Laboratoire Interactions, Dynamiques et Lasers
EMR9000 CEA, CNRS, Université Paris-Saclay

Modeling a novel laser-driven electron accelerator concept: Particle-In-Cell simulations at the exascale

Neïl ZAIM

March 6th, 2023

PHYSICS AT HIGH INTENSITY


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Experiments


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P. Bartoli

Theory/simulations


H. Vincenti
(head of numerical division)


P. Martin

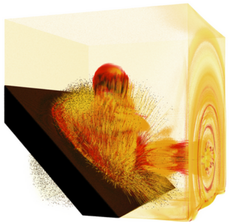

L. Fedeli

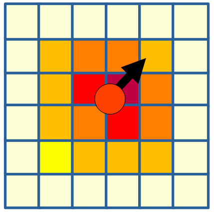

T. Clark


N. Zaim


A. Sainte-Marie

Outline

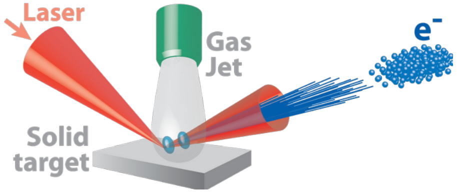




Laser-plasma interaction & the Particle-In-Cell method

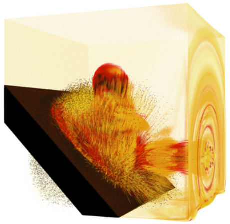
WarpX: a Particle-In-Cell code for the exascale era

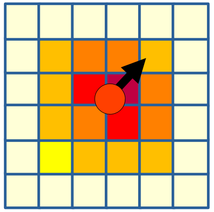
WarpX performances



Simulation of a new electron accelerator concept

Outline





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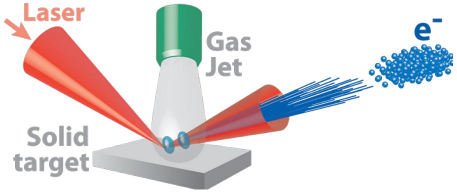
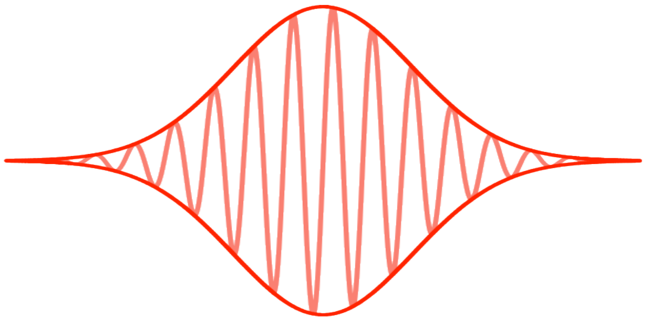


Simulation of a new electron accelerator concept

High-power Ti:Sapphire femtosecond lasers are the most intense light-sources available on Earth

Ultra-short **20-30 fs** “bullets” of light focused to extreme intensities



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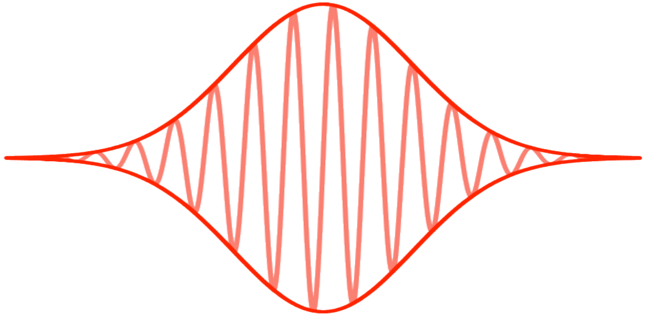

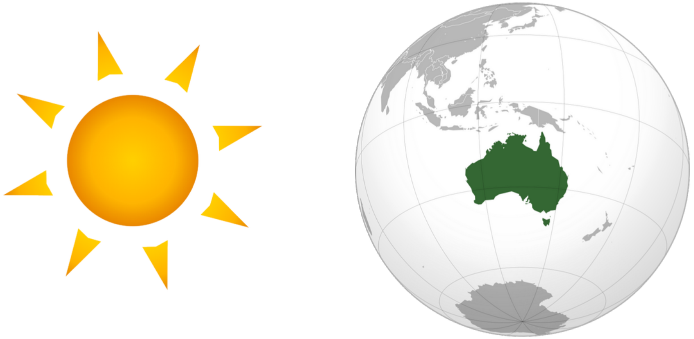

From **few TeraWatt** up to **several PetaWatt**
(few PW is power of the sunlight striking Australia!!)

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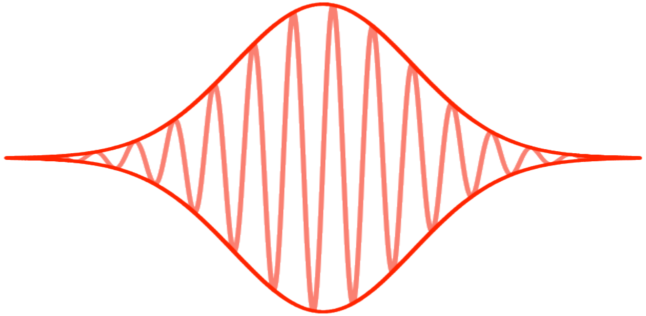
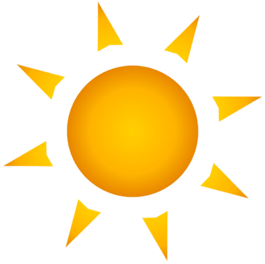
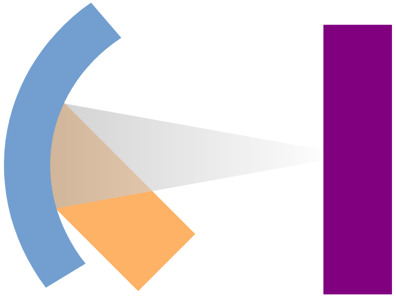




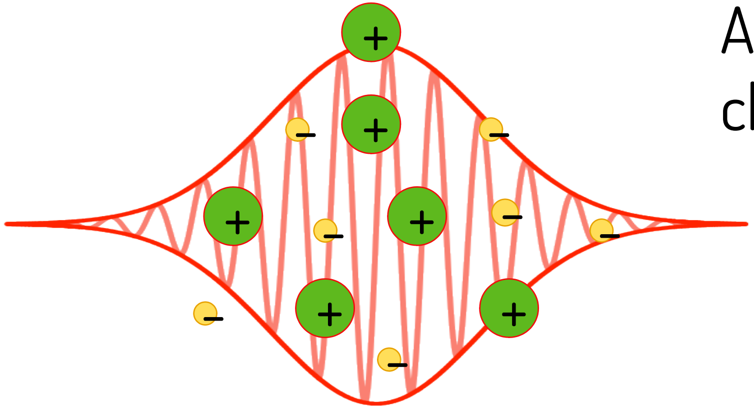


Intensity from **10^{18} W/cm^2** up to **10^{23} W/cm^2**

From **few TeraWatt** up to **several PetaWatt**
(few PW is power of the sunlight striking Australia!!)

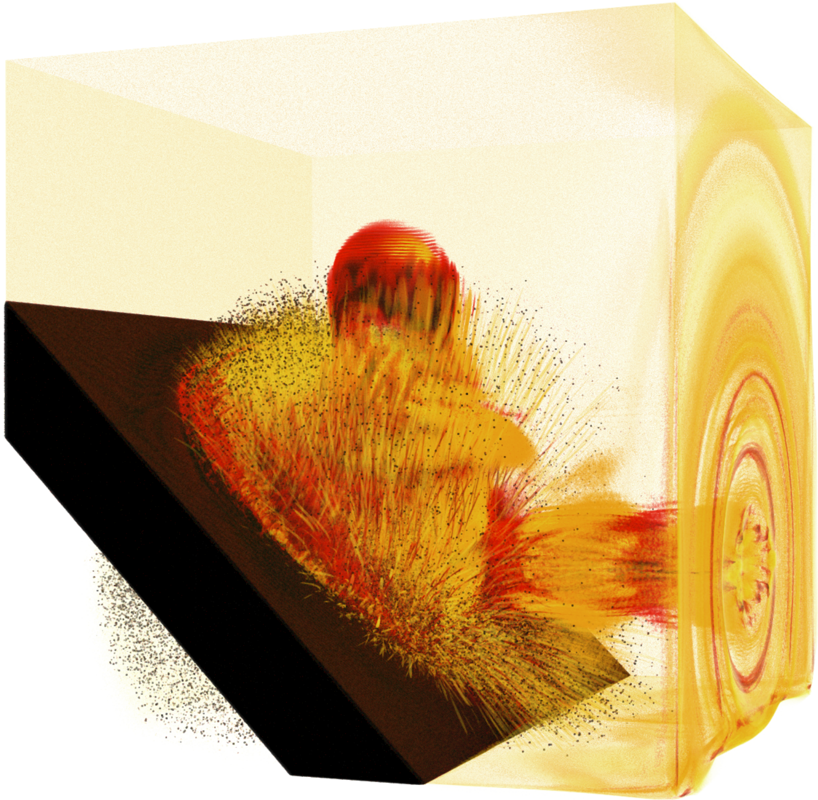
Focused down to a **few μm spot**
(wavelength is ~ 800 nm)

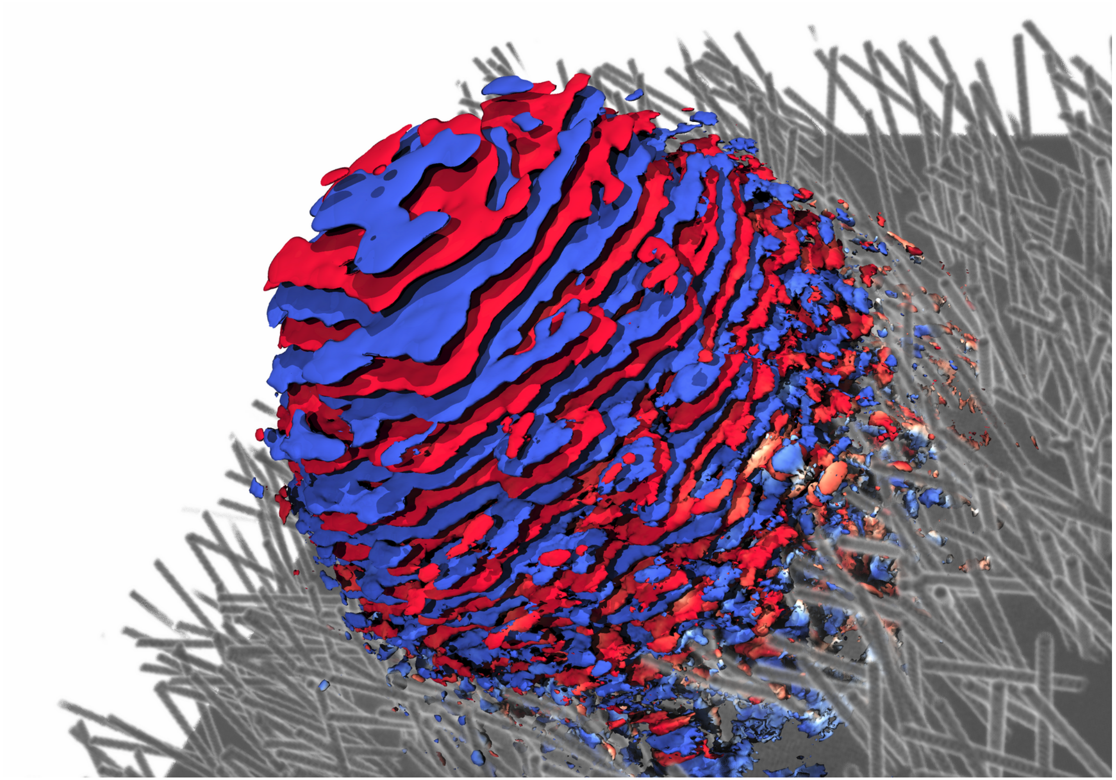
Any target irradiated with these lasers becomes a plasma almost instantaneously



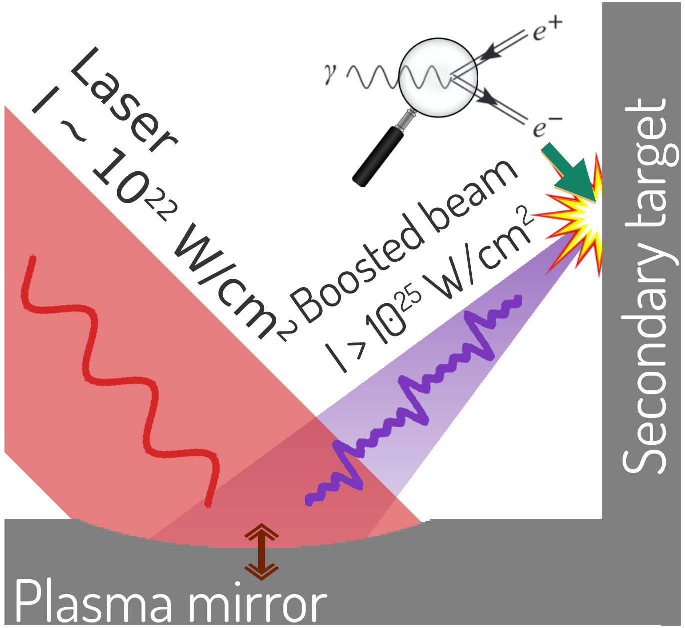
A "gas" of interacting charged particles

