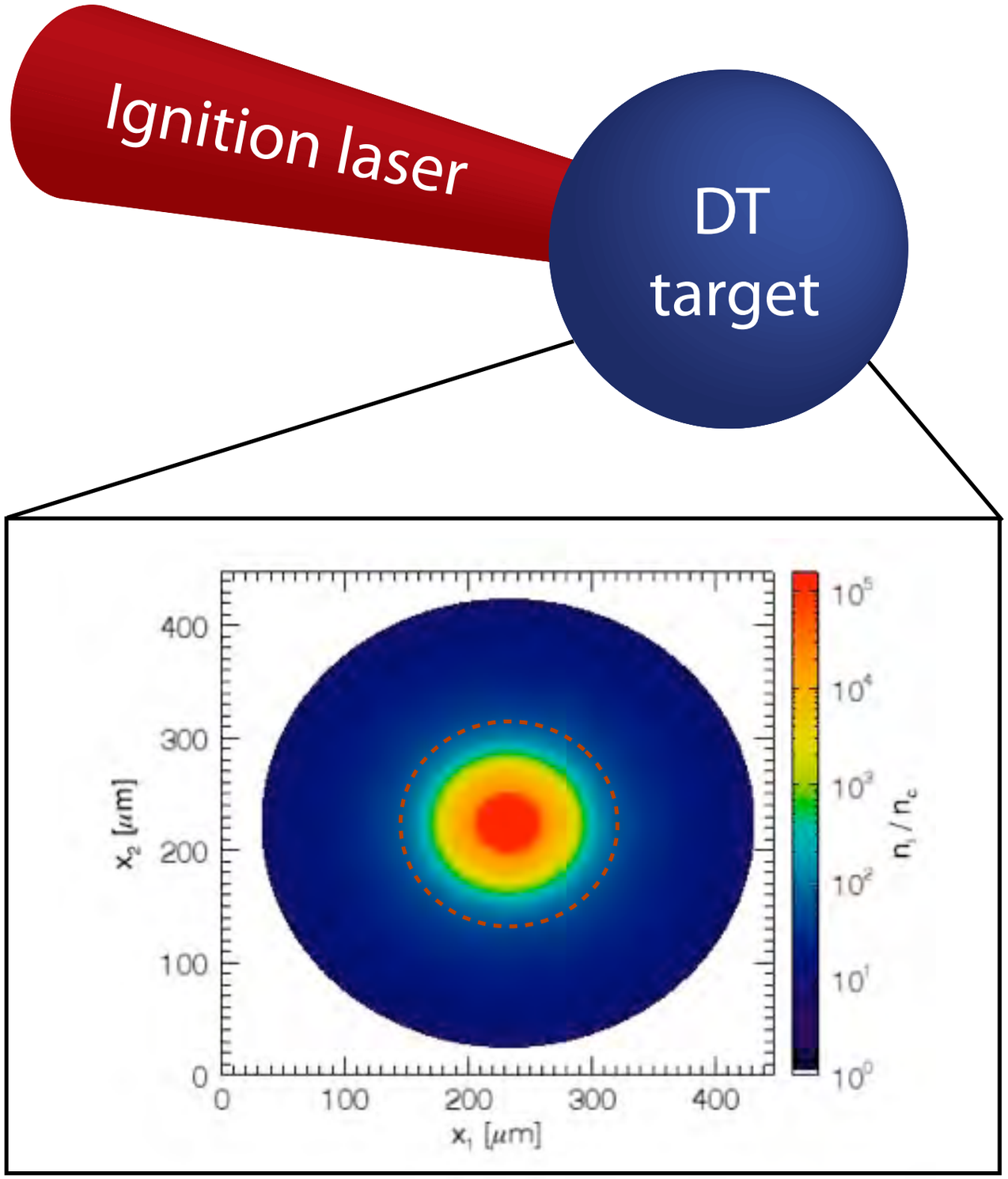
First full-scale FI modeling with realistic densities



Physical Parameters

Laser

- λ_0 = 1μm
- I_0 = 2×10^{20} Wcm^{-2} (100 kJ)
- W_0 = 30 μm
- **τ_0 = 15 ps**

Plasma

- **L = 450 x 450 μm^2**
- **n_{e0} = 1 n_c - 2×10^5 n_c**
- m_i/m_e = 3672

Numerical Parameters

- 42 cells/μm
- hybrid/full-PIC transition = 100 n_c
- Particles per cell = 64
- # time steps = 10^5
- cubic interpolation

