Smilei)

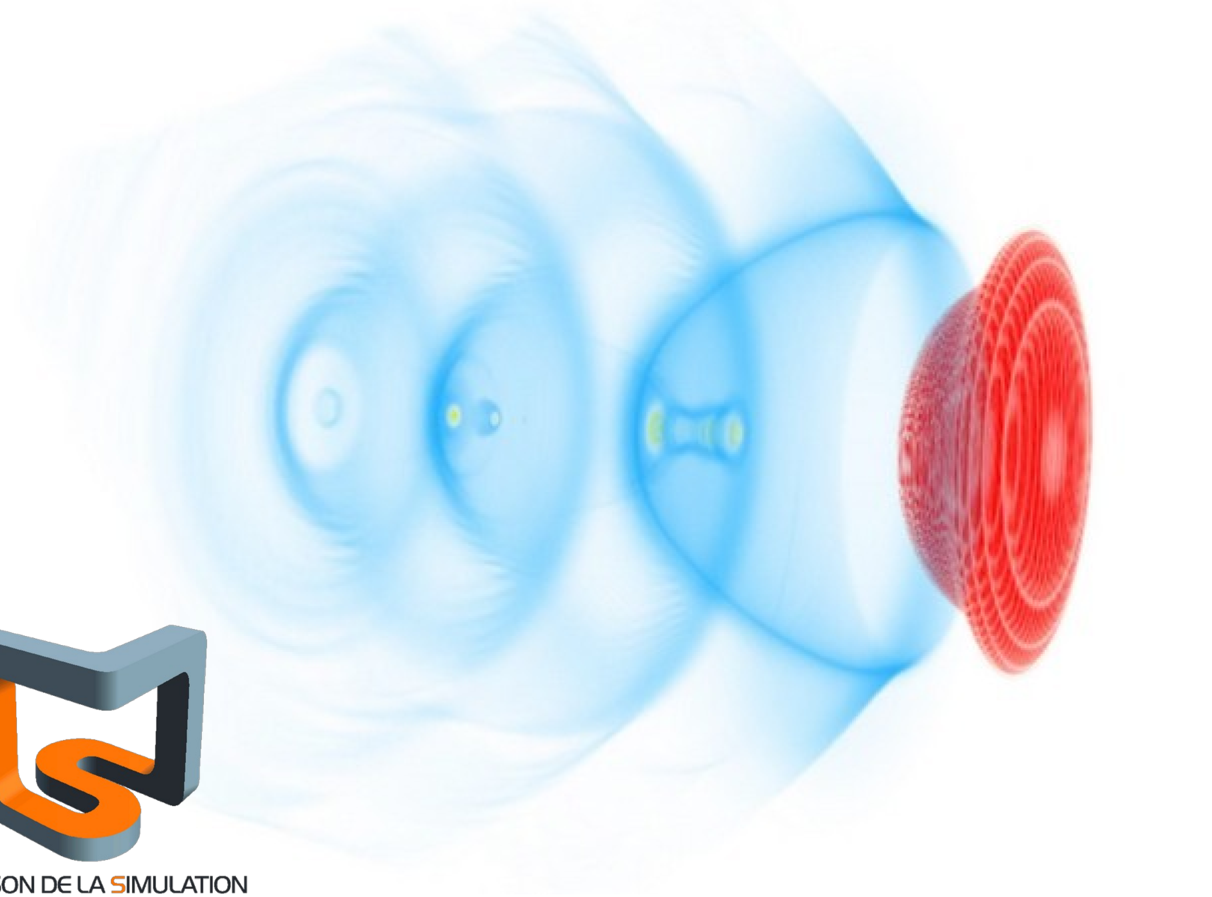
Building a plasma simulation ecosystem

A. Beck, LLR, Ecole polytechnique

G. Bouchard – A. Specka

M. Grech – F. Pérez – T. Vinci

M. Lobet – F. Massimo – J. Silvacuevas



European Strategy:

Townhall meeting #3

Milestones

"What are the important milestones for the next 10 years to get there from today ?"

=> Fast AND reliable codes:

1) Quasi - real time simulations for ~Hz repetition rate

2) Simulations capable of rendering experimental results

3) Both simultaneously

=> Brute force simulations of a large number of stages (exascale, next generation of supercomputers)

=> Maintainable and usable codes

Turn high tech complicated simulation code into a practical everyday tool: Code quality, shared knowledge, documentation, ease of use (interface for non expert)

All these milestones require mostly software engineering

Facilities and Funding

What is the role of the already planned future facilities in Europe and world-wide?

Computing centers provide HPC resources for the simulation campaigns.

Europe supports some applications towards exascale with 14 of “Centres of Excellence in HPC applications ” (Biomedicine, Combustion, Materials ...). Today, none of them is dedicated to high energy or plasma physics.

Is the R&D work for each of those deliverables already funded and, if not, what additional resources / support would be needed?

USA: Exascale Computing initiative => exascale supercomputer expected this year. $475 million for year 2021.
Exascale Computing Project => applications and software stack $250 million for year 2021. Plasma wakefield accelerator is listed as an objective.

Europe: Exascale systems annouced for 2023/2024 and is just now identifying scientific fields and pilot applications relevant to exascale. It is important that plasma acceleration is recognized as eligible for European exascale as it has been in the US.
EuroHPC: 8 Billion € for 2021-2030.