We are mainly interested in
ultra-intense laser-plasma interaction

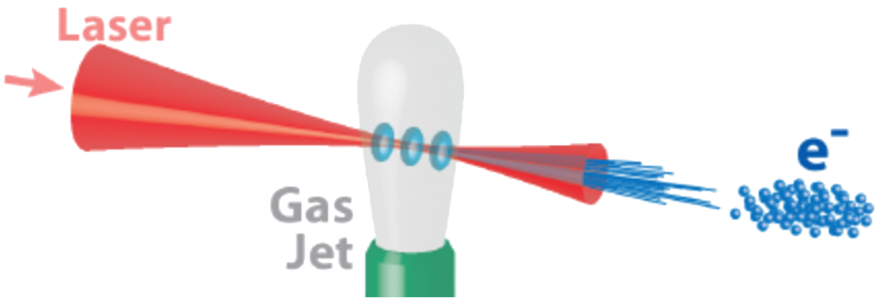




We are interested in laser-plasma interaction to **study extreme physical regimes & accelerate particles**



Use ultra-intense lasers to study the strong-field regime of QED



Laser-driven electron acceleration: compact high-energy e⁻ sources

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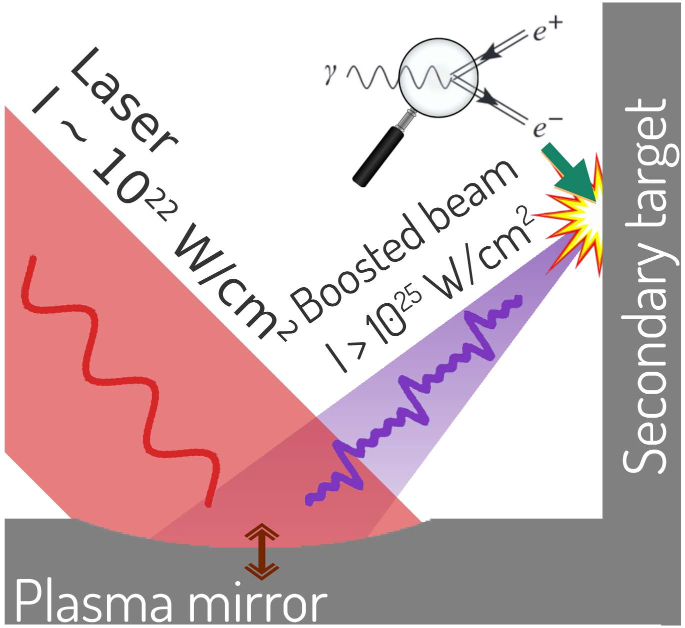

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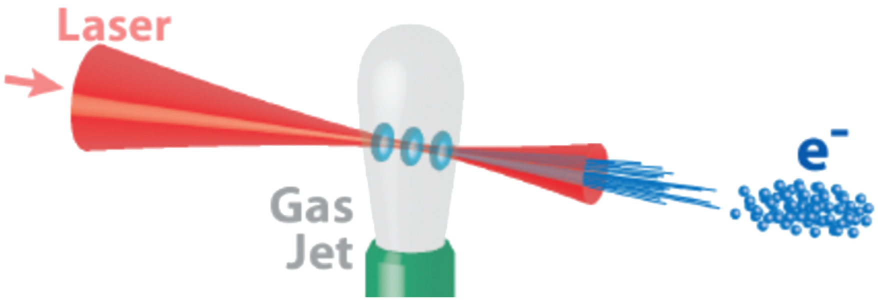
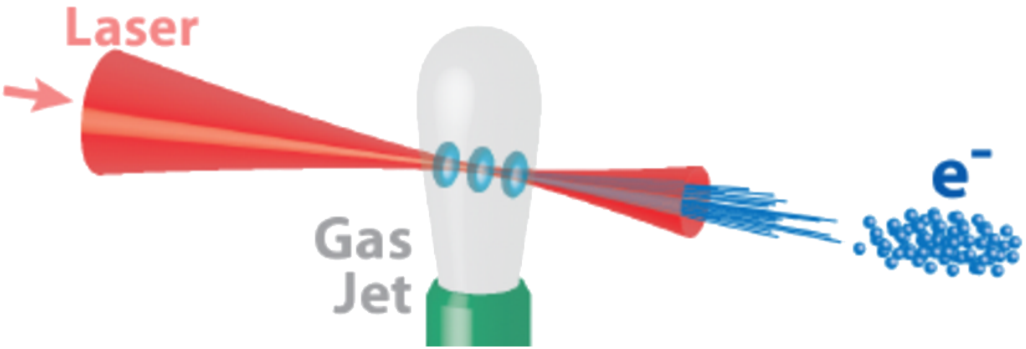
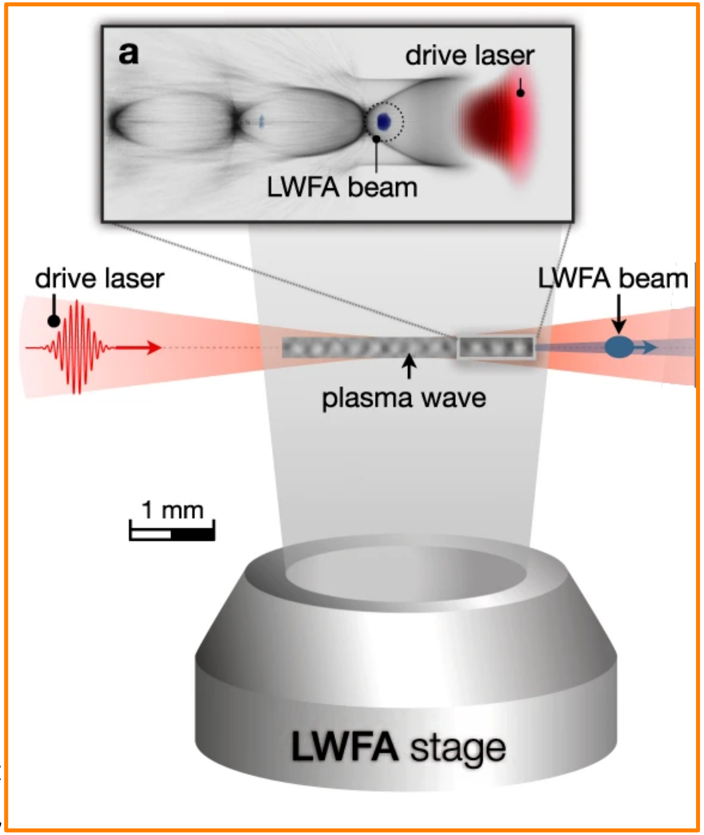


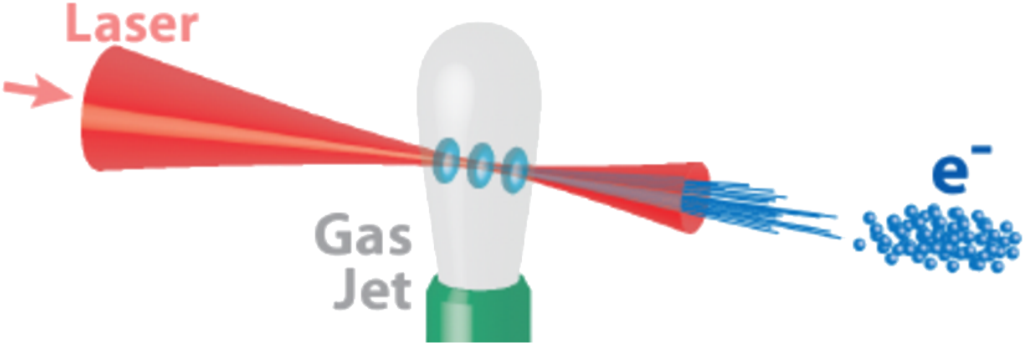
Laser-driven electron acceleration: compact high-energy e⁻ sources

In laser-driven electron acceleration schemes an ultra-intense laser typically interacts with a low density gas





This generally works well **but...**

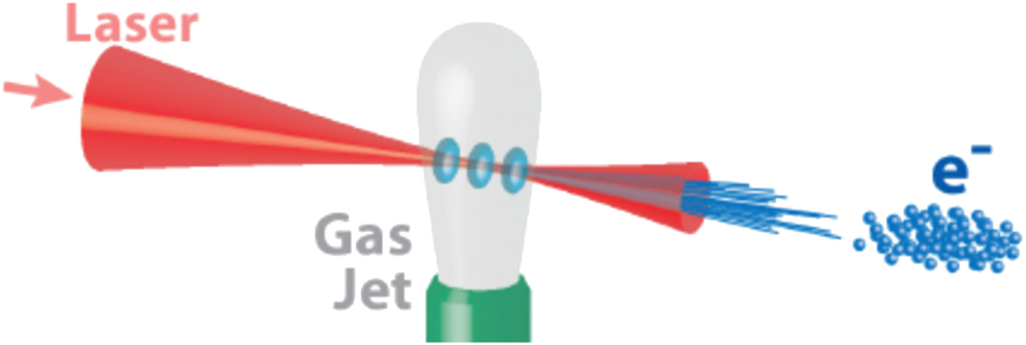


We can accelerate electron up to few gigaelectronvolts in few centimeters

Gonsalves et al. Phys.Rev.Lett. 122, 084801, 2019

This generally works well **but...**

having high charge & high quality at the same time is difficult



high quality — low charge

- or -

low quality — high charge

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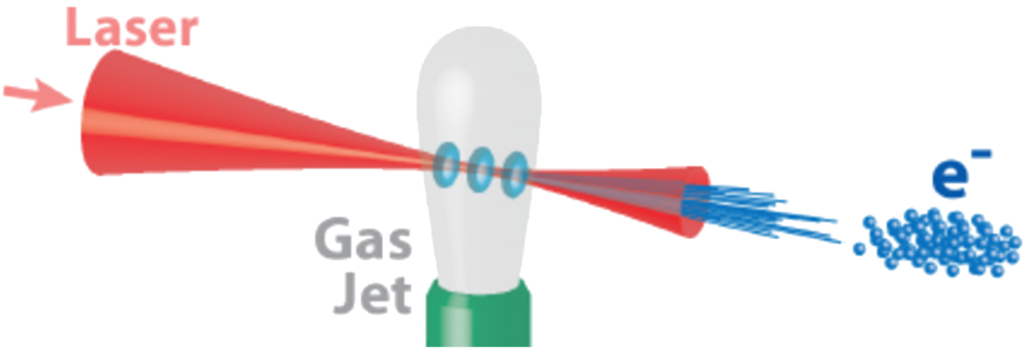


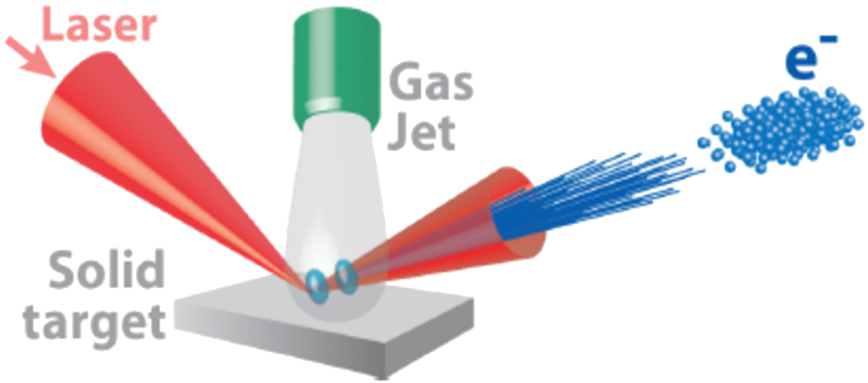
high quality ↑ low charge ↓

– or –

low quality ↓ high charge ↑

This is not good for many applications, e.g. FLASH radiobiology studies

We propose an approach that should give us high-charge, high-quality, ultra-short electron beams



high quality

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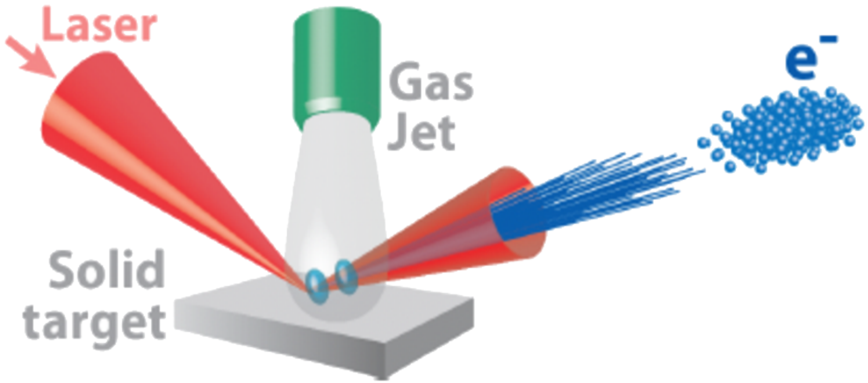


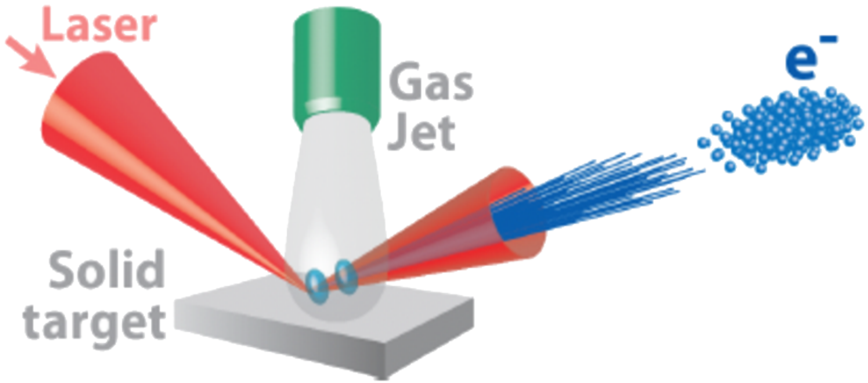
high quality

high charge

Does it actually work?