First full-scale FI modeling with realistic densities

Density

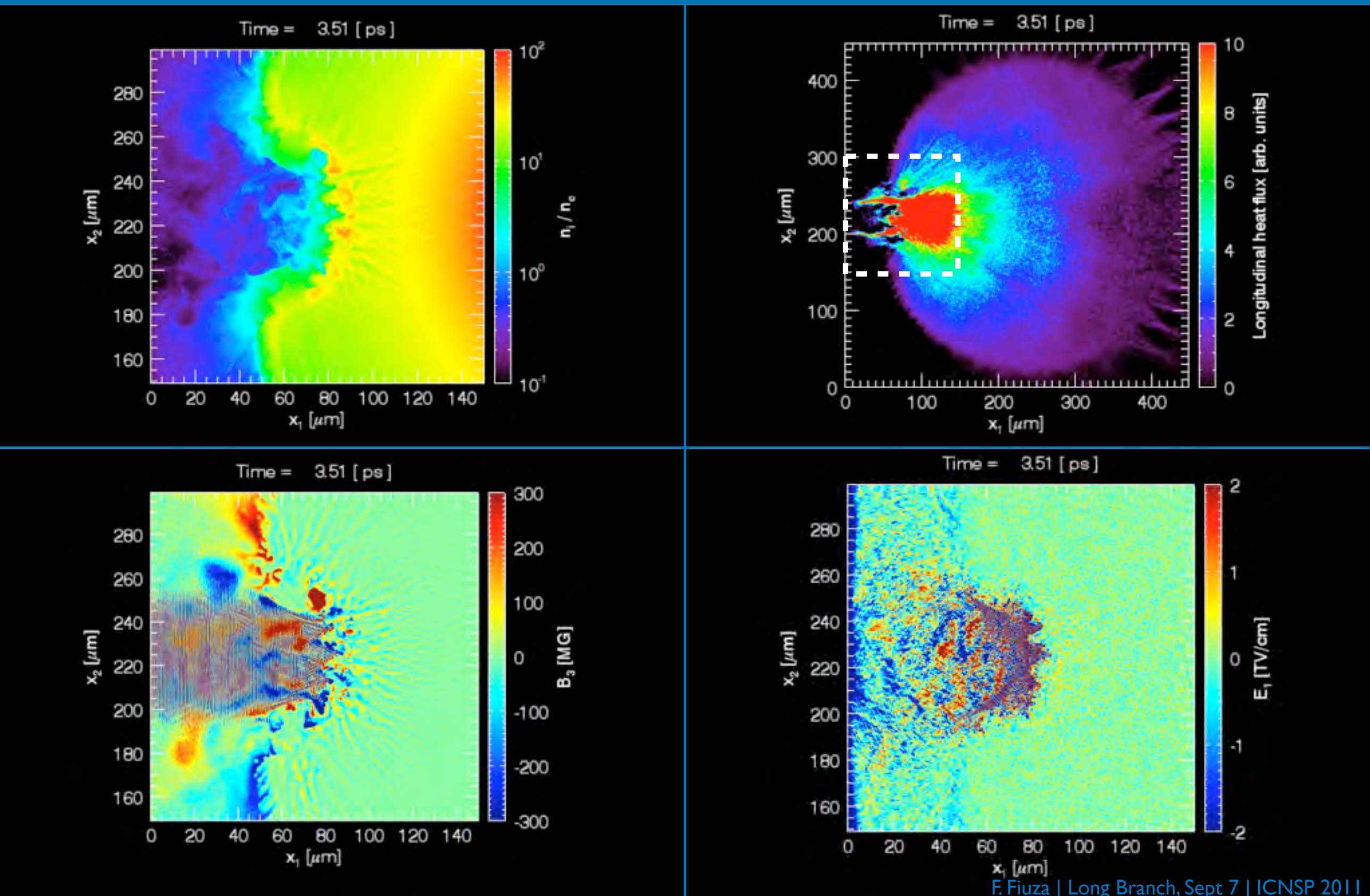
e^- heat flux

$I = 2x10^{20}\ Wcm^{-2}$

B-field

Longitudinal E-field