Open source ecosytem

Trainings
Benchmarks

Numerical Developers
Algorithms

Users
Features

Feedbacks

Comp. Allocation
Operation support

Smilei)
Input > Process > Output

Tech. collaboration

Computing Centers
Resources

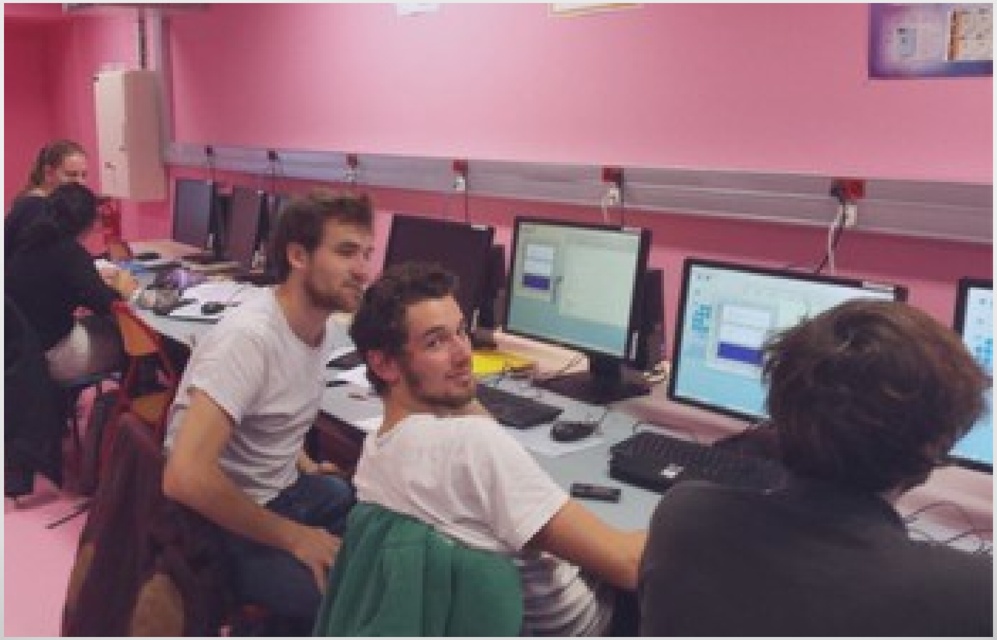
Optimization
Support

Computing Developers
Performance

Strong interconnections between the players of the ecosystem

Sharing knowledge

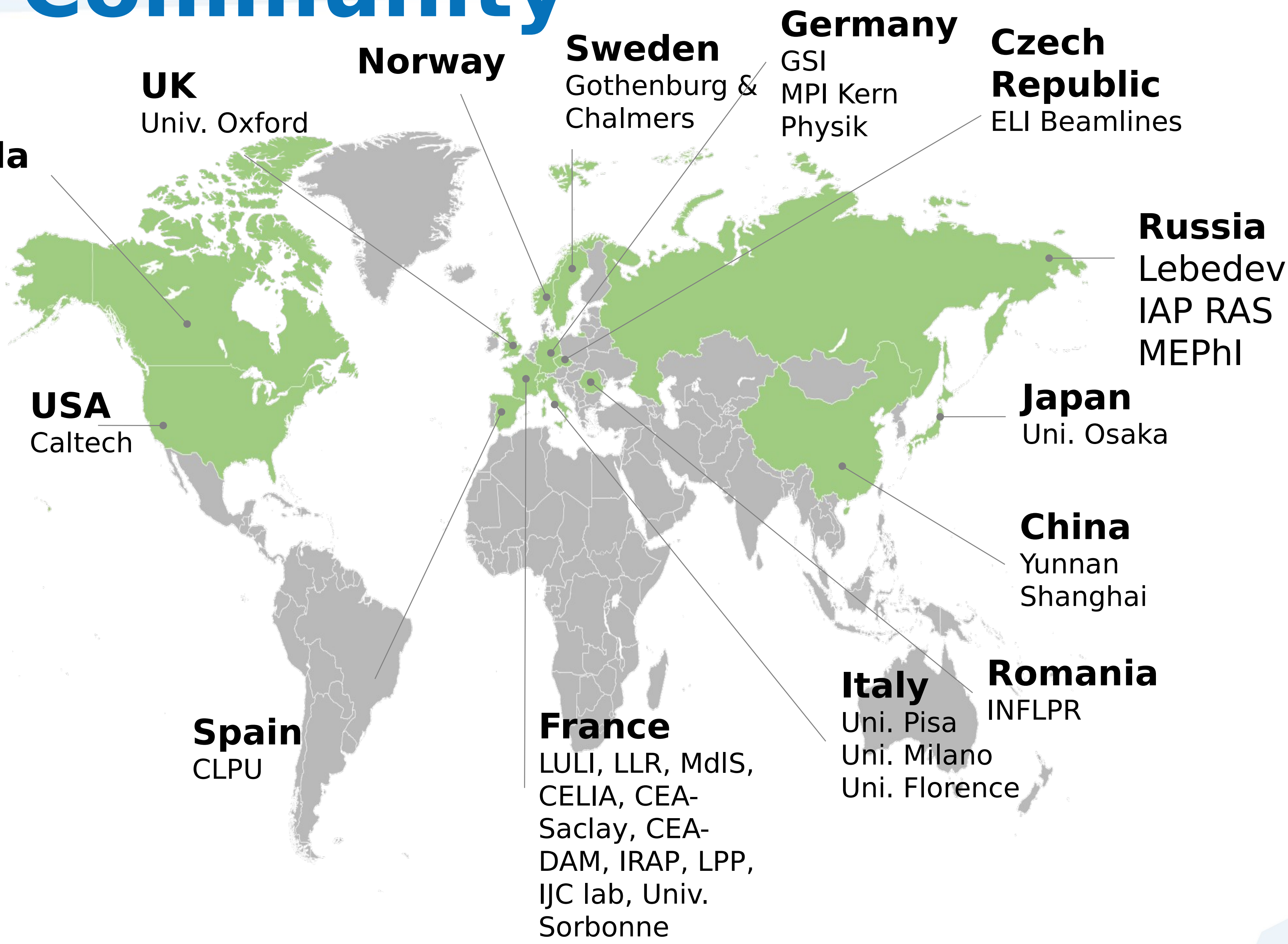
Practicals for
master students



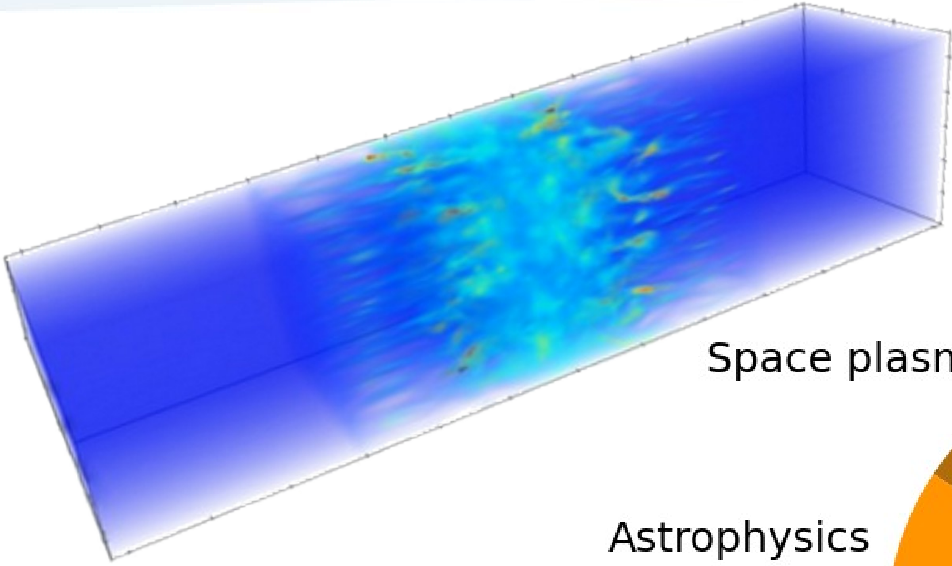
User training
& workshop

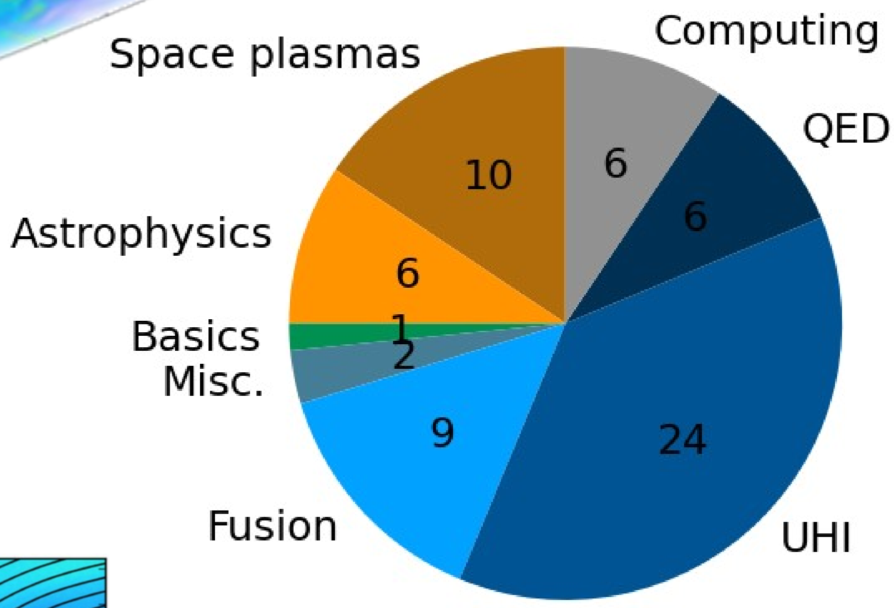
Tutorials available at
smileipic.github.io/tutorials