What are the best parameters to use in experiments?

We propose an approach that should give us high-charge, high-quality, ultra-short electron beams



high
quality

high
charge

Does it actually work?

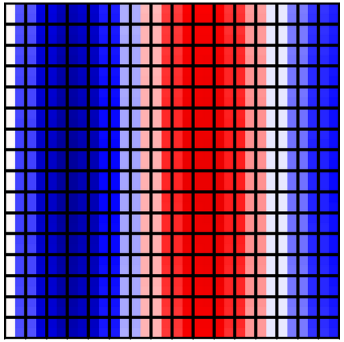
What are the best parameters to use in experiments?

→ **We need simulations**

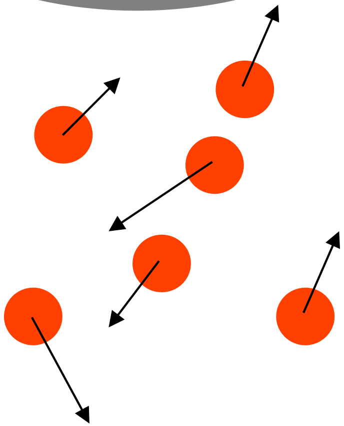
The Particle-In-Cell method is the standard tool to model relativistic kinetic plasmas

Particle-In-Cell codes are the tool of choice to model kinetic plasma phenomena

Electromagnetic fields



Charged macro-particles



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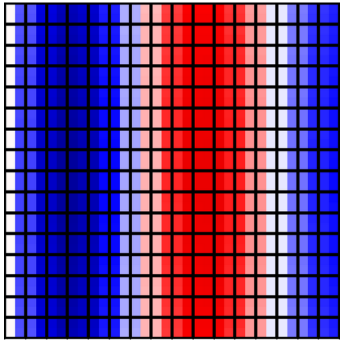
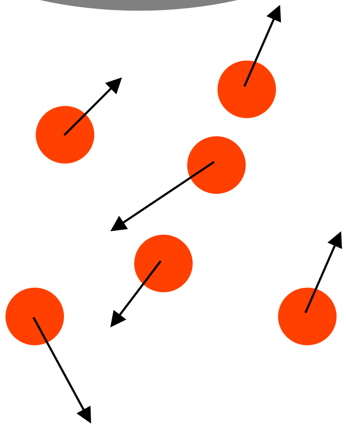


Usually simulated with an FDTD solver

Charged macro-particles



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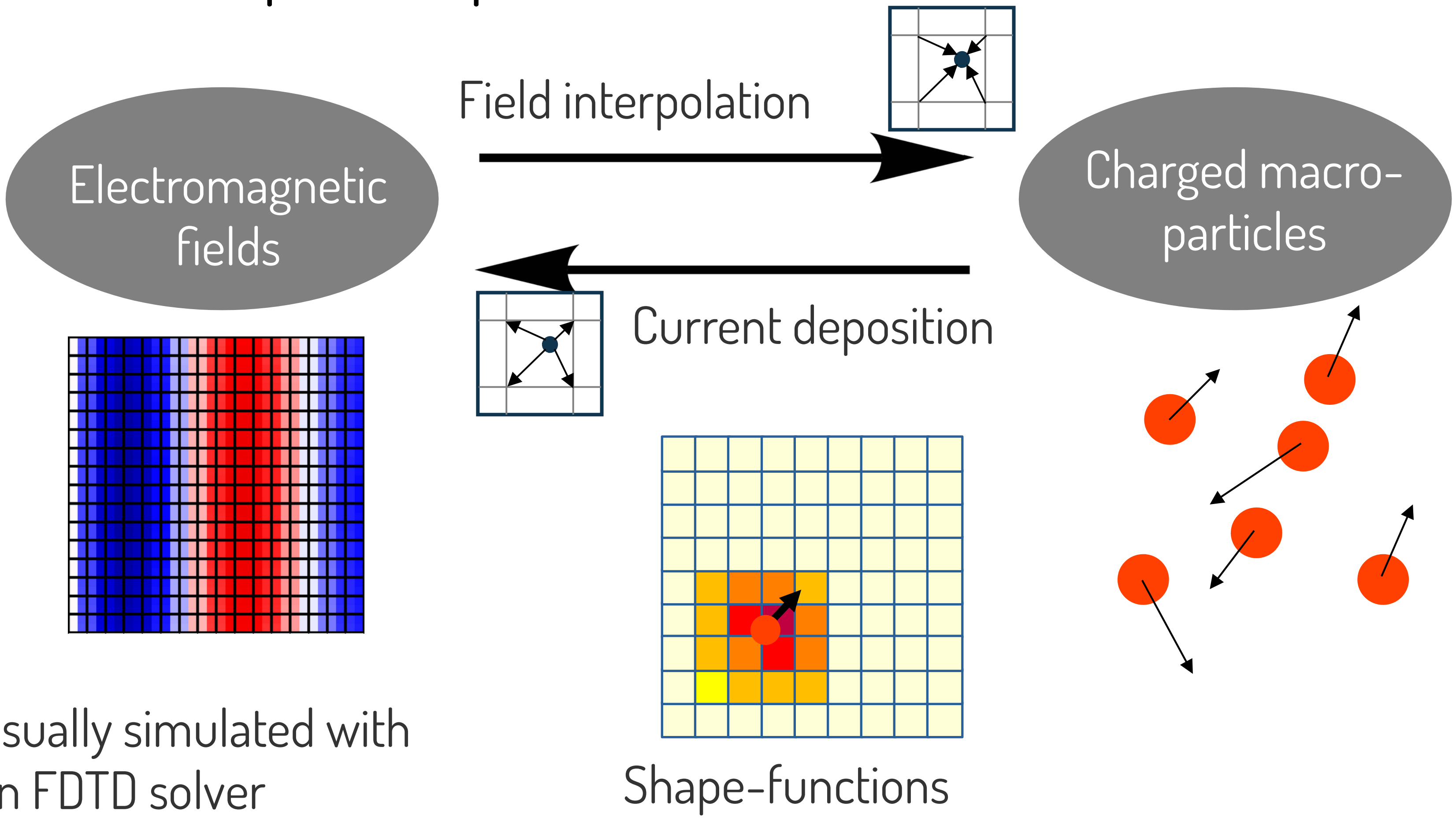
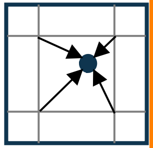


Particle-In-Cell codes are the tool of choice to model kinetic plasma phenomena

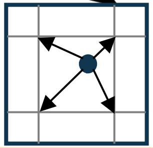
This is (typically) the most expensive part !

Electromagnetic fields

Field interpolation



Current deposition



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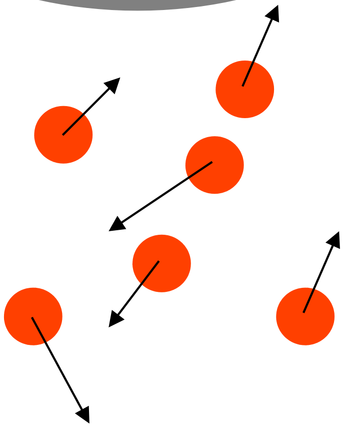
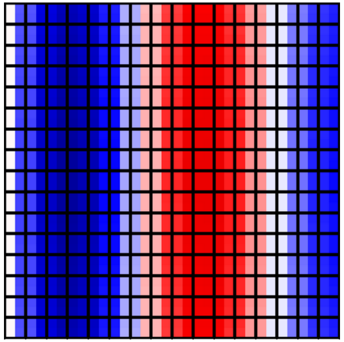
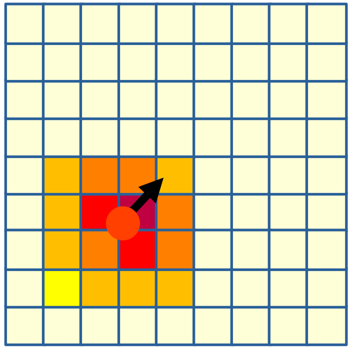


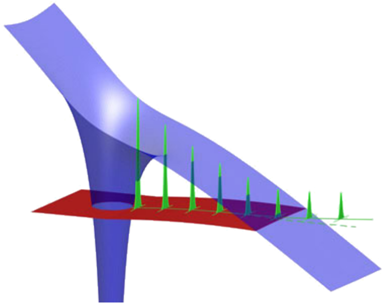




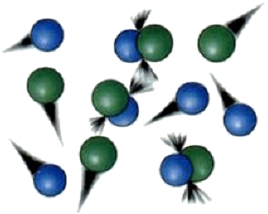
Usually simulated with an FDTD solver

Shape-functions

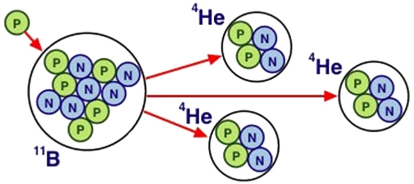
We can add more physical processes to the “core” Particle-In-Cell algorithm



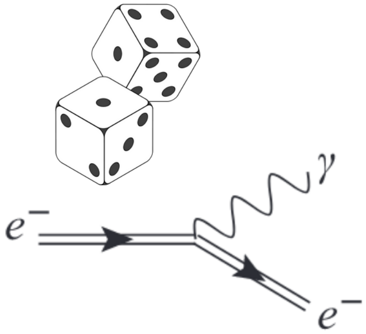
Ionization



Collisions

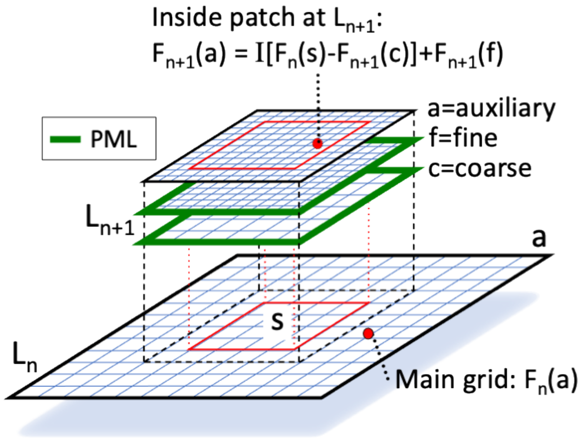


Nuclear fusion

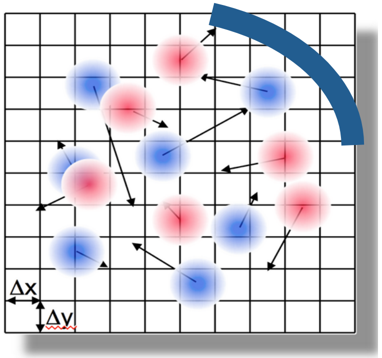


Strong-field QED

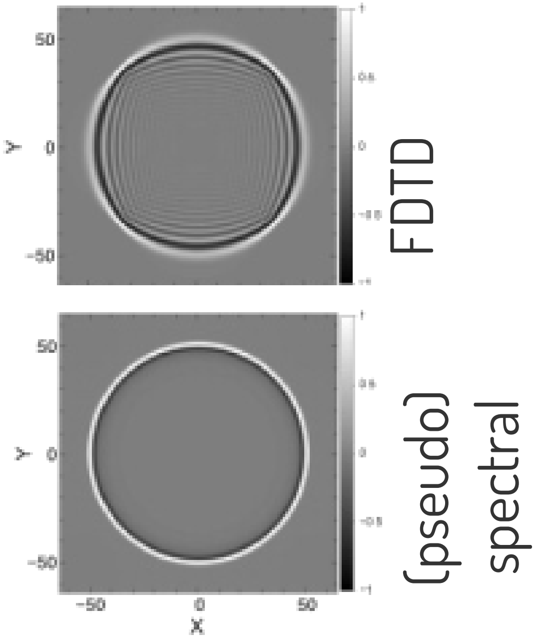
And we can also add sophisticated numerical methods