First full-scale FI modeling with realistic densities



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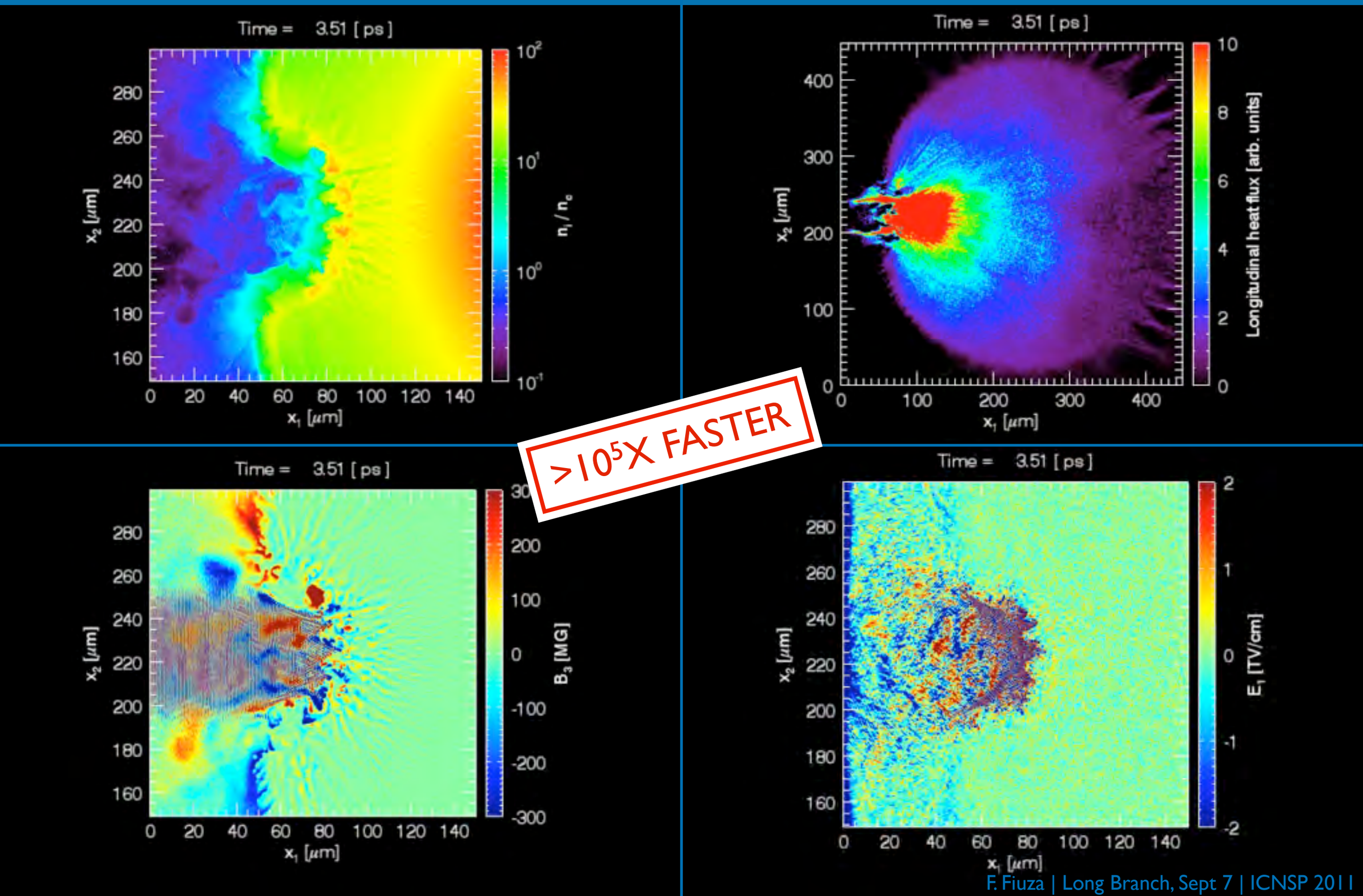
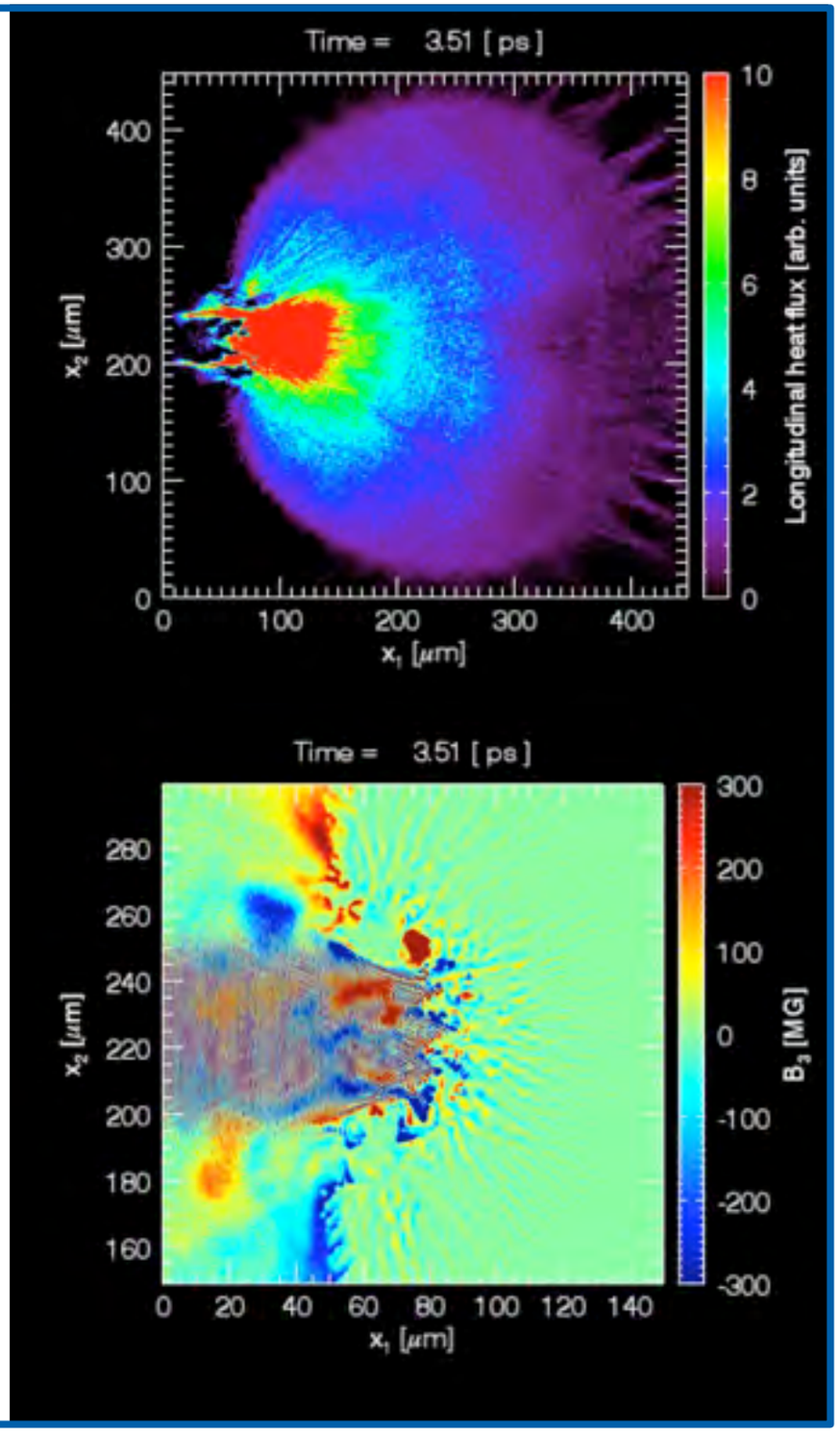
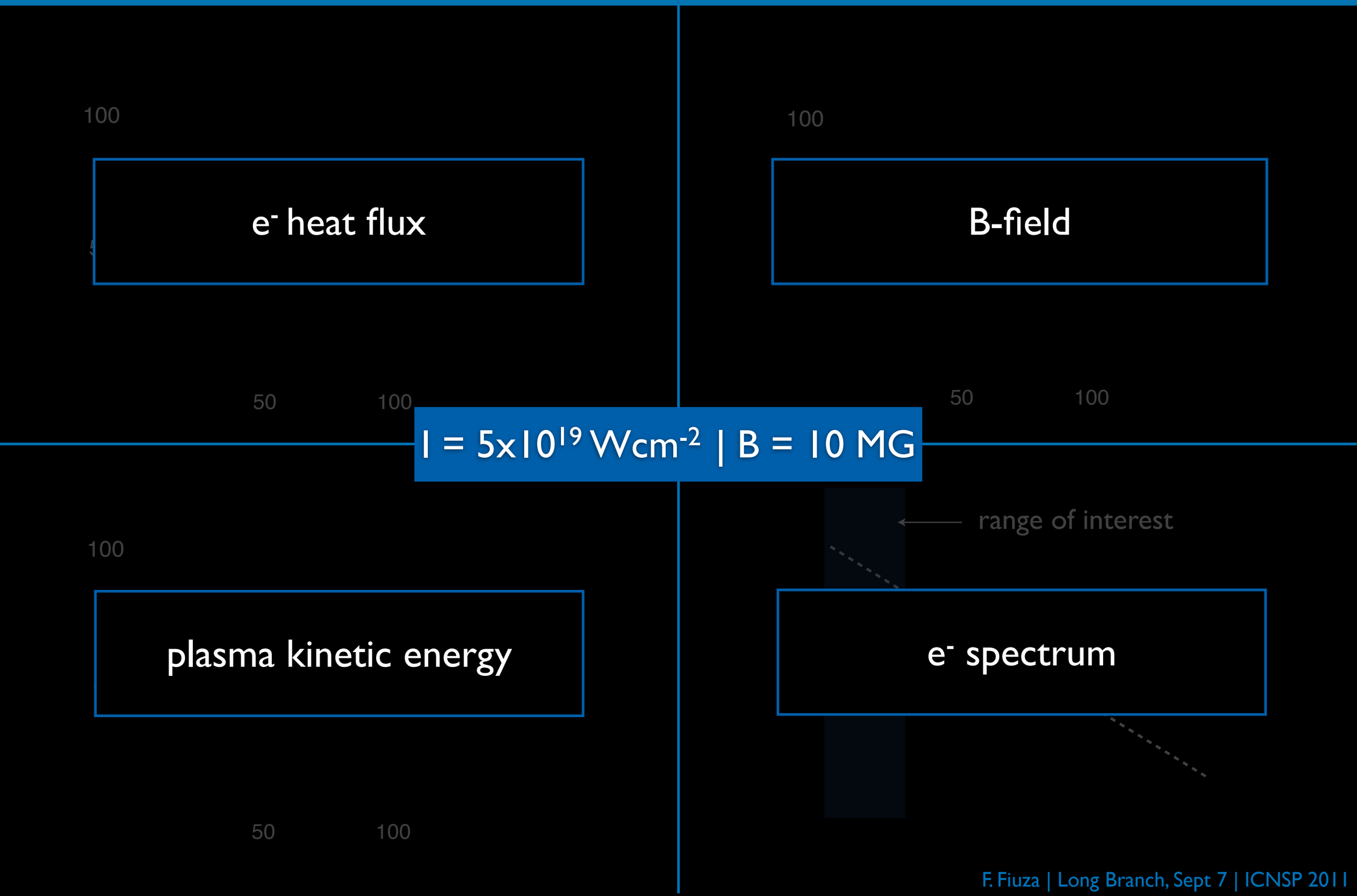