International Users Community

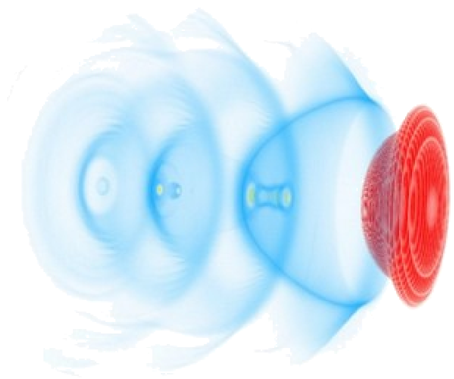


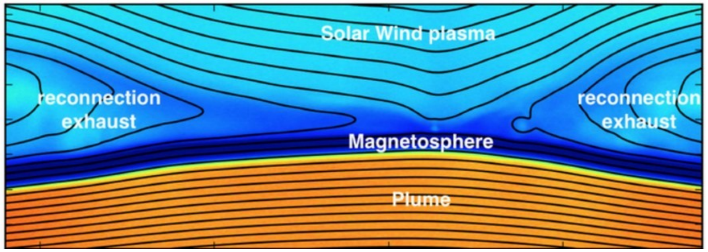
Joint effort between communities

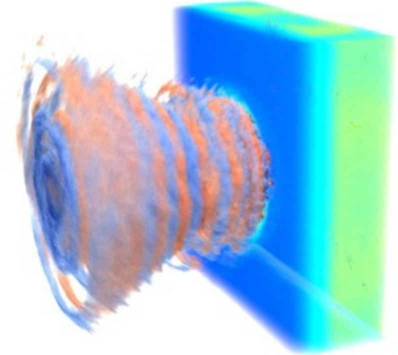




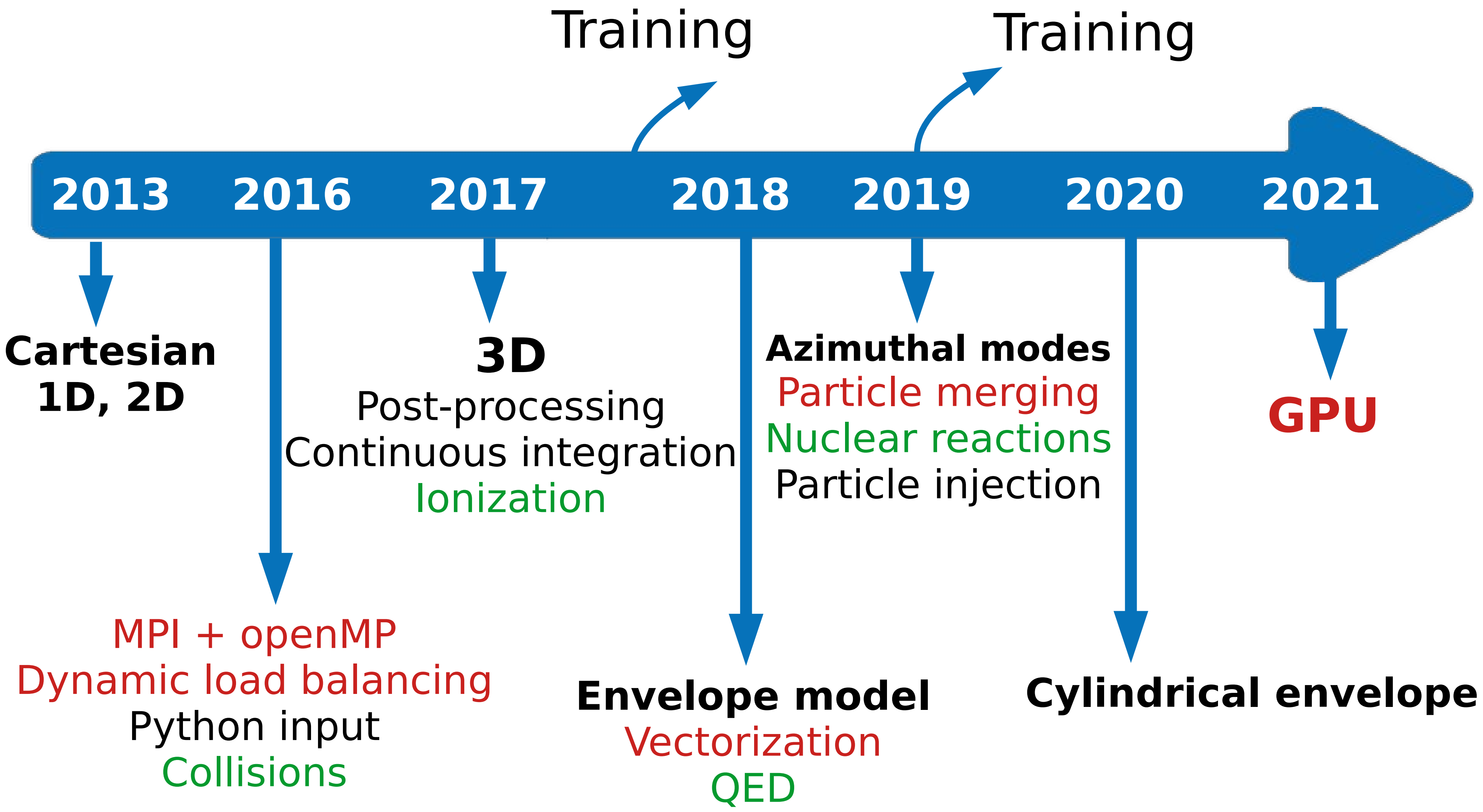
Publications distribution







Smilei) Timeline



Derouillat et al., *CPC* 222 (2018)

Features relevant for plasma acceleration

Physics	Numerics	HPC
• Ionization • QED	• Dispersion free solver • Envelope • Moving window • Azimuthal Decomposition • PML boundaries • Dynamic Load Balancing • Arbitrary laser/plasma profiles • Particles injection	• MPI • OpenMP • Taskification • GPU support • Vectorization

Towards fast and reliable simulations

1) Numerical methods and High Performance Computing are key.
2) Combining all features is the challenge.

Combining features is a lot of work

Ionization in alternating E field
Ammosov M. (1986)

Envelope Model
Mora P. (1997)

Azimuthal modes
Lifschitz et. al. (2008)

Ionization in Envelope

Azimuthal Envelope
Massimo et. al. (2019)

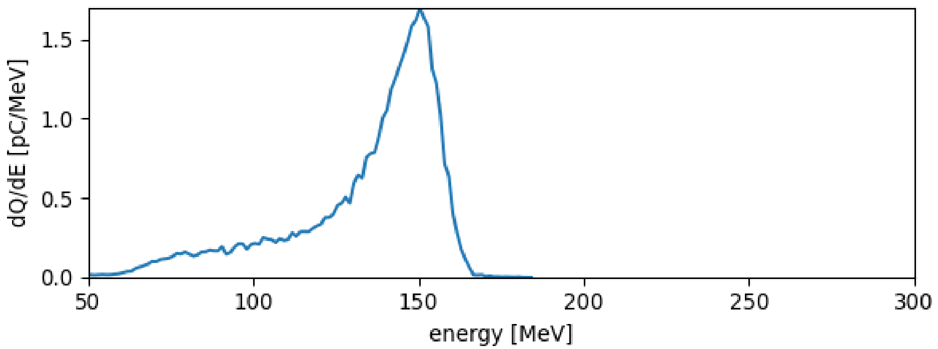
Ionization in Azimuthal Envelope
Massimo et. al. (2020)
https://doi.org/10.1103/PhysRevE.102.033204

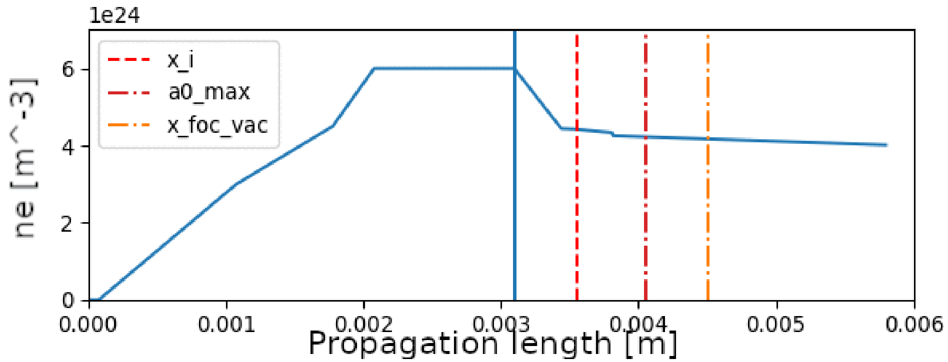
N^2 complexity
And N is getting very large !

Where do we stand today ?
A practical usecase

Simulations by unexperienced users at IJC Lab:
Ionization & downramp injection, ~5.2 mm propagation.
A simulation runs in ~12 minutes over 5 compute nodes.
1200 simulations are run in less than 6H on a national supercomputer.

- Use aggressive reduction
- Getting close to real time
- Manageable error (< 5%)
- Allows parameter scan for plasma cell design
- Will get better with the addition of improved boundary conditions, full GPU support, etc...



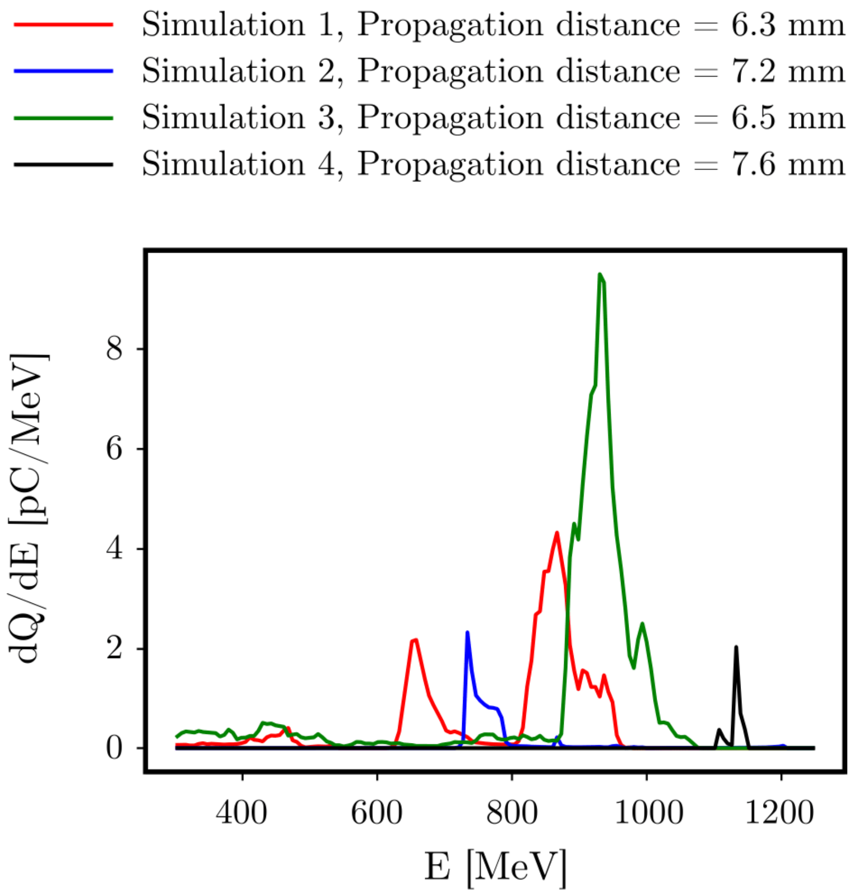


P. Drobniak, V. Kubytskyi, K. Cassou

Apollon Laser usecase

Simulation support to Apollon campaigns

- Target design
- Scan parameters of interest
- Guide ongoing campaigns (close to real time simulation)
- Interpretations of results



Massimo et. al. (2019)
Plasma Phys. Control. Fusion 61 124001

Milestones

"What are the important milestones for the next 10 years to get there from today ?"