Mesh refinement



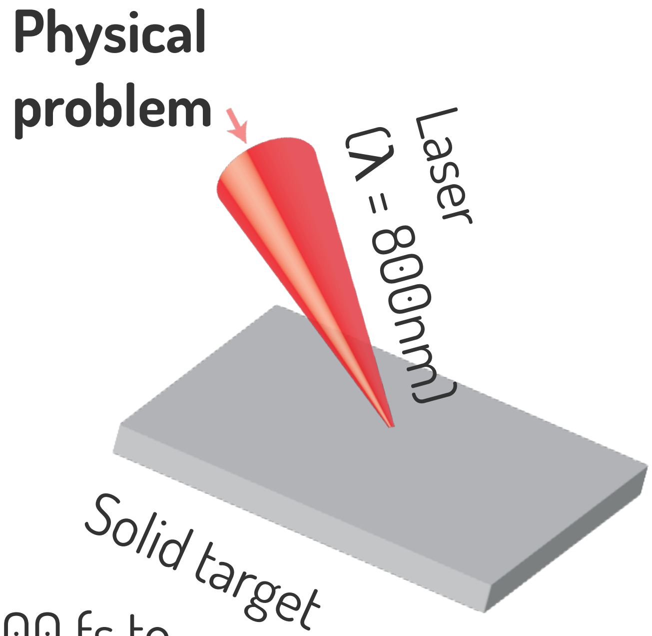
Complex surfaces



Advanced solvers

…

If we want to perform 3D simulations, we often end up needing a lot of computing power



200 fs to simulate

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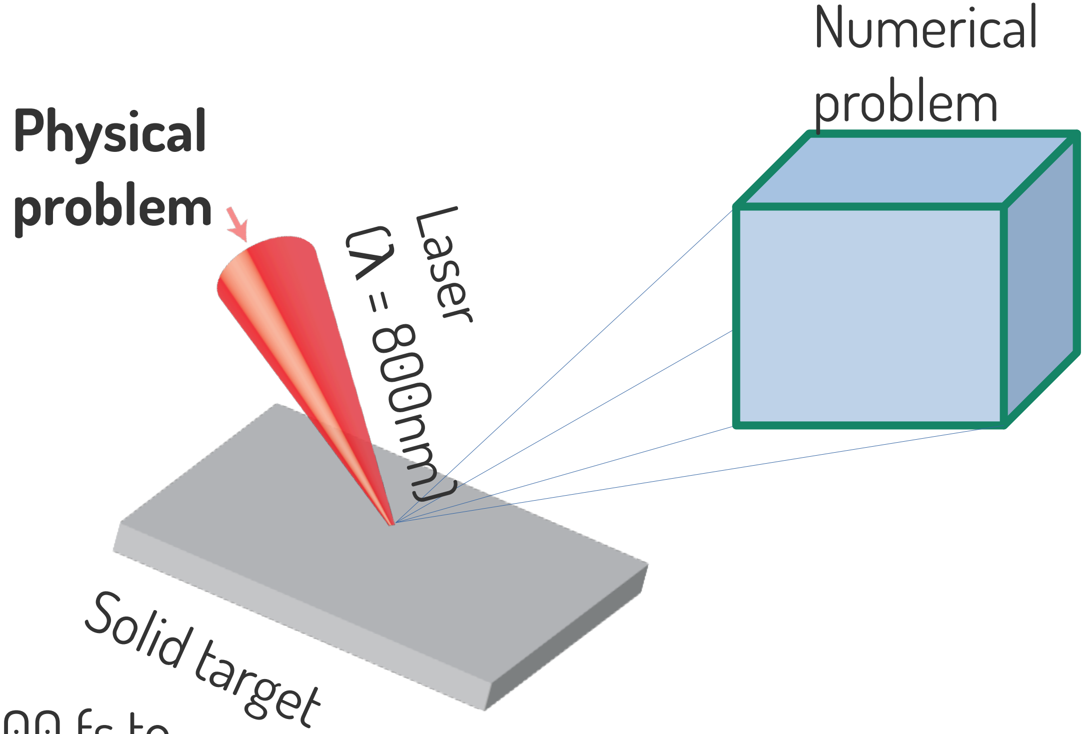

100x100x100 μm³ box
10 nm resolution
10s particles per cell
~ 6000 steps

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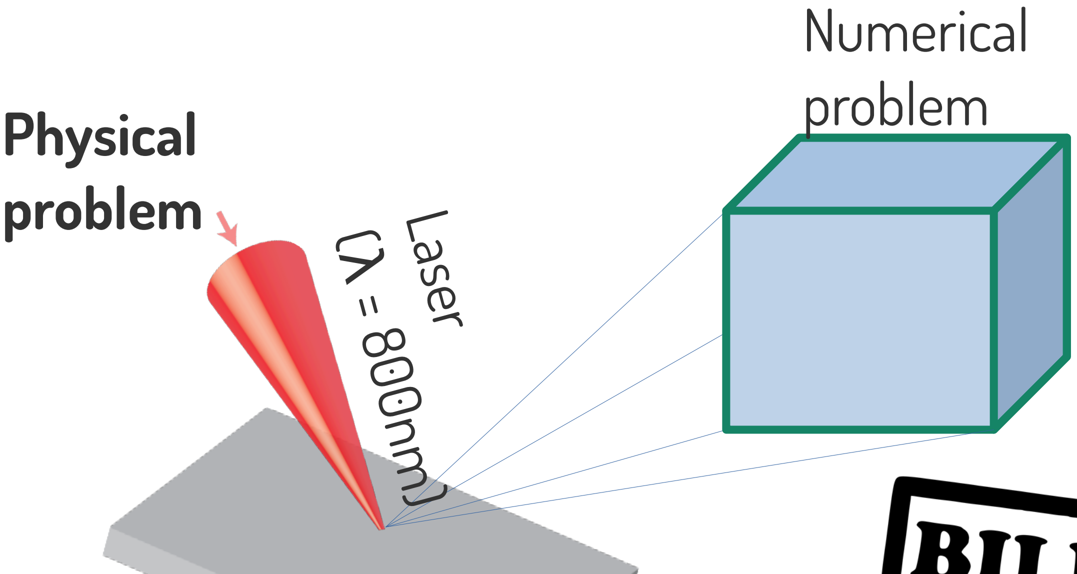

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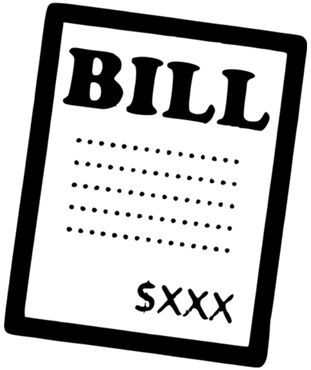
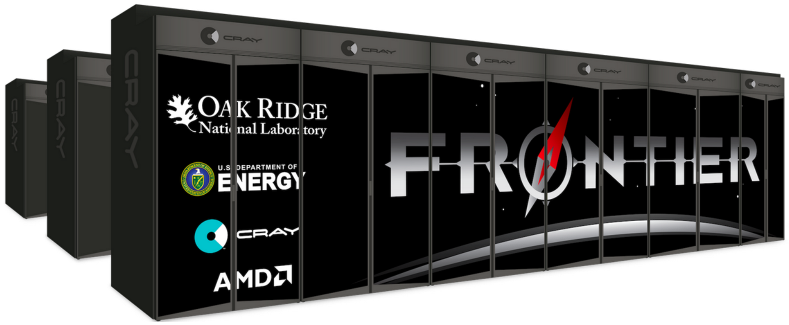


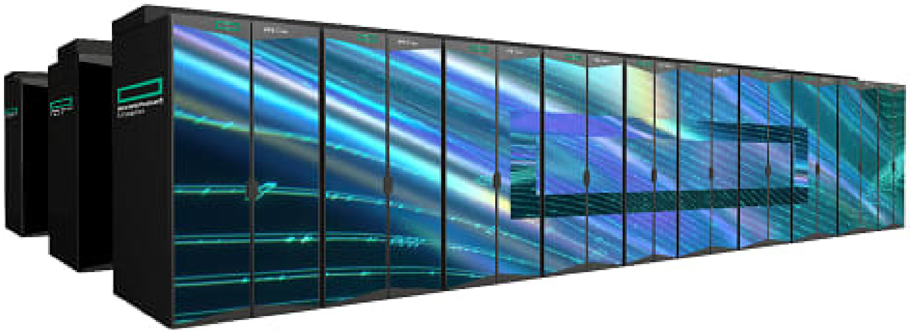
Computational cost

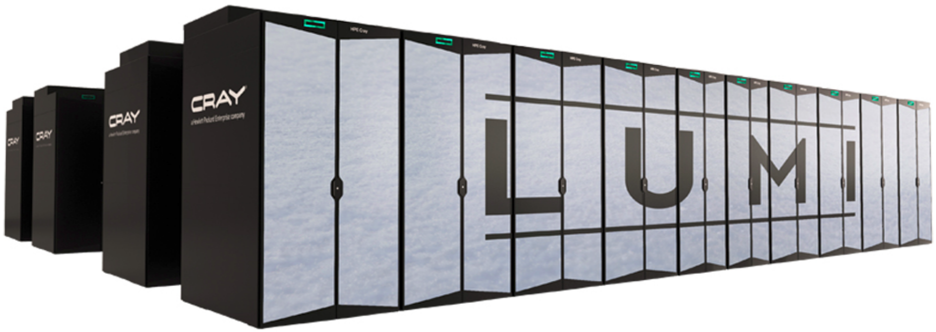
Tens of Terabytes of RAM!

Thousands to millions of CPU hours!

In order to perform large-scale Particle-In-Cell simulations we need supercomputers







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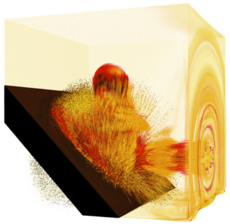

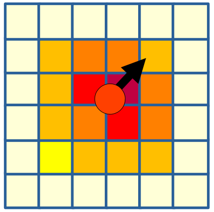

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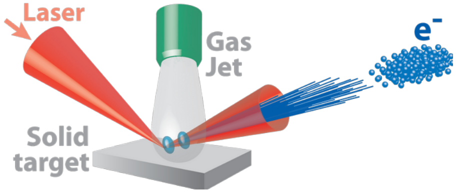
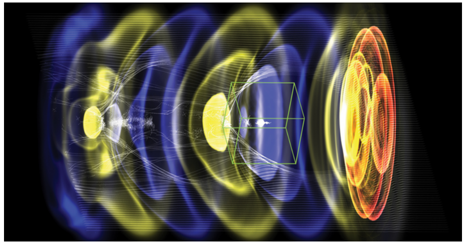


Simulation of a new electron accelerator concept

WarpX is an open-source Particle-In-Cell code for the exascale era.

30+ contributors



EXASCALE COMPUTING PROJECT

BERKELEY LAB

DE LA RECHERCHE À L'INDUSTRIE cea

Lawrence Livermore National Laboratory

SLAC NATIONAL ACCELERATOR LABORATORY

DESY.

CERN

MODERN ELECTRON

open source initiative Approved License®

Open-source & available on Github

Documentation: **ecp-warpx.github.io/**

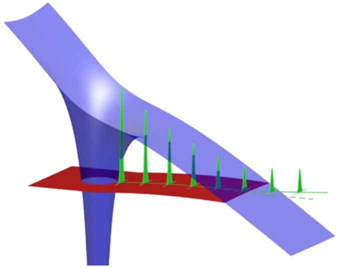
Gordon Bell prize winner @

SC22

From your laptop to the largest supercomputers in the world!