Stable interaction at ignition scale/energies

- **Interaction region is stable for long times**
- **Longitudinal heat flux ~70% laser flux**
- **Divergence is controlled to 20°-40°**
- **7% coupling efficiency to core**
- **Advecting B-fields can affect particle acceleration**
- **Wide range of EM instabilities develop at target surface**



Very high efficiencies are possible with 10 MG axial B-field



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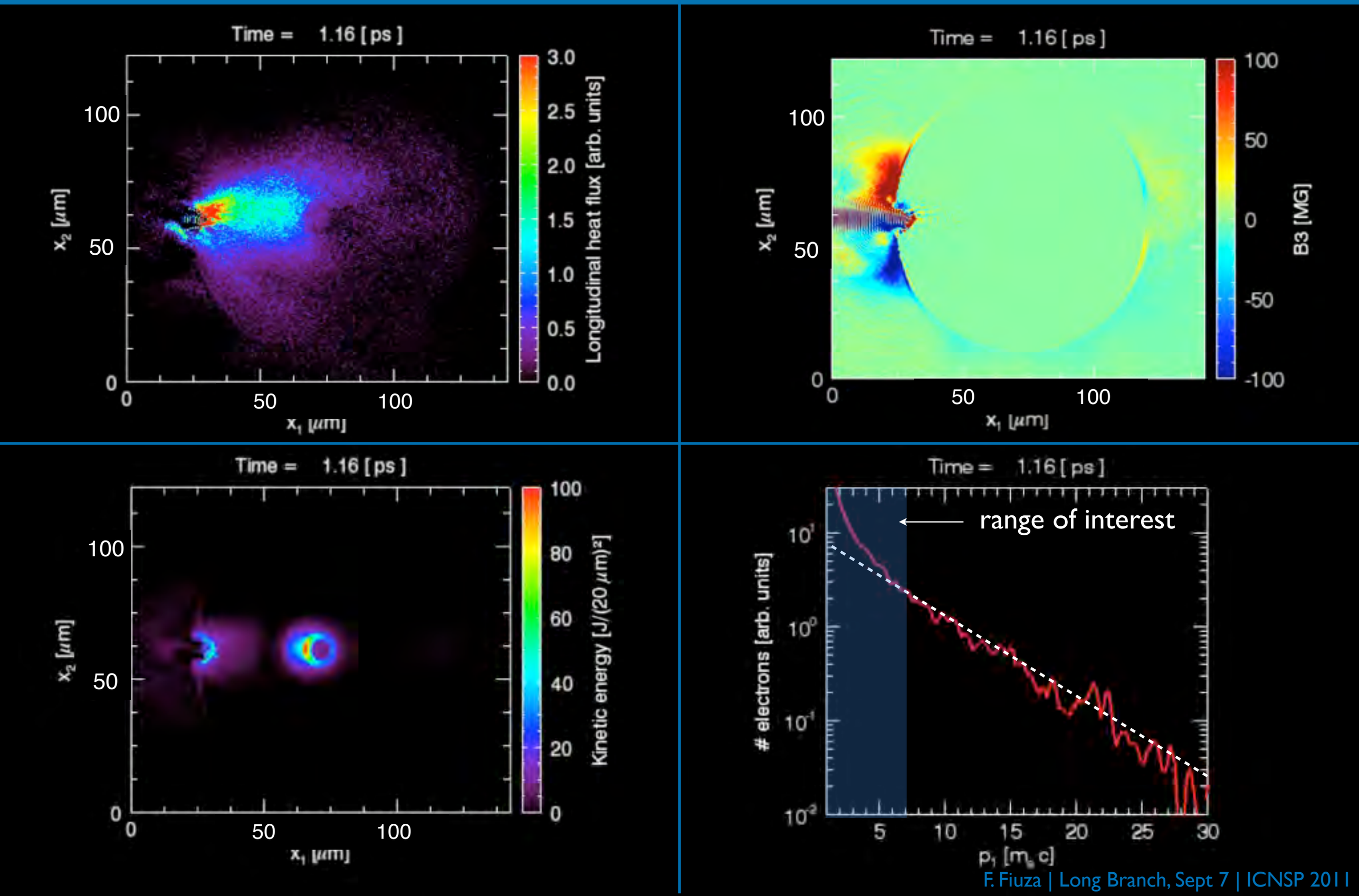