=> Fast AND reliable codes:

1) Quasi - real time simulations for ~Hz repetition rate

2) Simulations capable of rendering experimental results

3) Both simultaneously

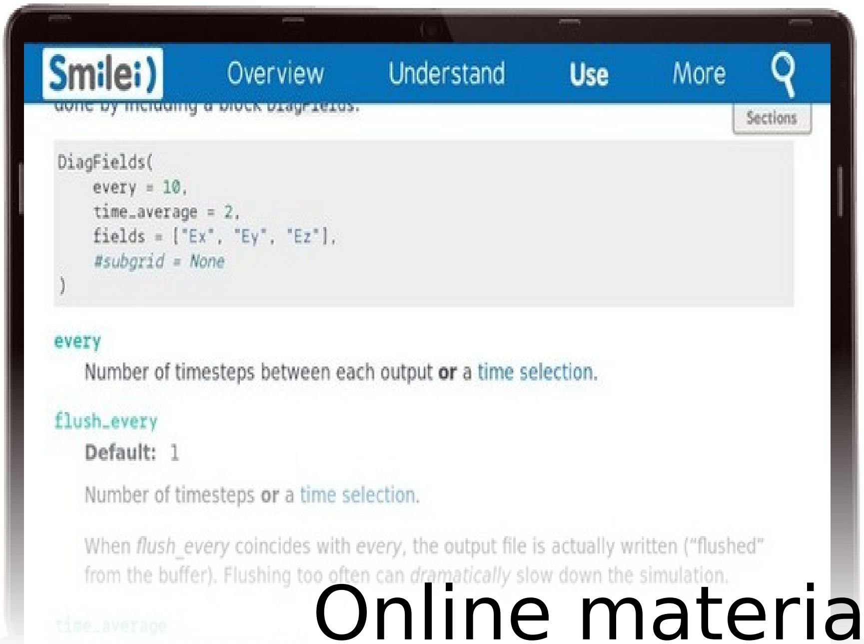
=> Brute force simulations of a large number of stages (exascale, next generation of supercomputers)

=> Maintainable and usable codes

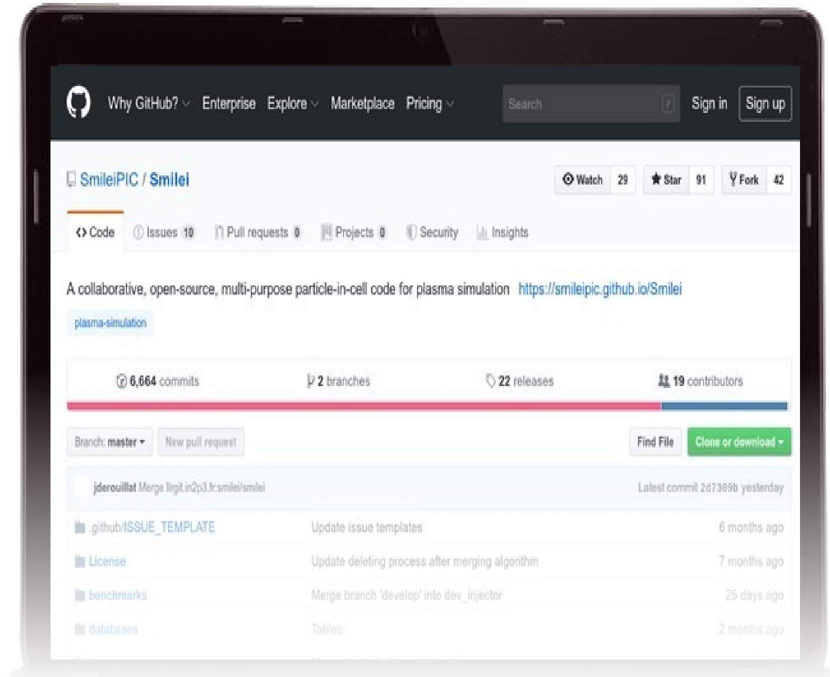
Turn high tech complicated simulation code into a practical everyday tool: Code quality, shared knowledge, documentation, ease of use (interface for non expert)

All these milestones require mostly software engineering

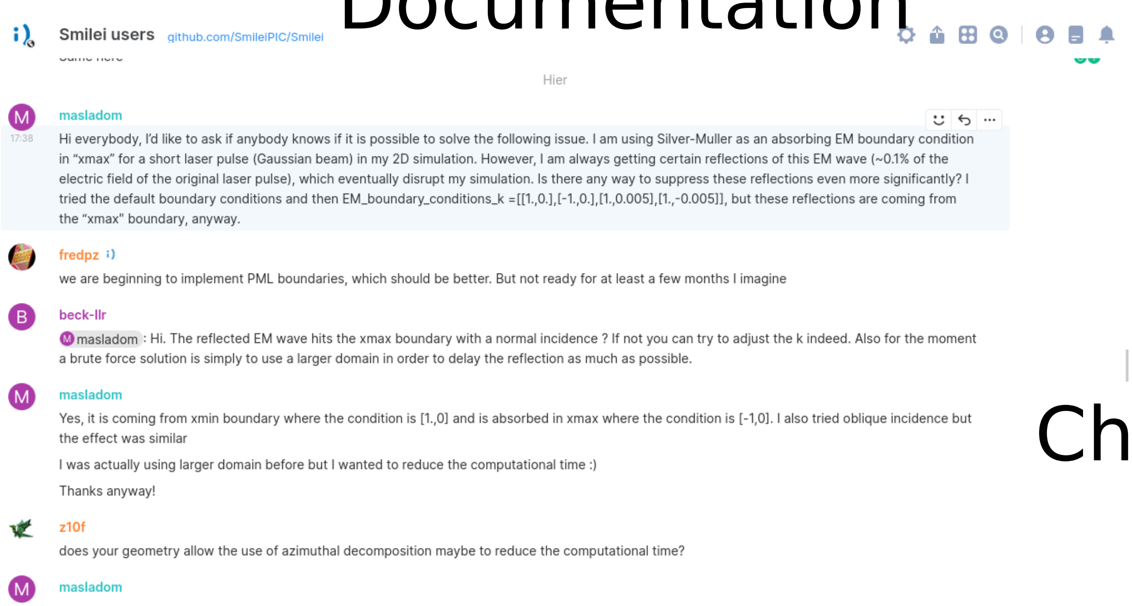
Building the community



Online material
Documentation

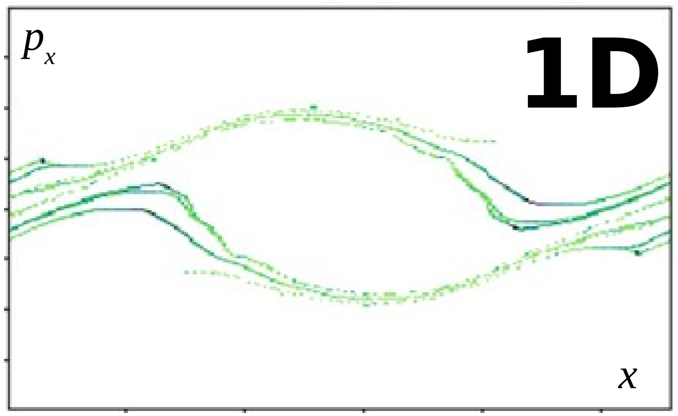


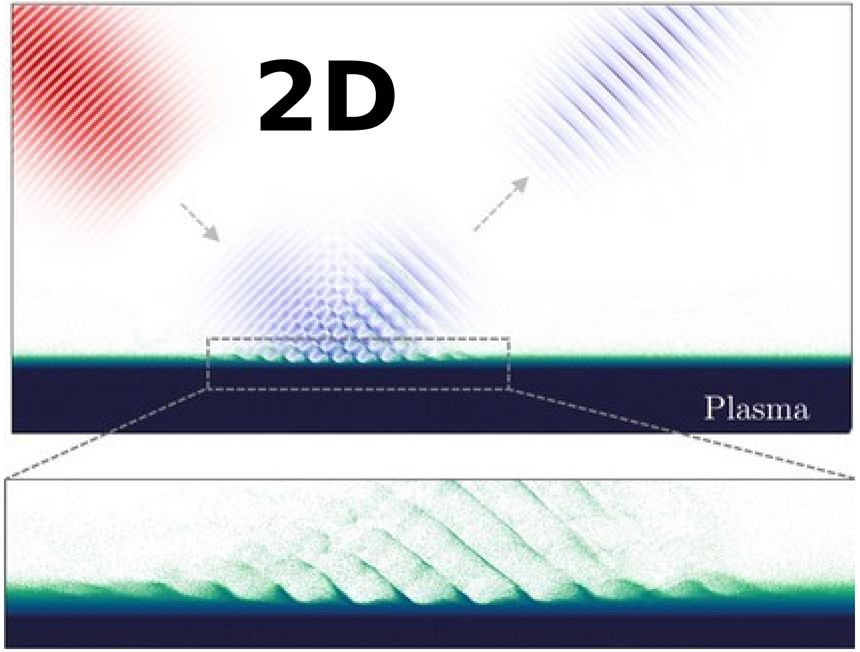
Free access
Issue reporting
Online support