WarpX offers a very rich set of features

Comprehensive additional physics modules set→



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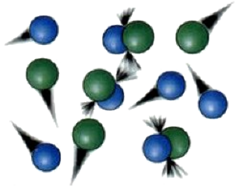

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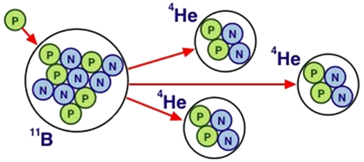
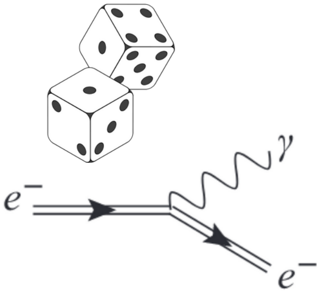
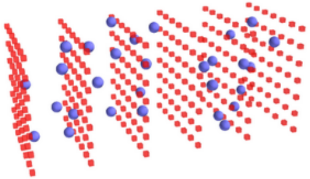


Nuclear fusion

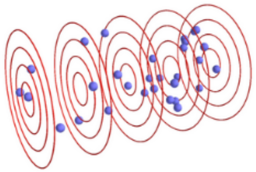


Strong-field QED

Cartesian & cylindrical geometries→

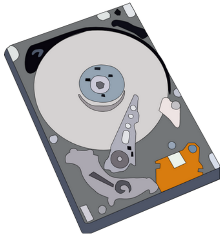


3D Cartesian grid



Cylindrical grid (schematic)

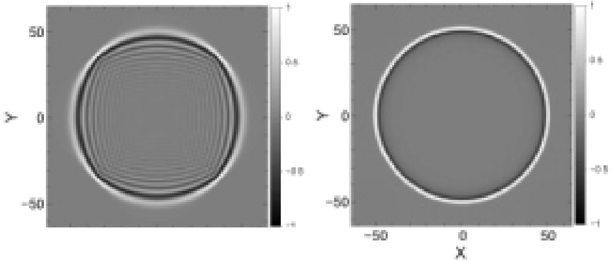
Scalable output→



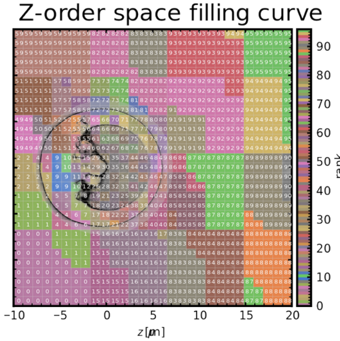
openPMD

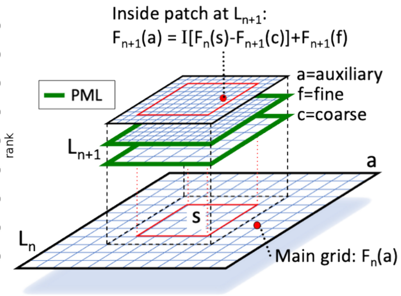
ADIOS

Advanced solvers→

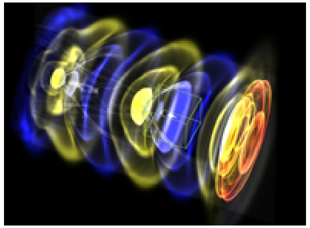


Advanced methods→



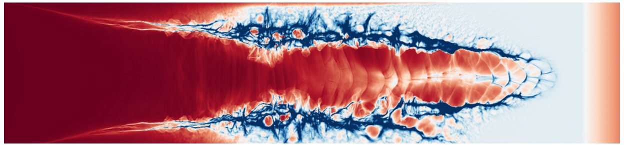


WarpX is used for many different applications!

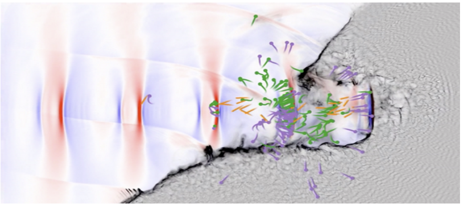


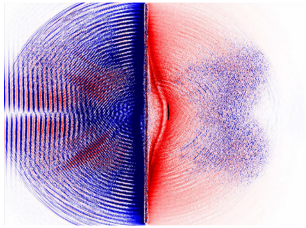
Plasma accelerators (LBNL, DESY, SLAC)

Laser-ion acceleration - advanced mechanisms (LBNL)



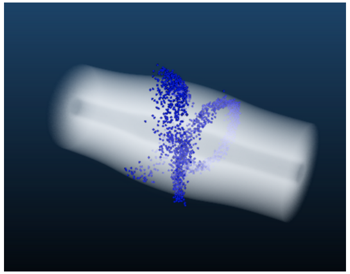
Plasma mirrors and high-field physics + QED (CEA Saclay/LBNL)



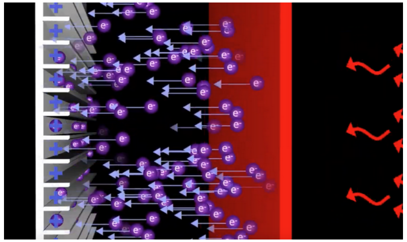


Laser-ion acceleration - laser pulse shaping (LLNL)

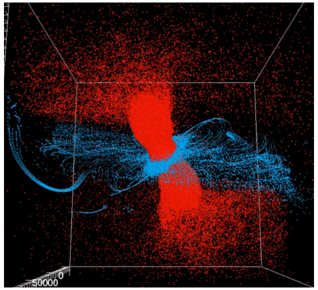
Fusion devices (Zap Energy, Avalanche Energy)



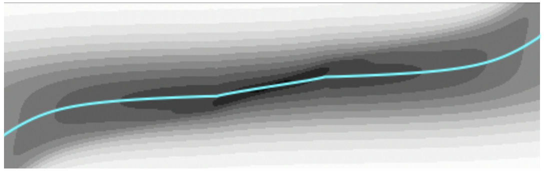
Thermionic converter (Modern Electron)



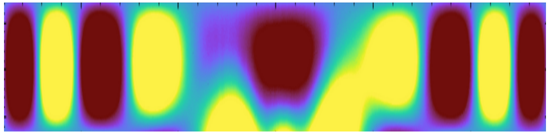
Pulsars, magnetic reconnection (LBNL)

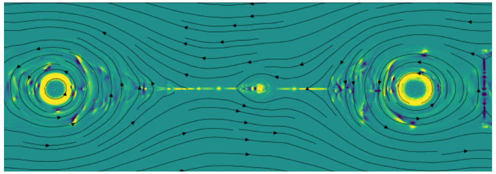


Magnetic fusion sheaths (LLNL)



Microelectronics (LBNL) - ARTEMIS





WarpX runs on GPUs (AMD, NVIDIA) and on CPUs (AMD, Intel, ARM...)

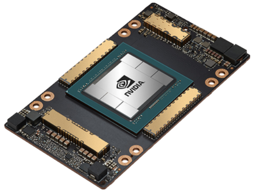
WarpX runs on GPUs (AMD, NVIDIA) and on CPUs (AMD, Intel, ARM…)

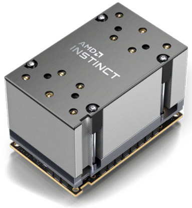
We achieve performance portability across different architectures thanks to **AMReX**

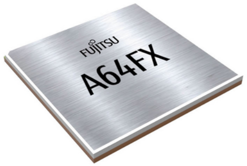
WarpX is built on top of the AMReX library, which provides performance portability

Single source approach

```cpp
using namespace amrex;

int N = 1'000'000;

Gpu::ManagedVector<double> a(N);
Gpu::ManagedVector<double> b(N);
Gpu::ManagedVector<double> c(N);
Gpu::ManagedVector<double> result(N);

/* OTHER CODE*/

auto d_a = a.data();
auto d_b = b.data();
auto d_c = c.data();
auto d_result = c.data();

ParallelFor(N,
    [=] AMREX_GPU_DEVICE (int i){
        d_result[i] = d_a[i]*d_b[i] + d_c[i];
    });
```







We express our algorithms as lambdas fed to “ParallelFor” functions

```
#ifdef AMREX_USE_OMP
    #pragma omp parallel for
#endif
for (WarpXParIter pti(*this, lev); pti.isValid(); ++pti)
{
    // ..
    amrex::ParallelFor(number_of_particles,
        [=] AMREX_GPU_DEVICE (int i)
        {
            // ..
        }
    // ..
}
```

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← AMReX also provides GPU-friendly containers, drop-in replacement for some STL features, parallel reductions...

“ParallelFor” now supports also compile-time optimization for runtime parameters

```
amrex::ParallelFor(TypeList<CompileTimeOptions<A0,A1,A2,A3>>{},
{runtime_option},
box, [=] AMREX_GPU_DEVICE (int i, int j, int k, auto control)
    {
        //...
        if constexpr (control.value == A0) {
        //...
        } else if constexpr (control.value == A1) {
        //...
        } else if constexpr (control.value == A2) {
        //...
        else {
        //...
        }
    //...
    });
```

←Thanks to template programming, under the hood, it generates all the possible combinations

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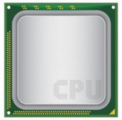
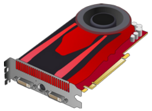
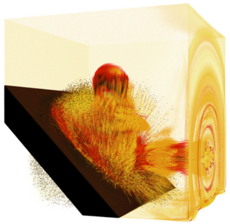
←Thanks to template programming, under the hood, it generates all the possible combinations

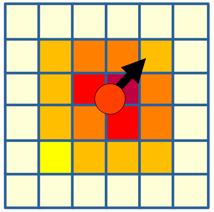
Helpful to reduce registry pressure on GPUs and for vectorization on CPUs





Outline

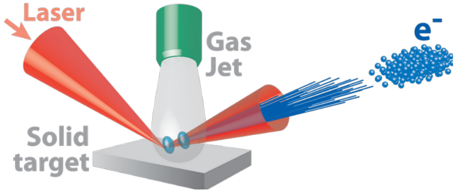




Laser-plasma interaction & the Particle-In-Cell method

WarpX: a Particle-In-Cell code for the exascale era

WarpX performances



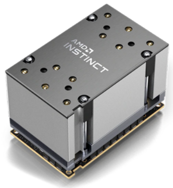
Simulation of a new electron accelerator concept

Let’s have a look at WarpX performances

TOP500 The List.

1st 

Frontier
AMD MI250X



2nd 

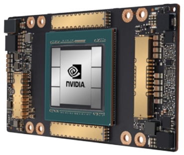
Fugaku
Fujitsu A64FX

5th 

Summit
NVIDIA V100

8th 

Perlmutter
NVIDIA A100



A Particle-In-Cell code is **memory bound**: we expect **only few % peak FLOP/s efficiency**

	DP PFlop/s	Linpack Benchmark	HPCG Benchmark
Perlmutter A100	3.38	12.9%	223%
Summit V100	11.79	8.3%	435%

L.Fedeli et al. SC22 proceedings (2022)

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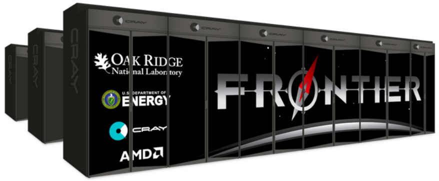

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→ **Specific tuning for Fugaku (3.3X perf. in SP)** Atos

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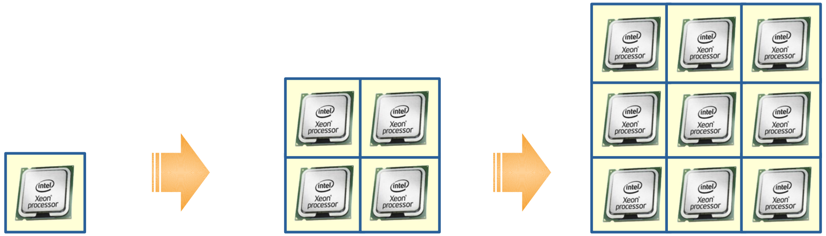
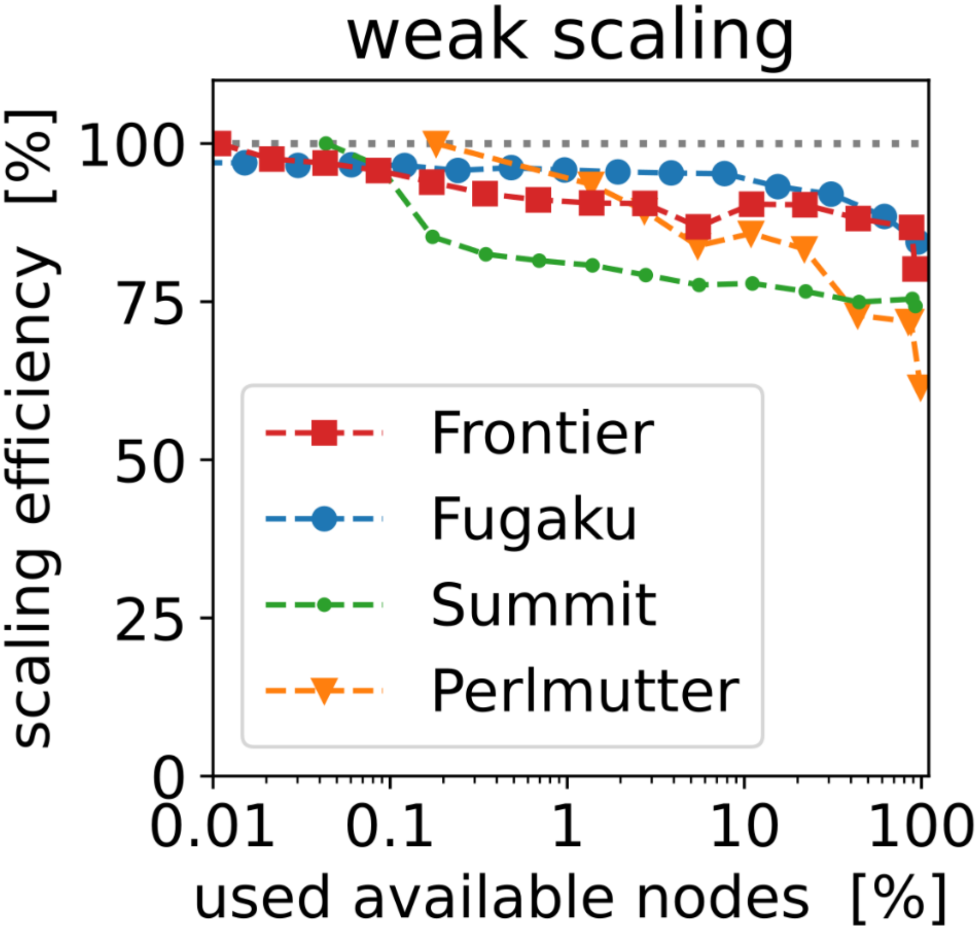
WarpX **very well** over 4-5 orders of magnitude