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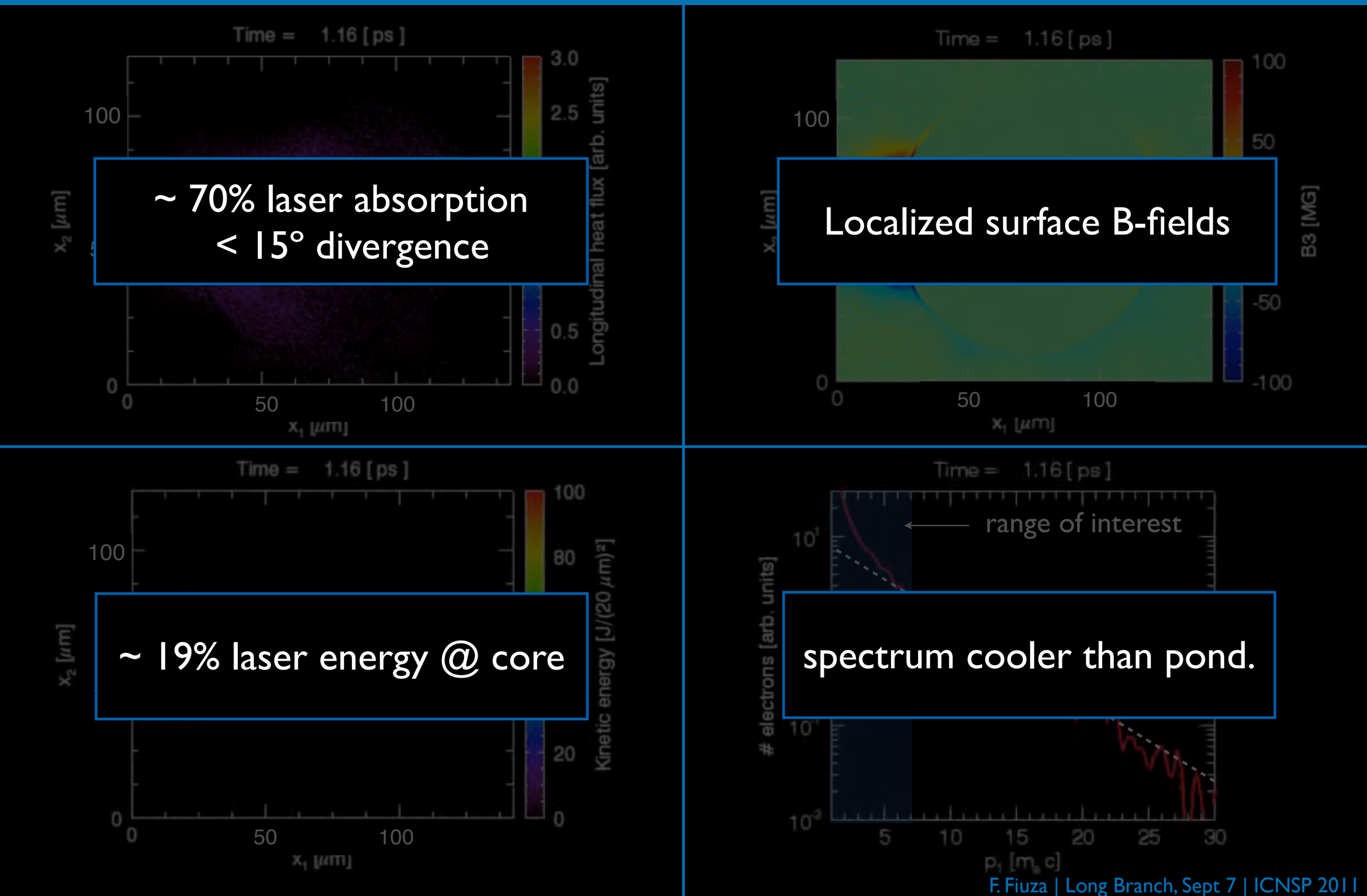

Summary from first full-scale simulations

	Laser intensity (Wcm^{-2})	Heat flux (%)	Divergence half-angle (°)	Core efficiency (%)
No cone	$2x10^{20}$	70	20-40	7
No cone	$2x10^{20}$	70	25-45	4
No cone	$5x10^{19}$	70	20-45	7
Cone	$5x10^{19}$	70	25-35	11
10 MG B-field	$5x10^{19}$	70	< 15	19
40 MG B-field	$5x10^{19}$	70	-	26

Full-size target

Scaled-down target

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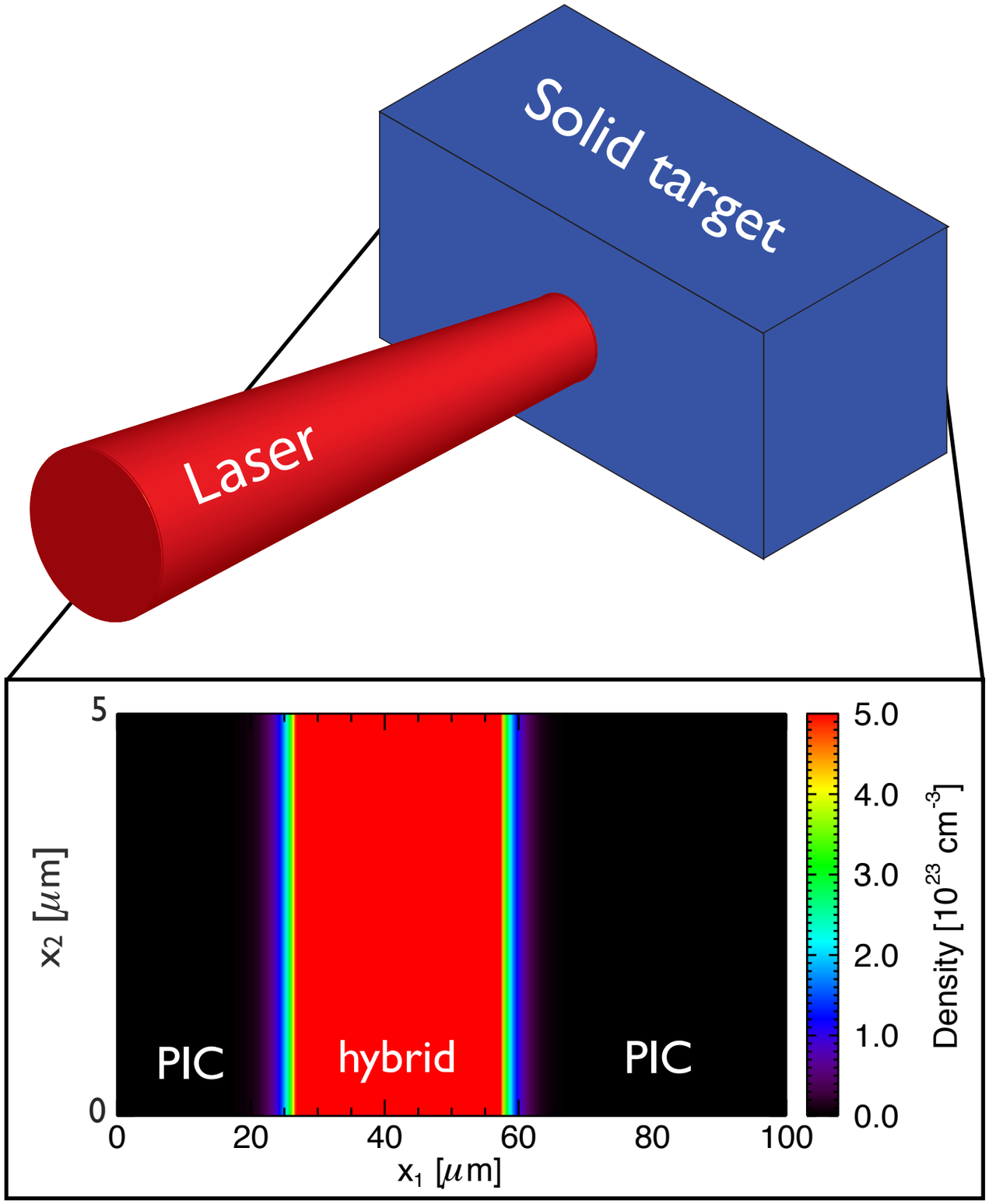
Ion acceleration from laser-solid interactions