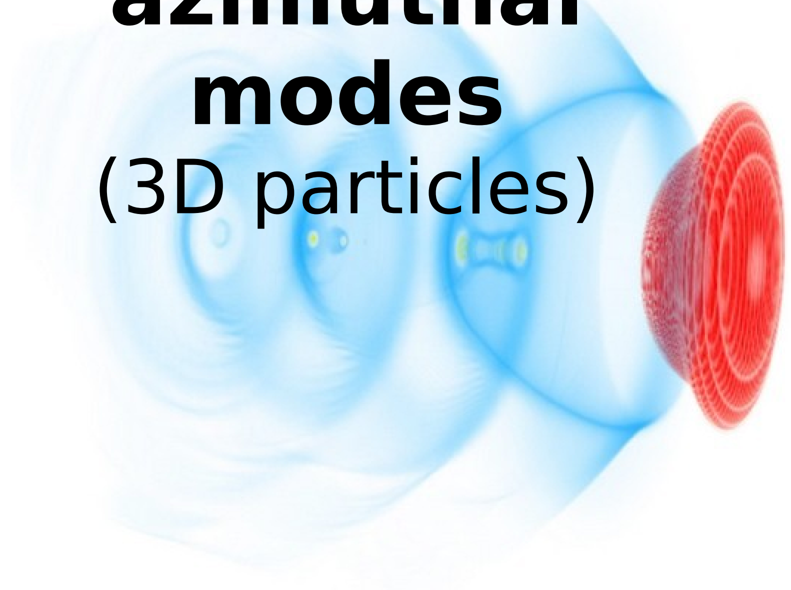
Chat with developers
and other users

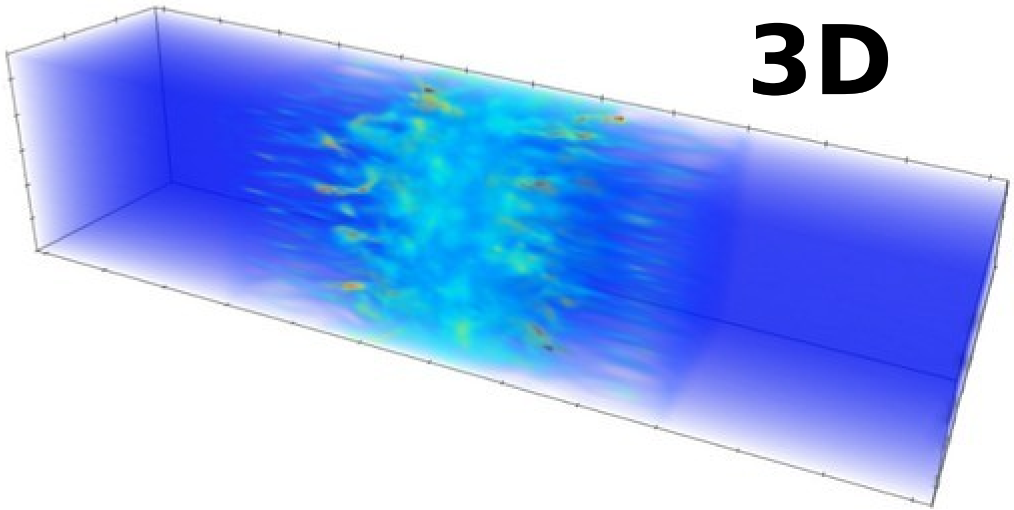
Multiple geometries





Cylindrical azimuthal modes
(3D particles)

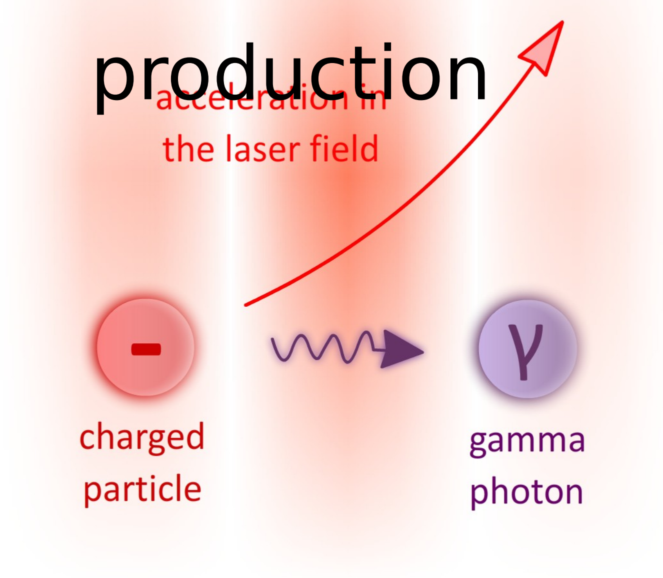




Additional physics

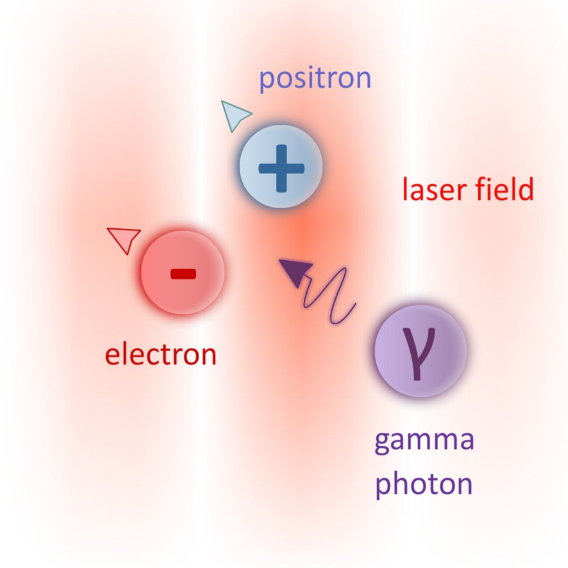
Radiation reaction

+ photon production



Non-linear Breit-Wheeler

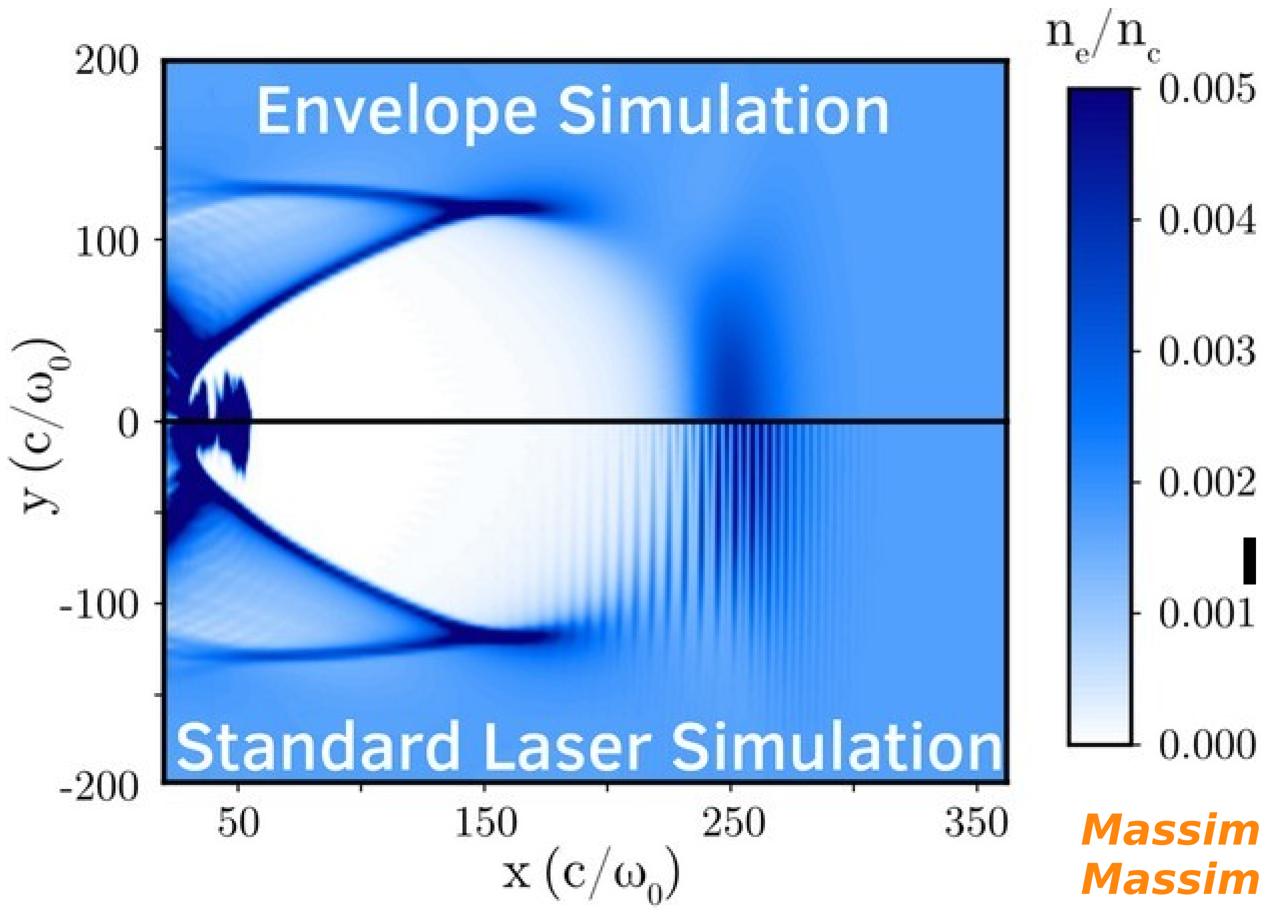
pair cascades



Lobet et al., JPCS (2016)
Niel et al., PRE** 97 **(2018); PPCF** 60 **(2018)