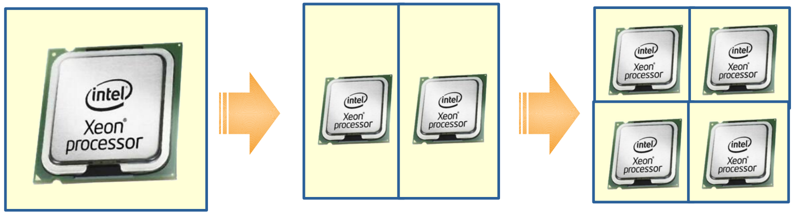


Nodes

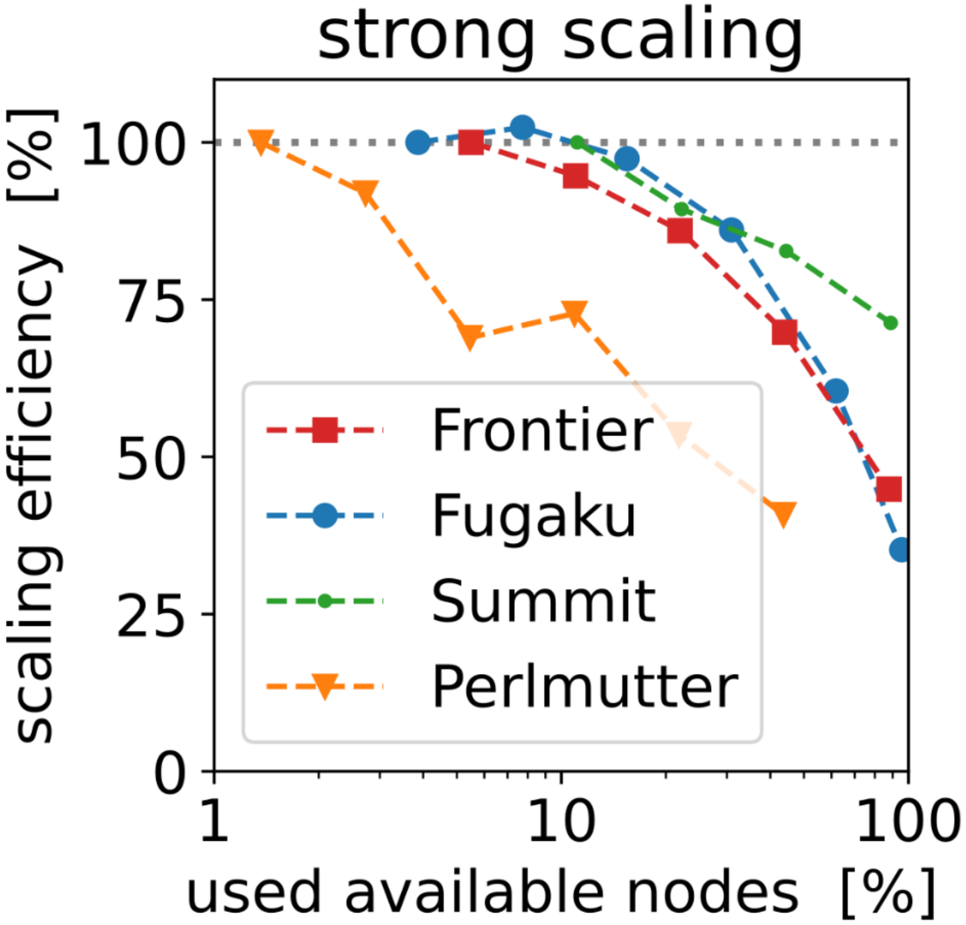
Frontier: 1 – 8,576 (pre-acceptance)
Fugaku: 1 - 152,064
Summit: 2 - 4,263
Perlmutter: 1 – 1,088 (pre-acceptance)

L.Fedeli et al. SC22 proceedings (2022)

WarpX can be **strong-scaled by an order of magnitude** when needed

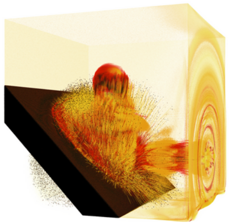
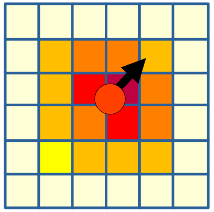


Nodes
Frontier: 512 – 8,192 (pre-acceptance)
Fugaku: 6,144 - 152,064
Summit: 512 - 4,096
Perlmutter: 15 – 480 (pre-acceptance)



L.Fedeli et al. SC22 proceedings (2022)

Outline

Laser-plasma interaction & the Particle-In-Cell method

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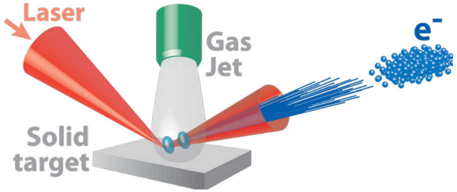
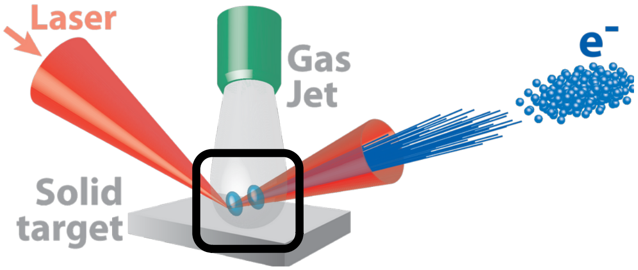
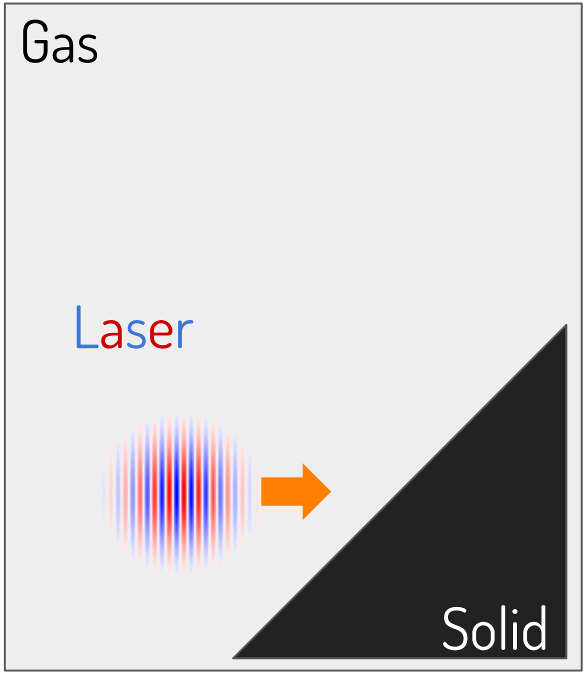


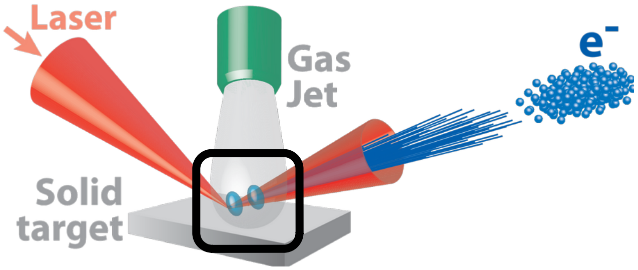
Simulation of a new electron accelerator concept

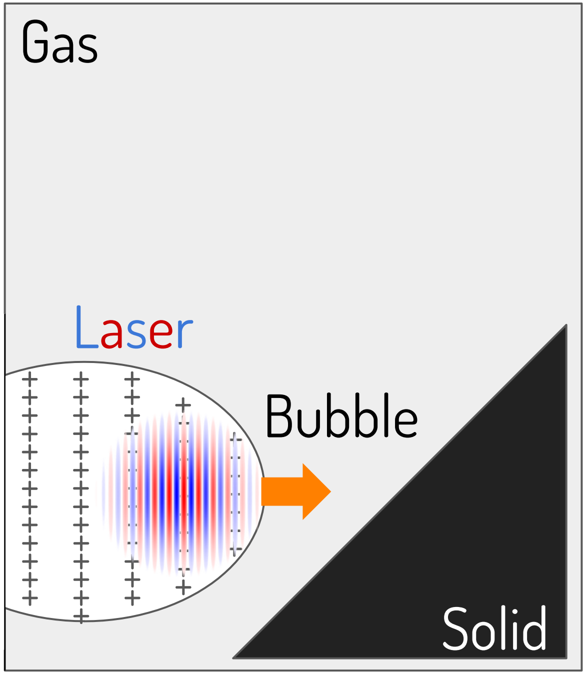
An ultra-short laser beam propagates in a low density gas



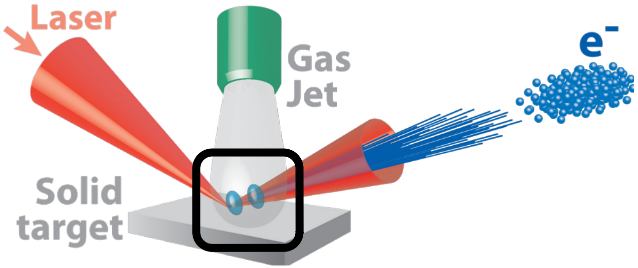


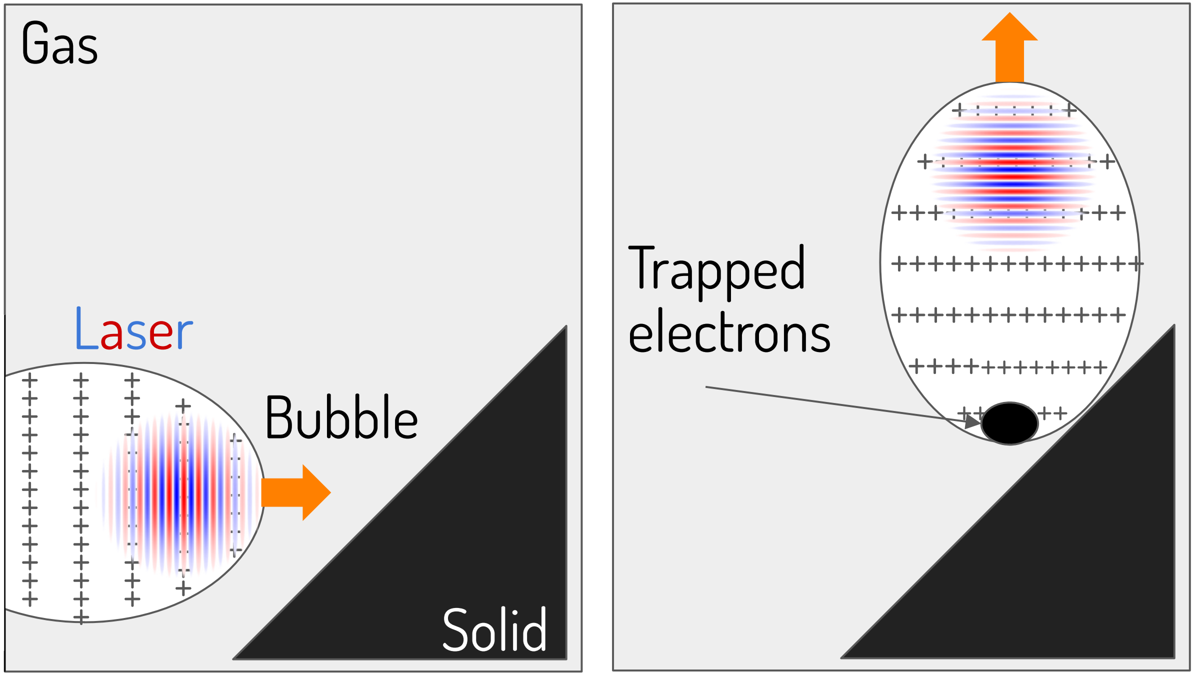
The laser pushes electrons away and generates a positively charged “bubble”