Physical Parameters

Laser

- λ_0 = 1 μm
- I_0 = 5x10^{19}
- W_0 = 5 μm
- τ_0 = 350 fs (1D); 200 fs (2D)

Plasma

- L = 30 x 5 μm^2
- n_{e0} = 1000 n_c (1D) - 500 n_c (2D)
- m_i/m_e = 1836

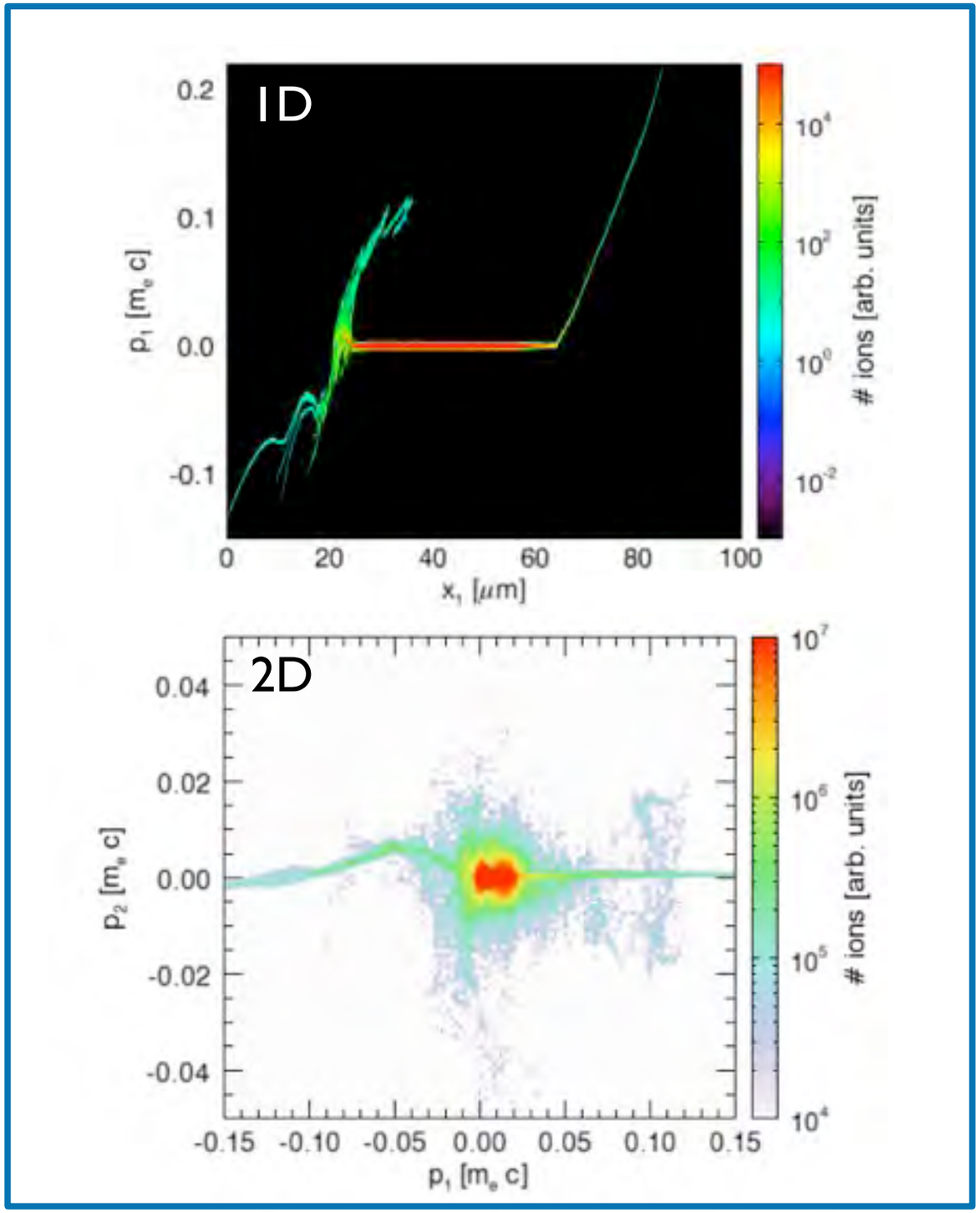
Numerical Parameters

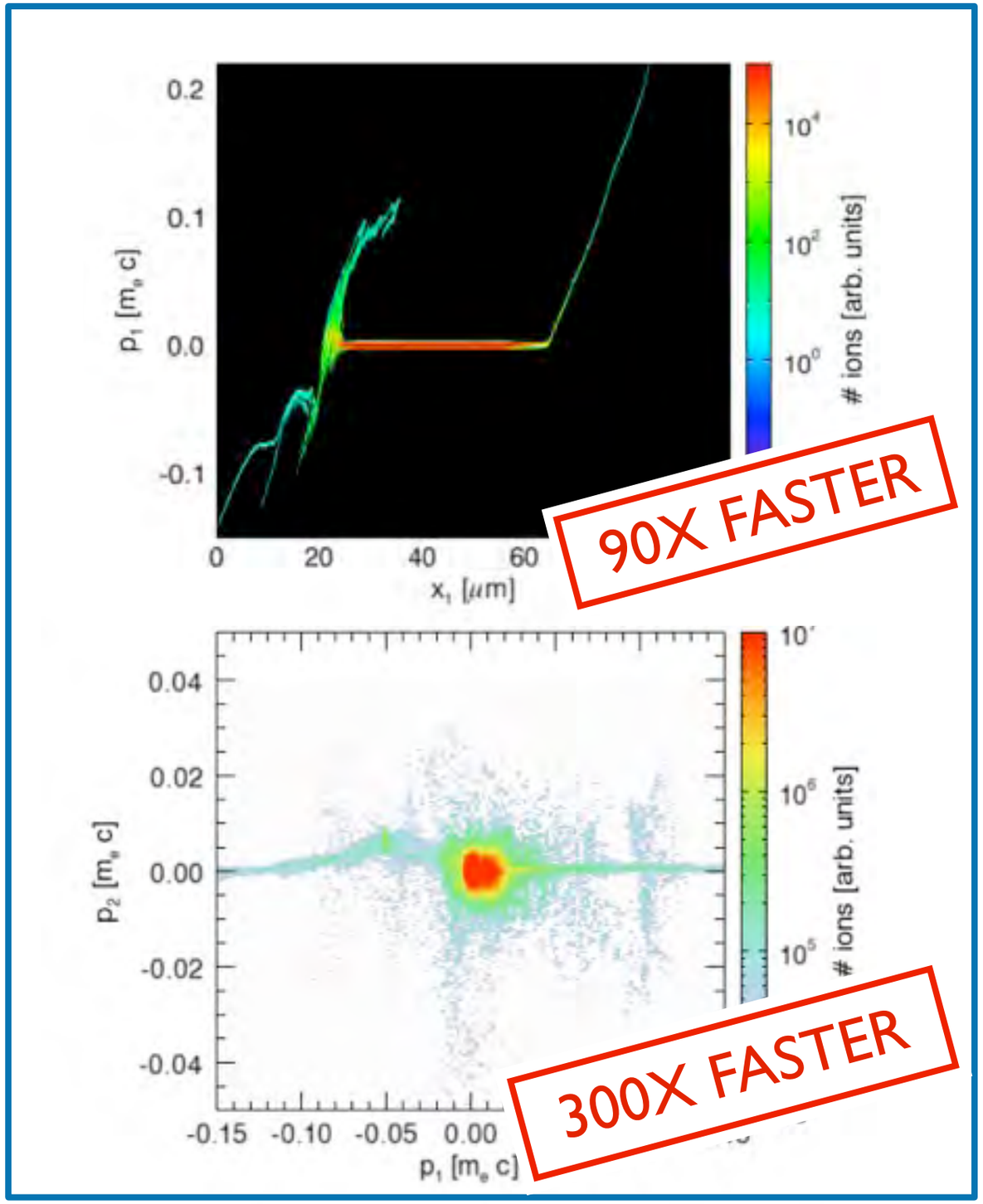
- 400 cells/μm (full-PIC)
- 42 cells/μm (hybrid-PIC)
- hybrid/full-PIC transition = 100 n_c
- Part. per cell = 200 (1D) - 9 (2D)
- cubic interpolation