Advanced numerical methods

- Full-PIC = resolve the laser wavelength
- Approximation : reduced equations on laser envelope



Envelope simulation:

20 x faster in 3D

100 x faster in AM

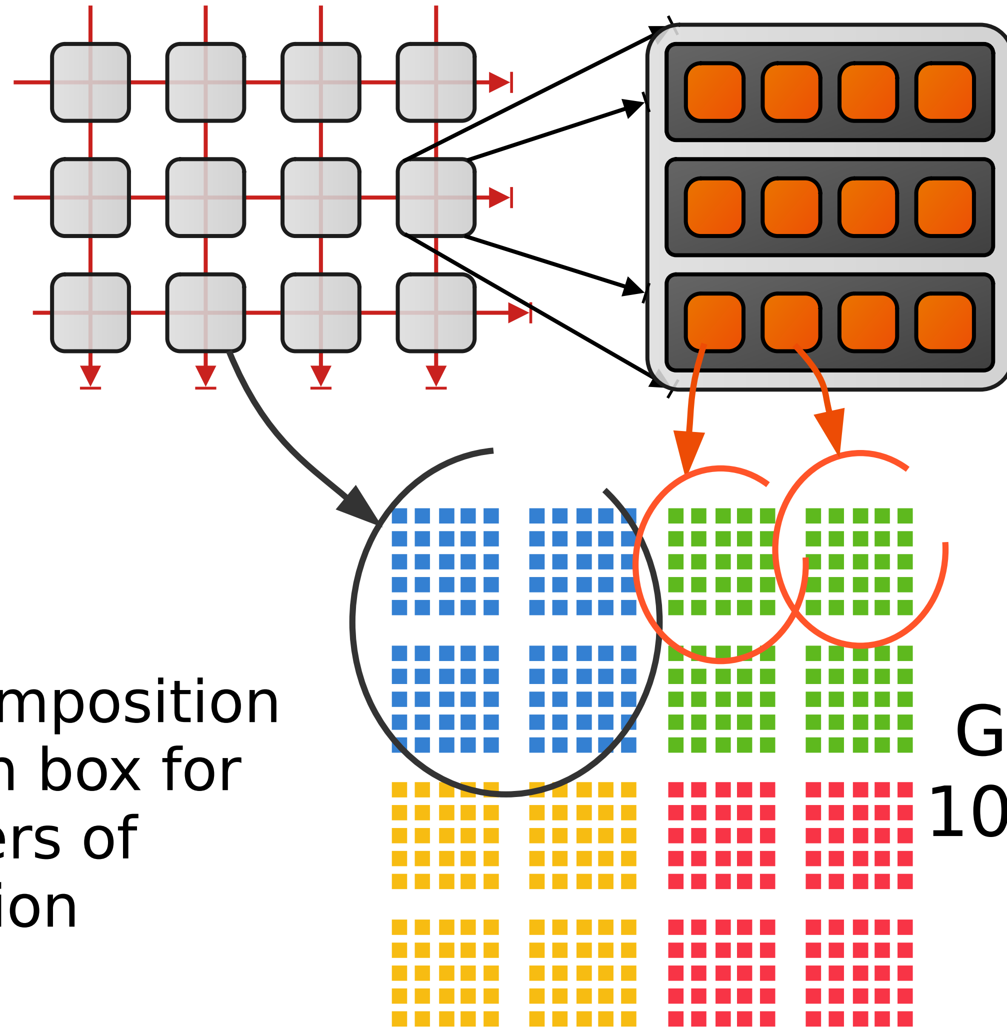
Ionization compatible

Massimo et al., PPCF (2019)
Massimo et al., IOP Proceedings (2019)
Massimo et al., PRE (2020)

Parallel computing

Many nodes
+ network

MPI protocol



Many cores
per node

OpenMP directives

Hierarchical decomposition of the simulation box for multiple layers of parallelization

Good scaling to 100 000s of cores

Smilei

Is part of the French national benchmark for supercomputing

Happi post-process

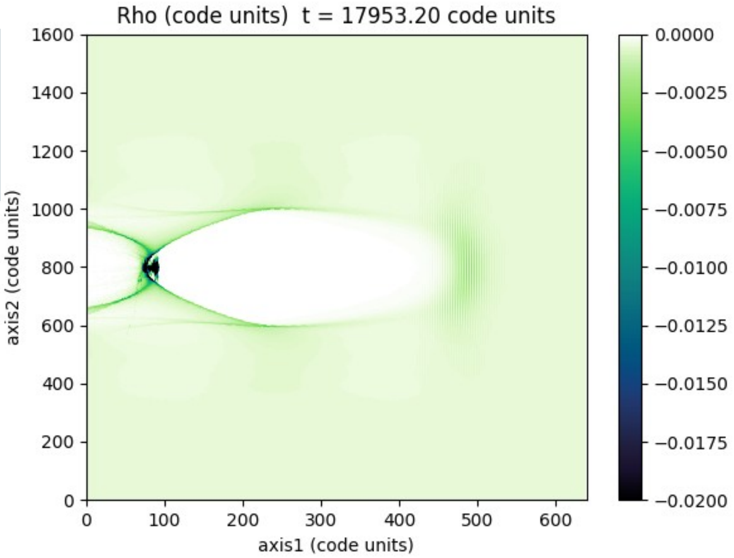
- The repository includes a *python* module

```
$ ipython
In [1]: import happi; S = happi.Open(“simulation_directory”)
```

- Plot results

```
In [2]: rho = S.Probe(0,”Rho”)

In [3]: rho.plot(timestep=180000, vmin=-0.02)
```



- Data manipulation

```
In [4]: data_array = rho.getData()
In [5]: rho.toVTK()
```

Integrate into the global ecosystem

Smilei

Complies

Contributes

openPMD

P-I-C-S-A-R

Standard for Particle-Mesh Data

PIC code library

Smilei)

Open-source
PIC code

Collaborative, user-friendly

GitHub • Python interface

Educational resources

Online documentation • Tutorials

High-performance

MPI-OpenMP • Load balancing • vectorization

Physics

Ionisation • Collisions • Strong-field QED

Advanced solvers

Spectral solvers • Multi-geometries • Laser envelope

M. Grech
F. Perez
T. Vinci

M. Lobet
F. Massimo
J. Silvacuevas

MAISON DE LA SIMULATION

A. Beck
G. Bouchard

… and many more

Derouillat et al., CPC** 222 **(2018)

Smilei)