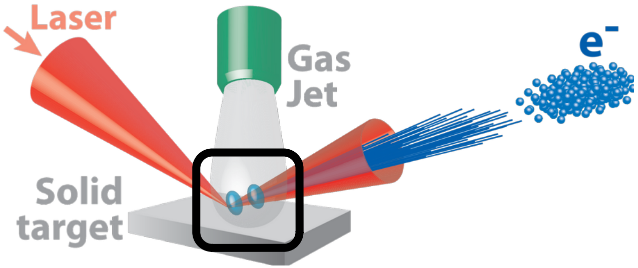


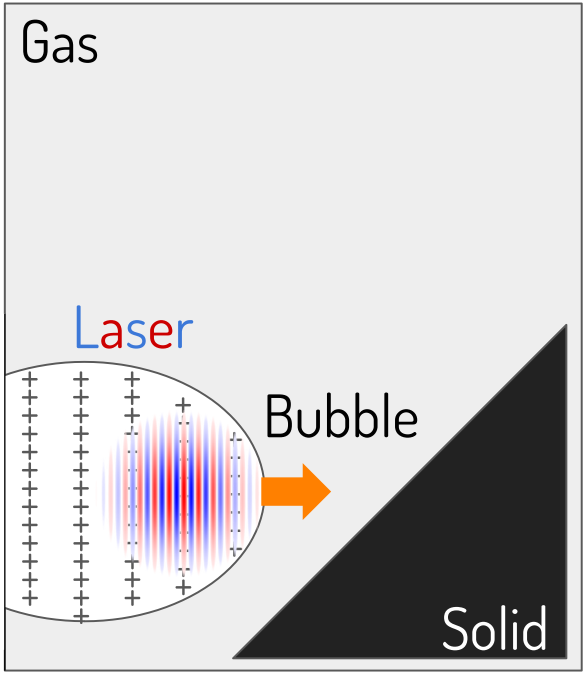
The laser is reflected by the high-density plasma and the bubble traps some of its electrons

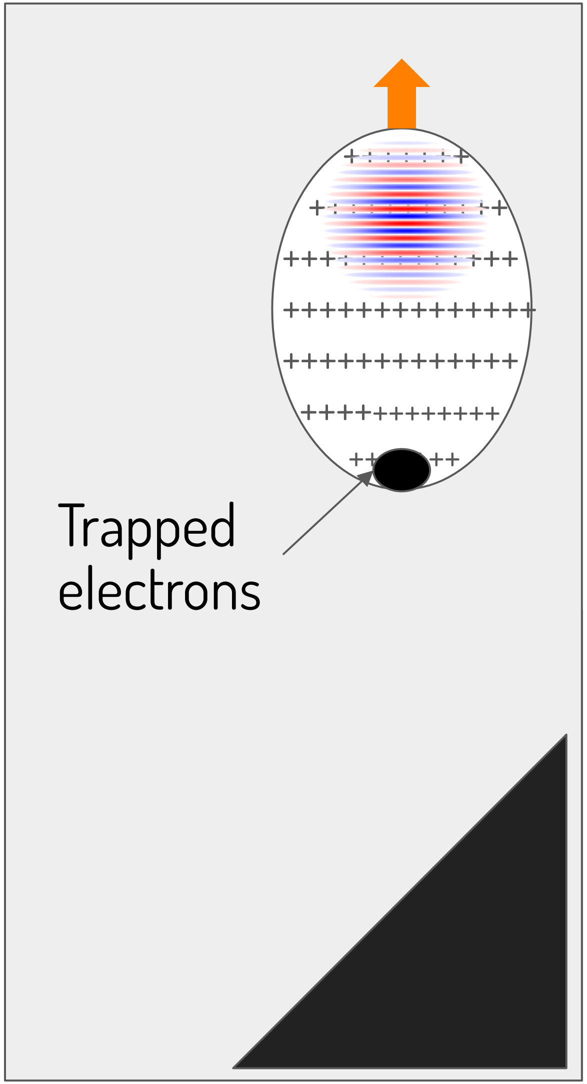




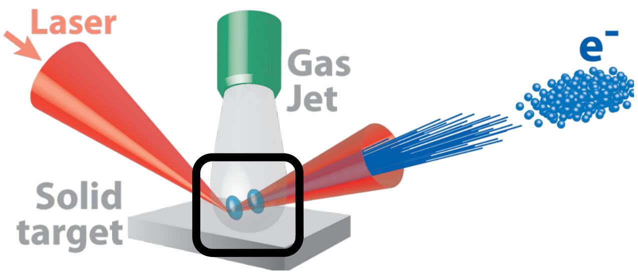
The bubble accelerates electrons over few millimeters





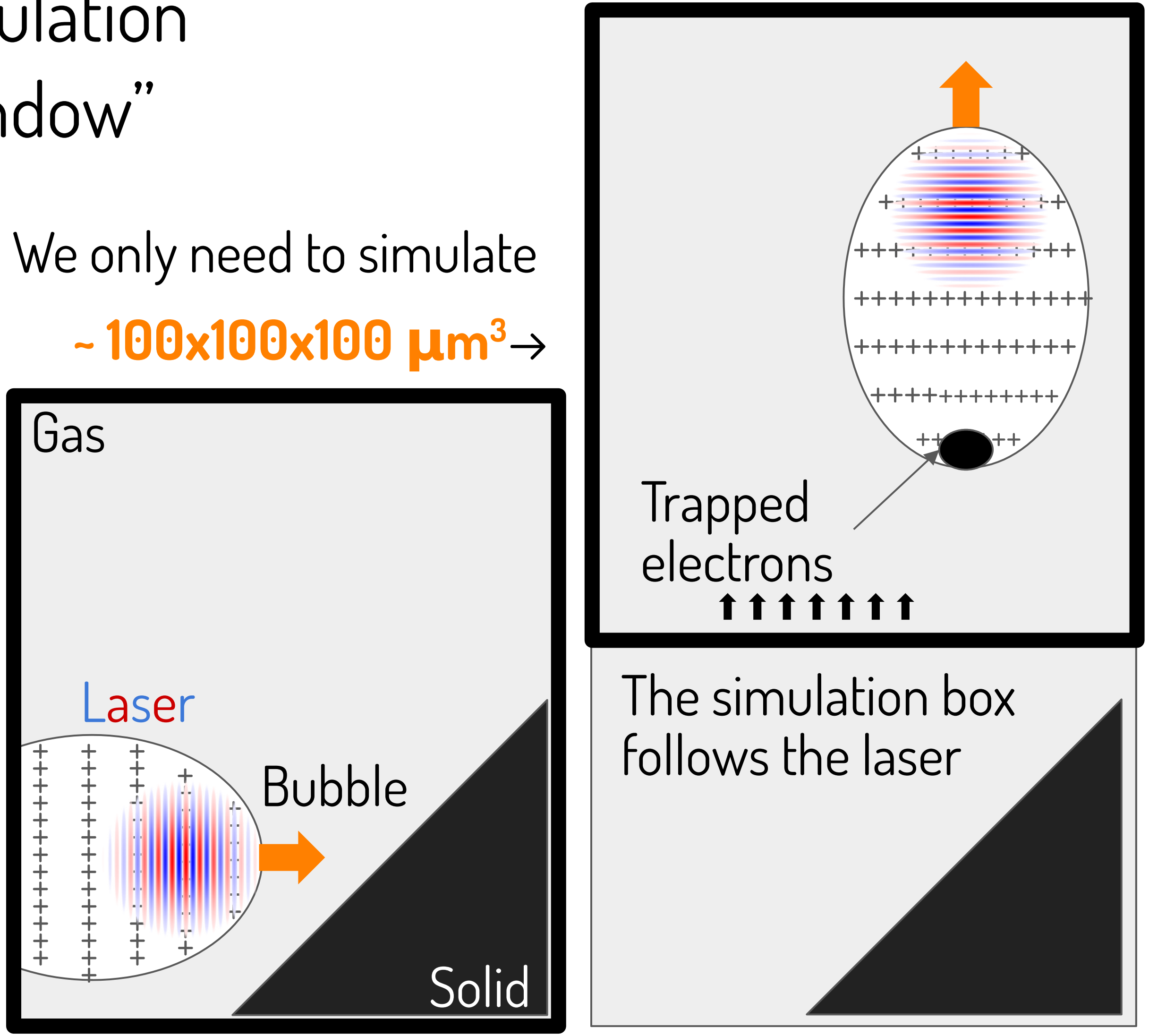


We can have smaller simulation boxes with a “moving window”

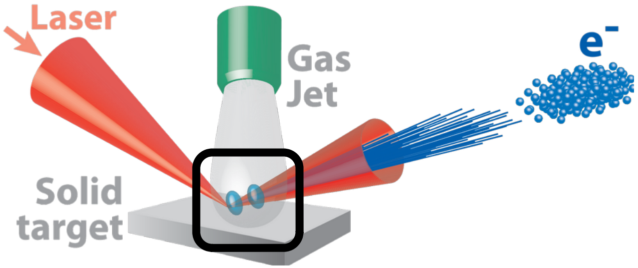


We only need to simulate

~ 100x100x100 µm³→



The main challenge concerns laser-solid interaction



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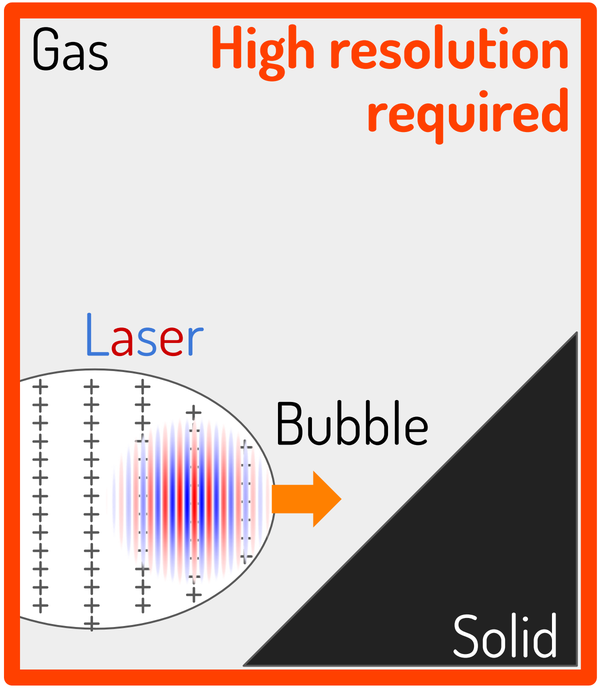
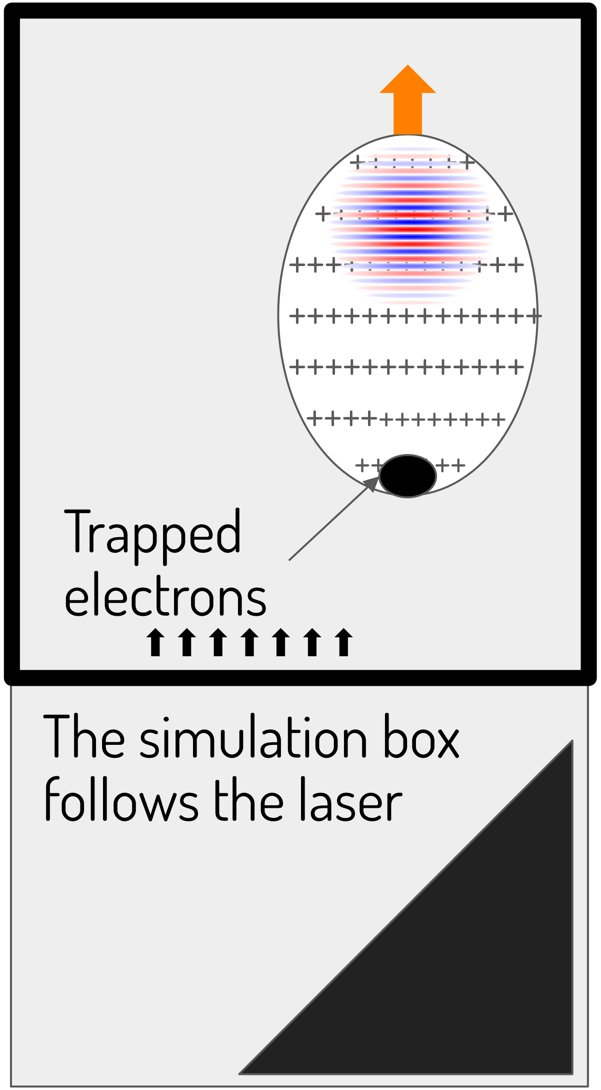