Monte Carlo Coulomb collisions modeled in all simulations

Very large speed-ups can be achieved while maintaining the accuracy

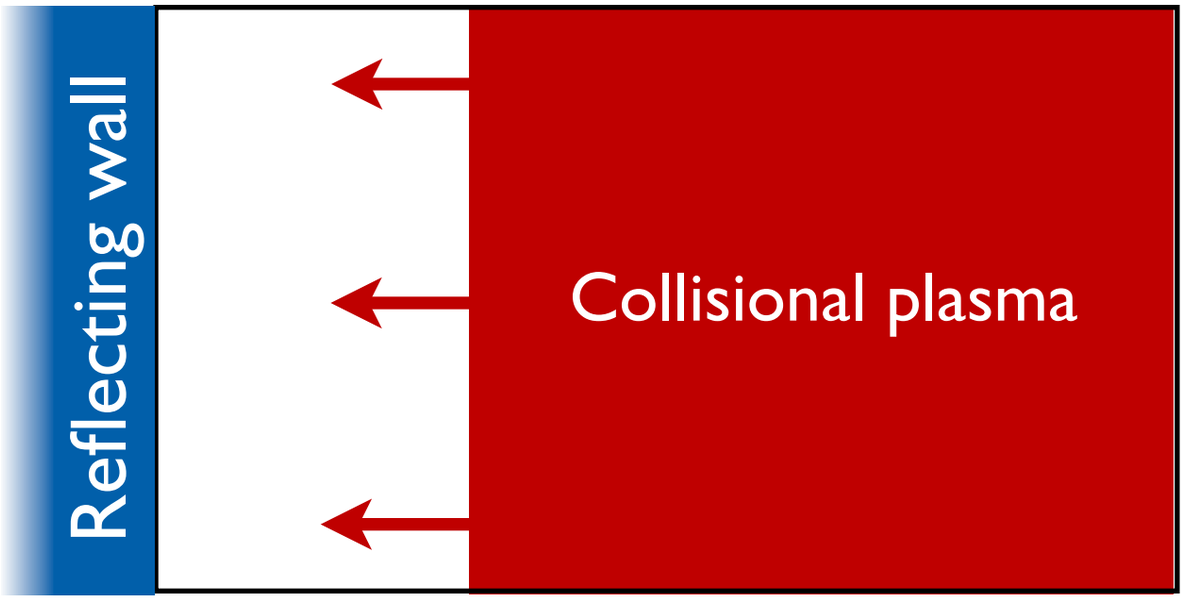
OSIRIS	h-OSIRIS



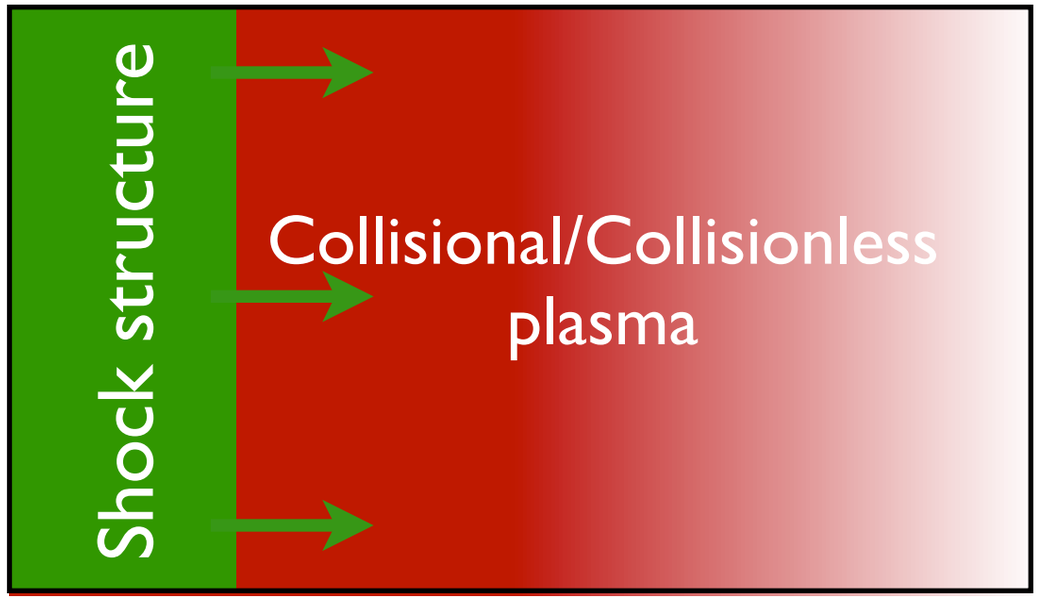


Modeling shocks in astrophysical scenarios

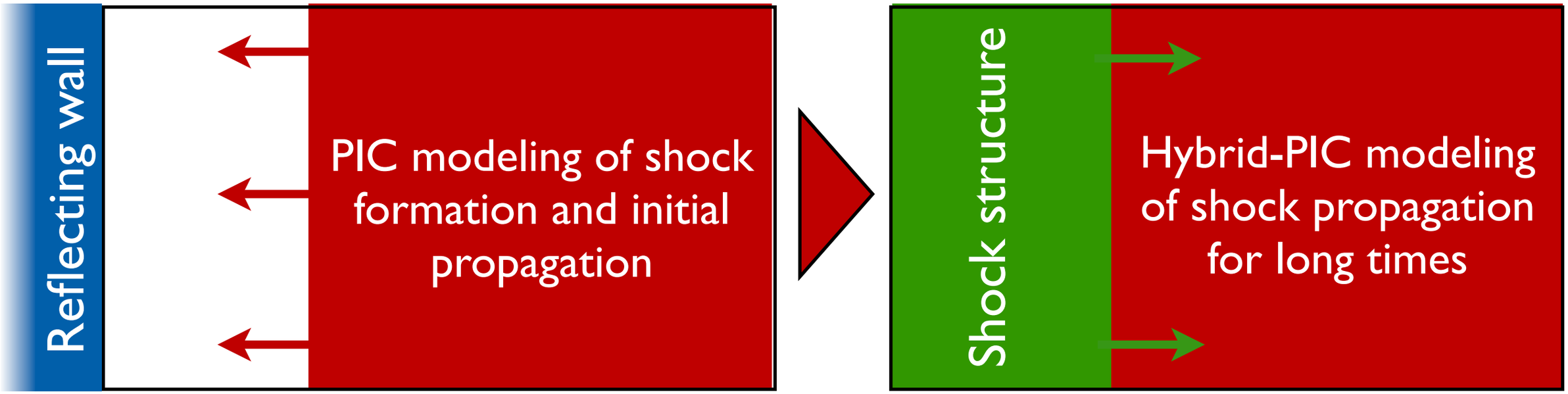
Collisional hybrid-PIC shock simulations



Shock collisionless/collisional transition



Ab initio multi-scale hybrid-PIC simulations of shock formation and propagation



Conclusions

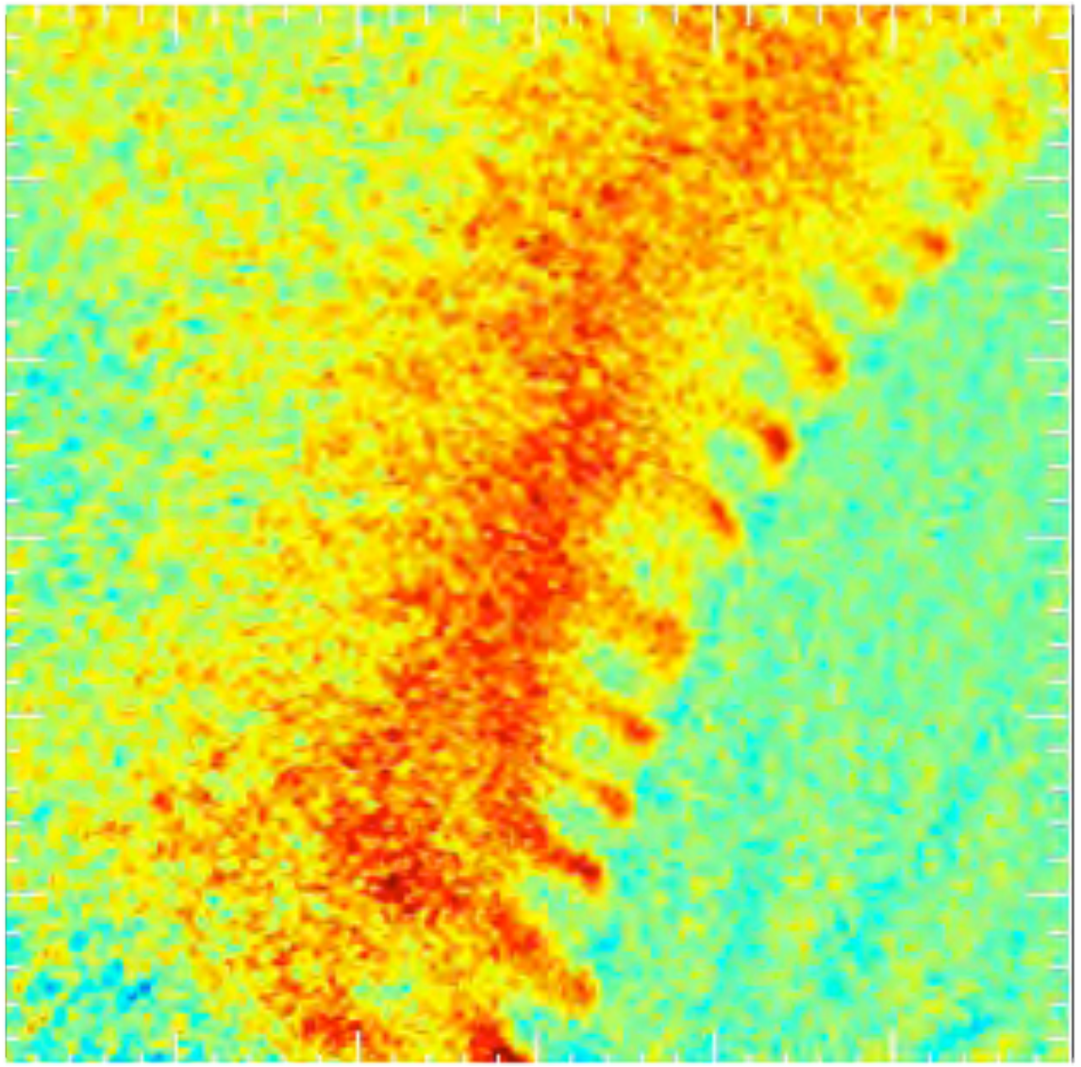
Fast ignition with intense lasers

- **7-20% coupling efficiency in realistic conditions**
- **Interaction is stable at ignition conditions**
- **10 MG axial B-field can provide collimation**
- **e^- cooler than pond. scaling indicate possibility to use ultrahigh laser intensities**
- **Longer simulation times reveal wide range of EM instabilities**

HEDP modeling

- **New algorithm allows for full-scale modeling of high energy density scenarios (matching experimental parameters)**
- **Numerical consistency is crucial in hybrid-PIC**
- **Realistic target geometries are important (physical size + isolated boundaries)**

Future perspectives

Next steps

- Model appropriate for shock ignition scenarios (work in progress)
- Full-scale 3D modeling of ion acceleration in laser-solid interactions
- Modeling of collisional/collisionless transitions (temporal/spatial) in astrophysical scenarios