Open-source
PIC code

M. Grech
F. Perez
T. Vinci

M. Lobet
F. Massimo
J. Silvacuevas

MAISON DE LA SIMULATION

A. Beck
G. Bouchard

maisondelasimulation.fr/smilei

github.com/SmileiPIC/Smilei

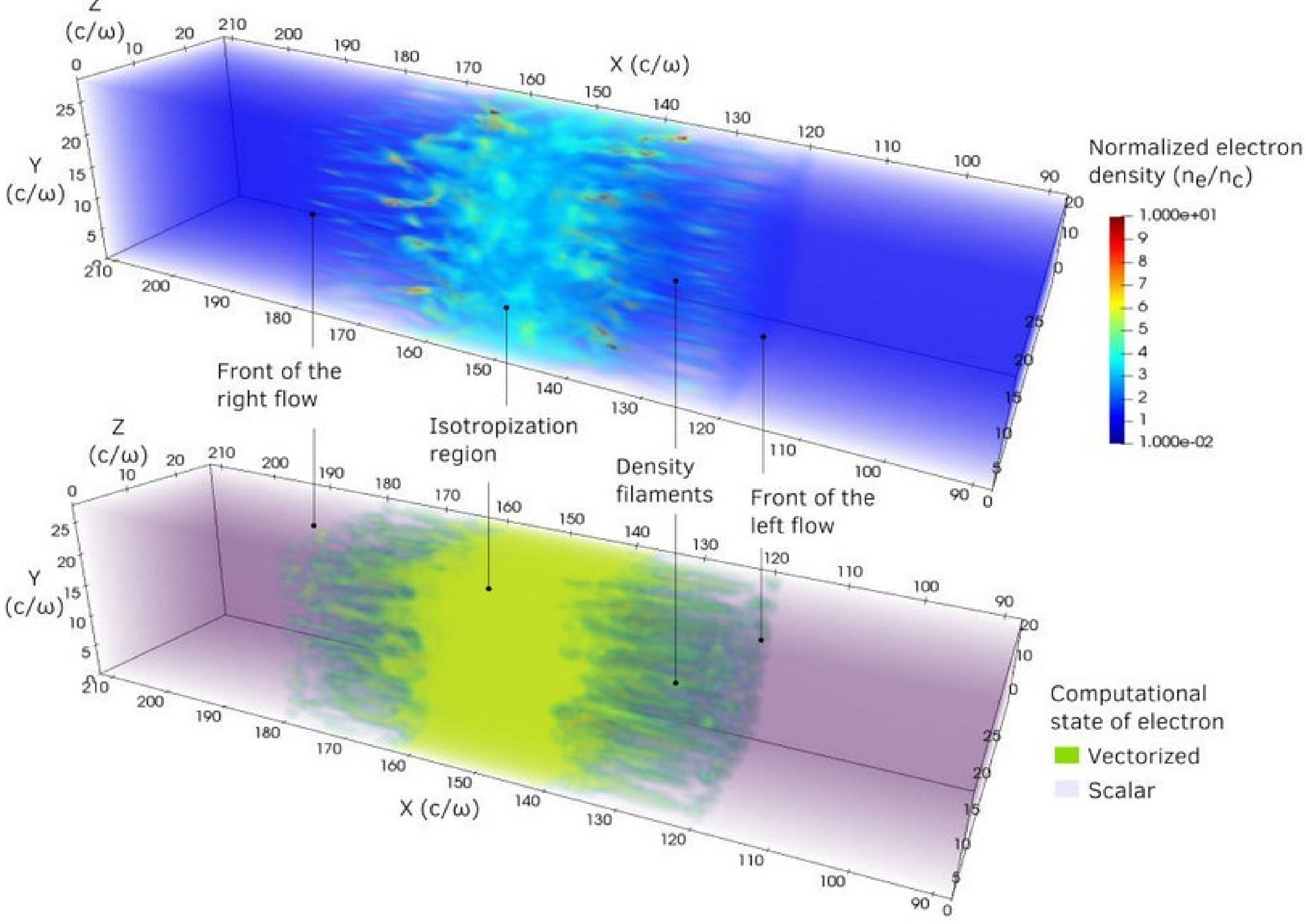
... and many more

app.element.io/#/room/#Smilei-users:matrix.org

Derouillat* et al., *CPC* 222 *(2018)

High Performance

Vectorization activated only where there are many particles per cell



Beck et al., CPC 244 (2019)

Many options for solvers

- Charge-conserving current deposition

  Esirkepov, CPC *135* ***(2001)***

- Orders of interpolation:

  2 or 4

  (3 or 5 points)

- Several FDTD schemes:

  “Yee”, “Cowan”, “Lehe”

  Nuter et al., EPJD *68* ***(2017)***

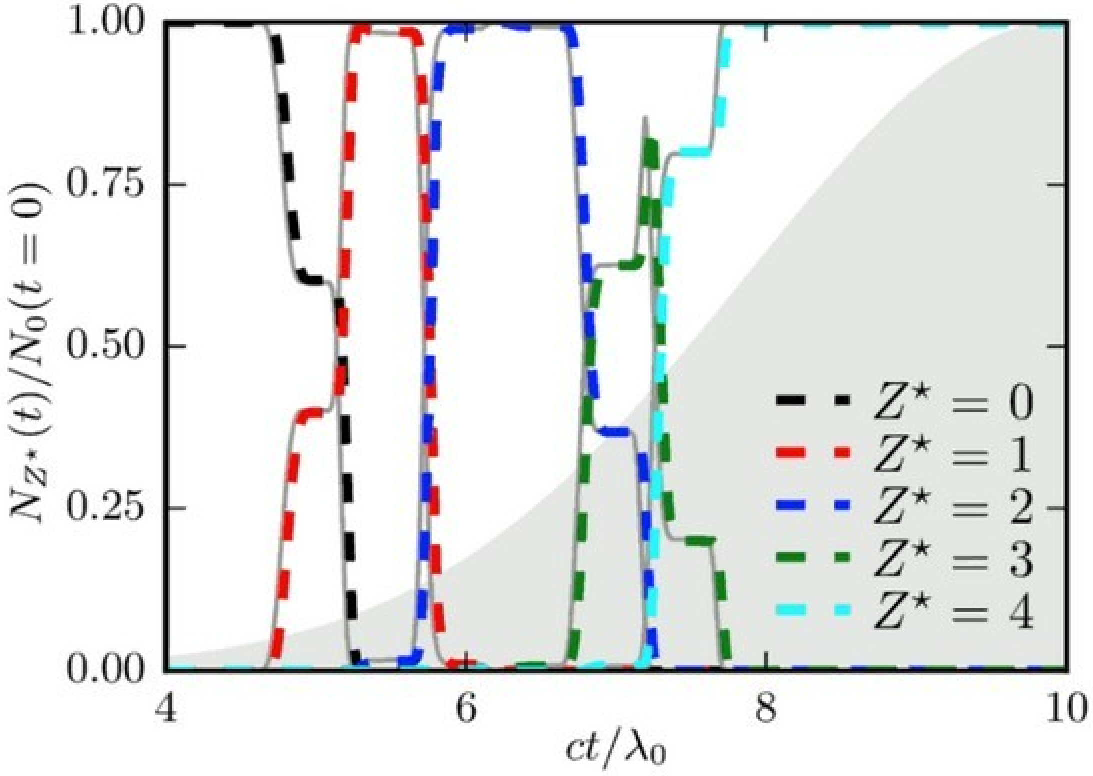
- Spectral solver available *via* ***PICSAR*** *(beta)*

  picsar.net

Ionization by fields

- Monte-Carlo
- Multiple events in 1 timestep
- May define a custom ionization rate

Carbon ionization state *vs* time

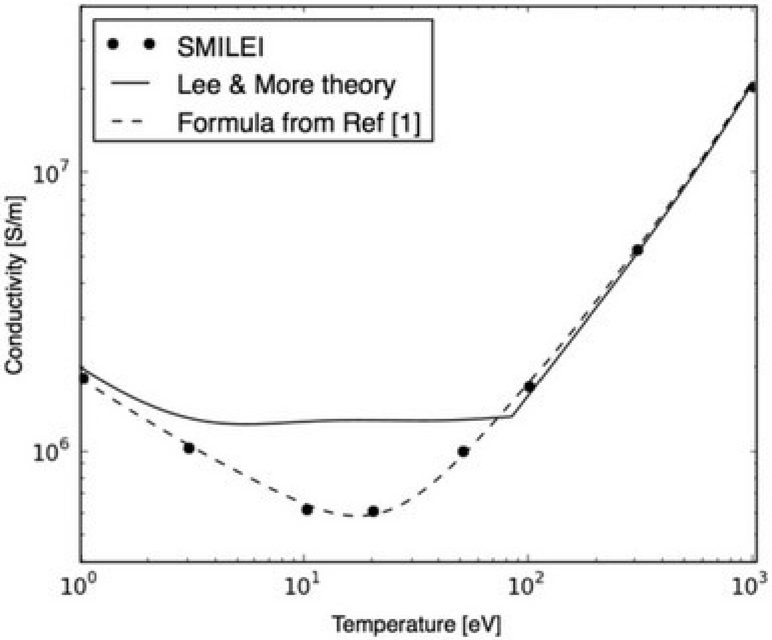


Nuter** et al., **POP 18 (2011)

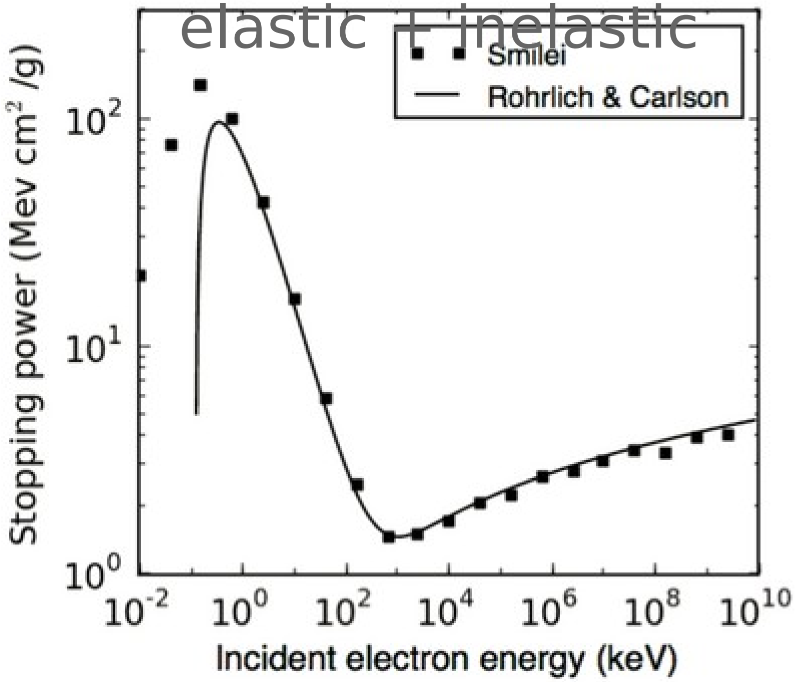
Processes between pairs of particles

- Collisions
- Collisionnal ionization
- Nuclear reactions (D-D fusion in progress)

Conductivity of Cu
in wide temperature range



Electron stopping power in Al
elastic + inelastic



Balance the workload between processors

Uniform plasma (balanced)

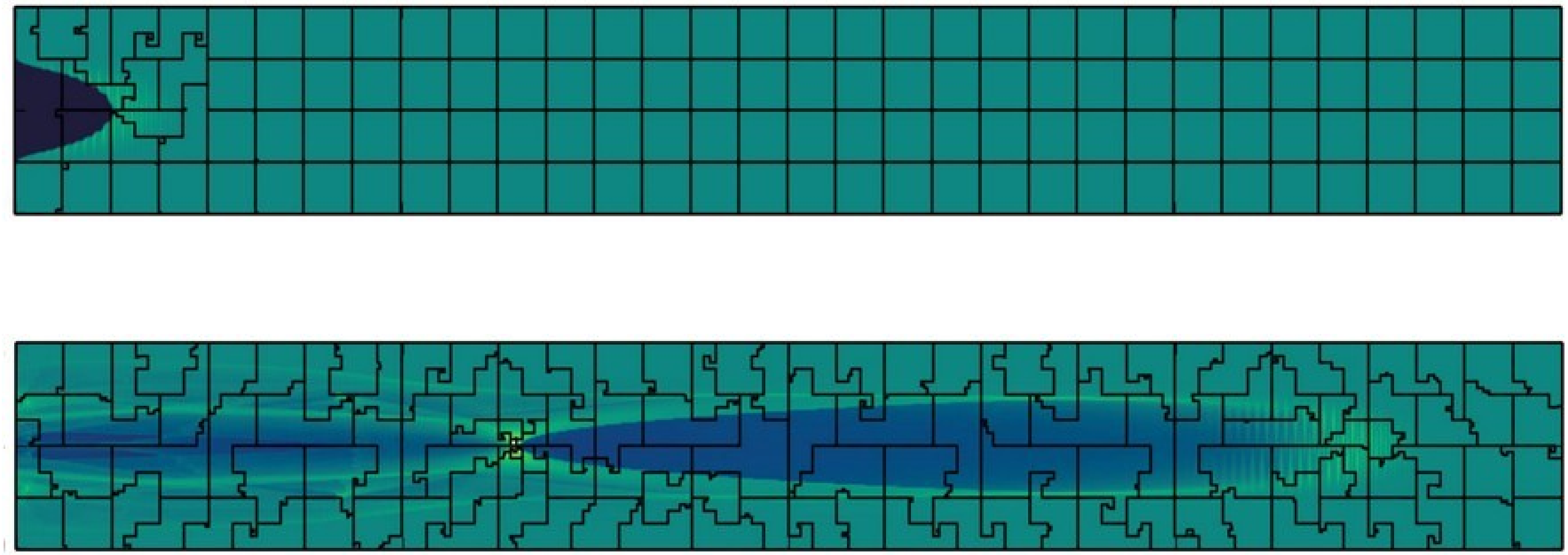
Local plasma

(imbalanced)

The decomposition evolves according to the computing imbalance

Balance the workload between processors

Domains automatically adapt
to the simulation evolution

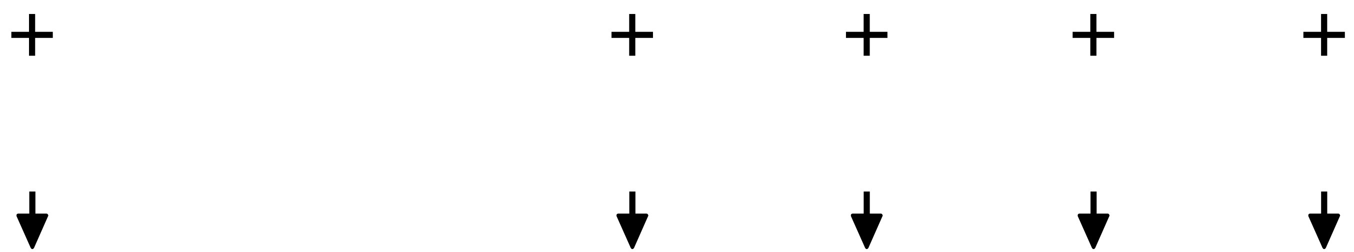


Laser wakefield simulation ~ 2x faster

Vectorization: do multiple operations at once

Scalar

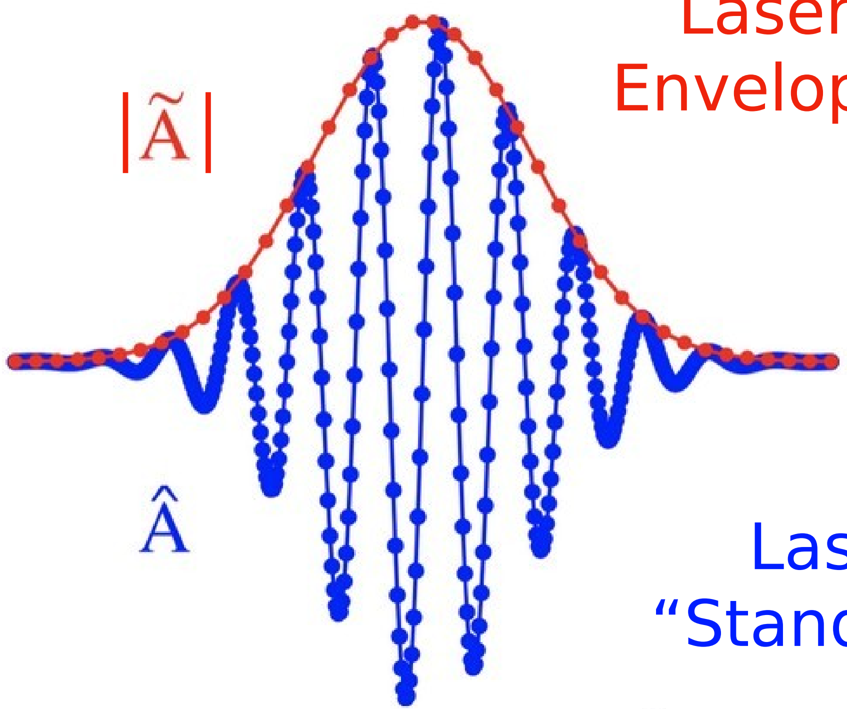
Vectorized



Theoretically, almost 4x faster

Requires extensive work on data structure & operators

Envelope: wave equation



Terzani and Londrillo,
CPC (2019)

Laser Complex Envelope

$$\hat{A}(\mathbf{x},t) = Re\left[\tilde{A}(\mathbf{x},t)e^{ik_0(x-ct)}\right]$$

+

D'Alembert Equation:

$$\nabla^2\hat{A} - \partial_t^2\hat{A} = -\hat{J}$$

Envelope Equation:

$$\nabla^2\tilde{A} + 2i\left(\partial_x\tilde{A} + \partial_t\tilde{A}\right) - \partial_t^2\tilde{A} = \chi\tilde{A}$$

Plasma
Susceptibility

Envelope: particle motion

Ponderomotive force:
Acts as a radiation pressure on charged particles.
Expels the electrons from high-intensity zones.

Equations of motion for the macro-particles:

$$\frac{d\bar{\mathbf{x}}_p}{dt} = \frac{\bar{\mathbf{u}}_p}{\bar{\gamma}_p} \qquad r_s = q_s/m_s$$

$$\frac{d\bar{\mathbf{u}}_p}{dt} = r_s \left(\bar{\mathbf{E}}_p + \frac{\bar{\mathbf{u}}_p}{\bar{\gamma}_p} \times \bar{\mathbf{B}}_p \right) - r_s^2 \frac{1}{4\bar{\gamma}_p} \nabla \left(|\tilde{A}_p|^2 \right)$$

Lorentz Force (plasma fields)

Ponderomotive force (laser envelope)

B. Quesnel and P. Mora, Physics Review E 58, 3719 (1998)