We need a resolution of **~10 nanometers** for laser-solid interaction →



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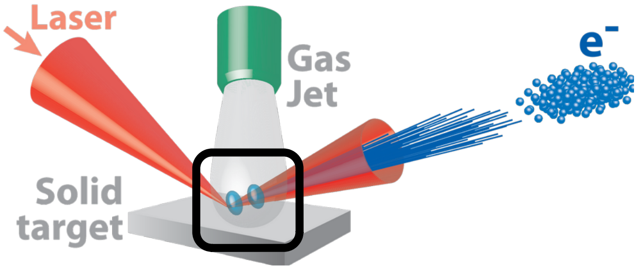
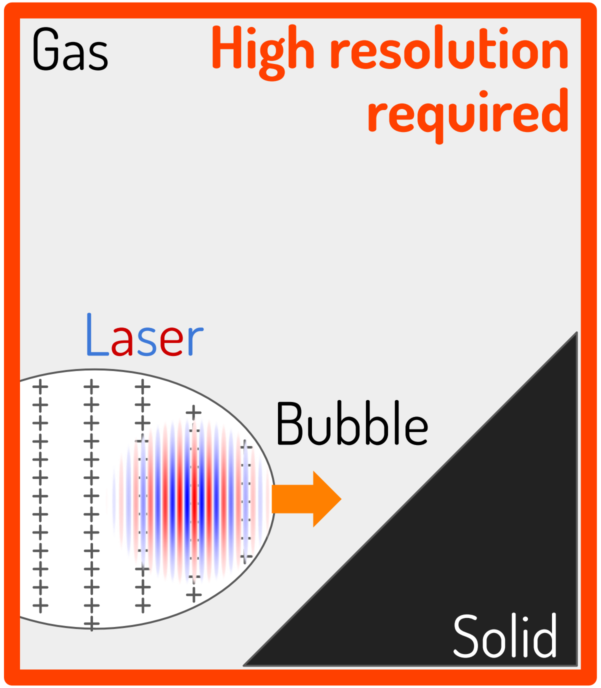
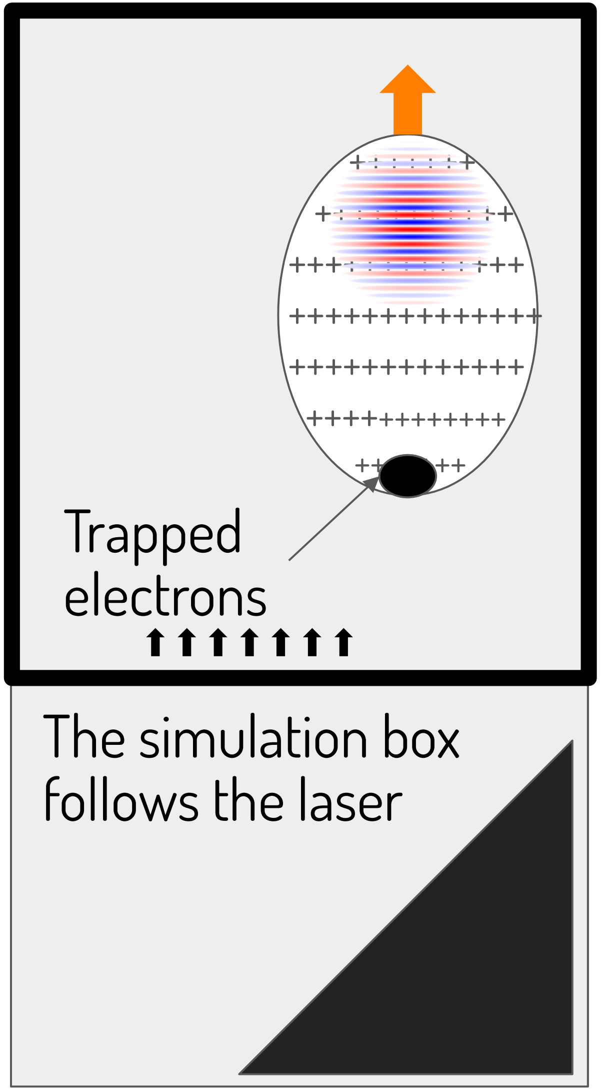


We only need to simulate

~ 100x100x100 μm^3 →





Enabled by **very good weak scaling** →

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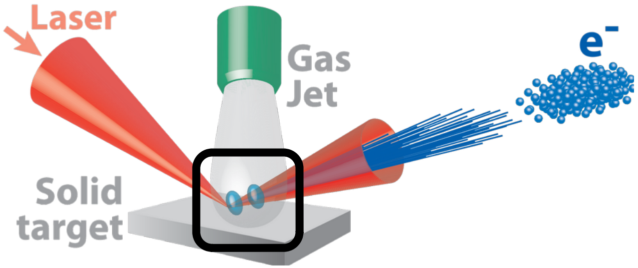

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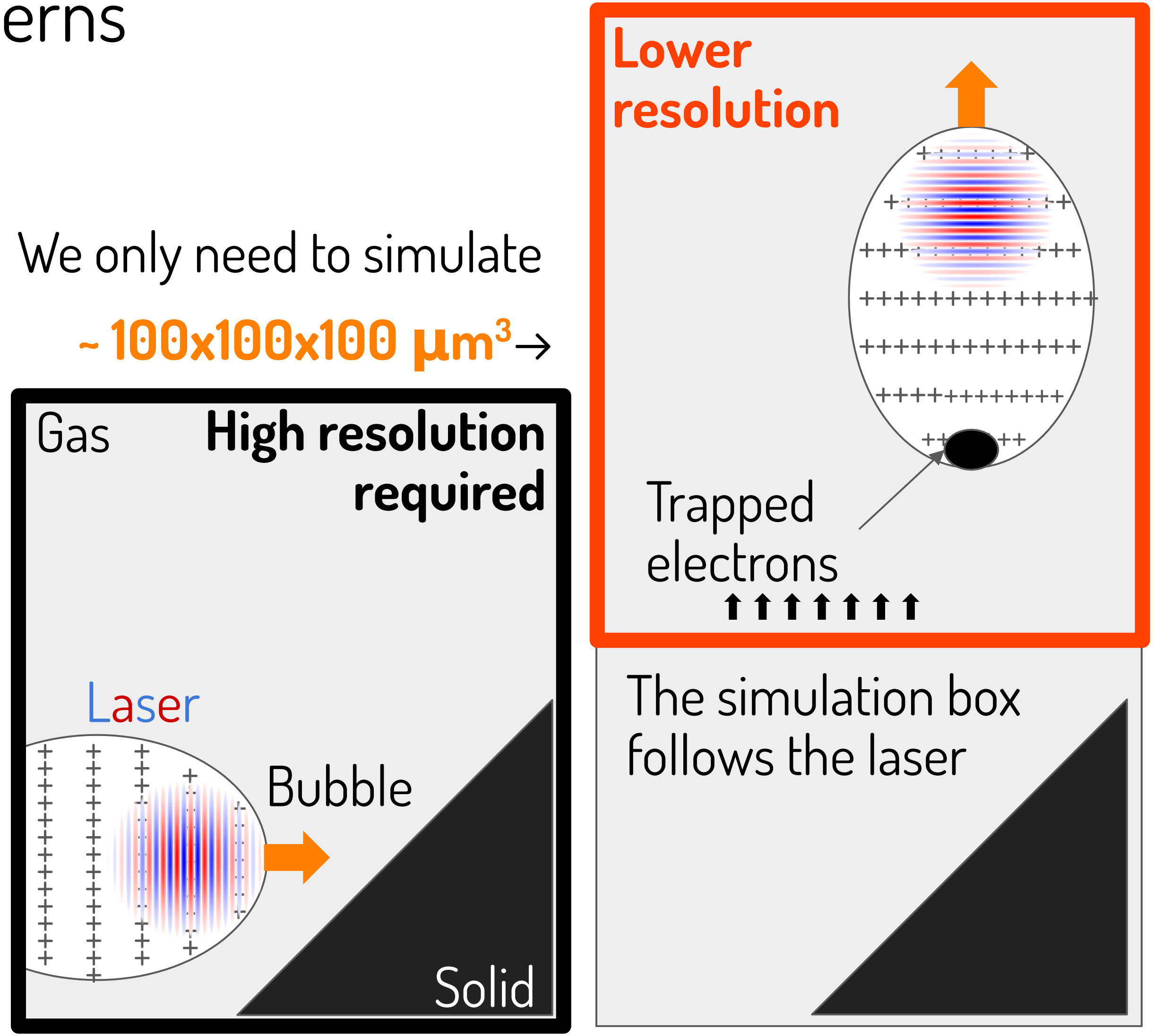

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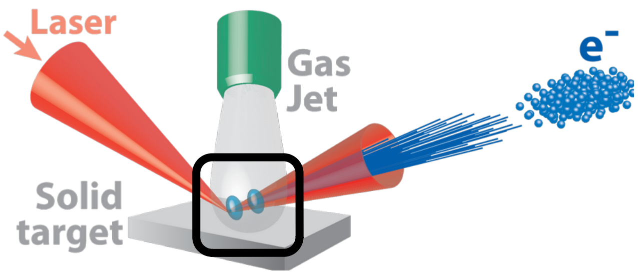
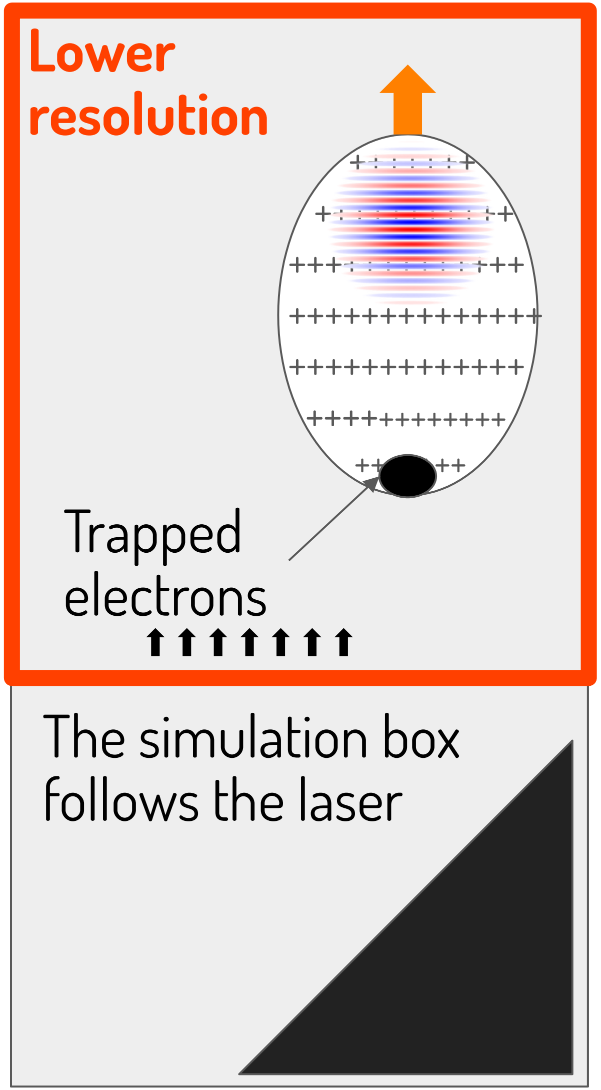


Enabled by **very good strong scaling** →



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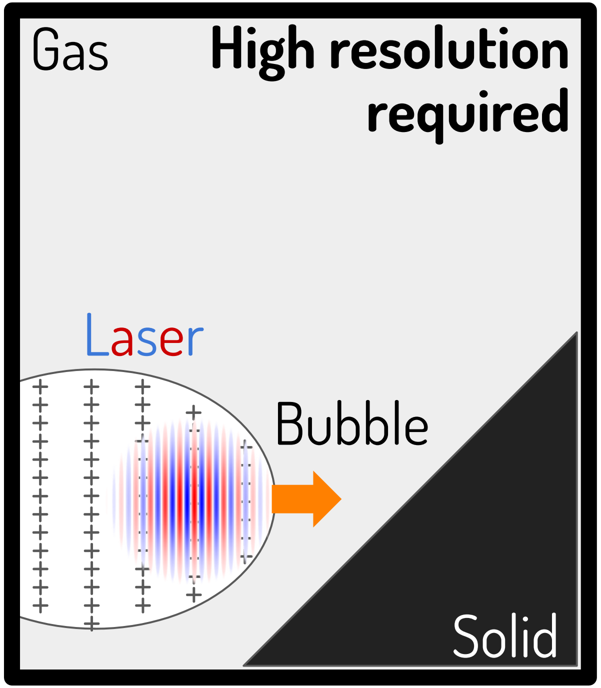
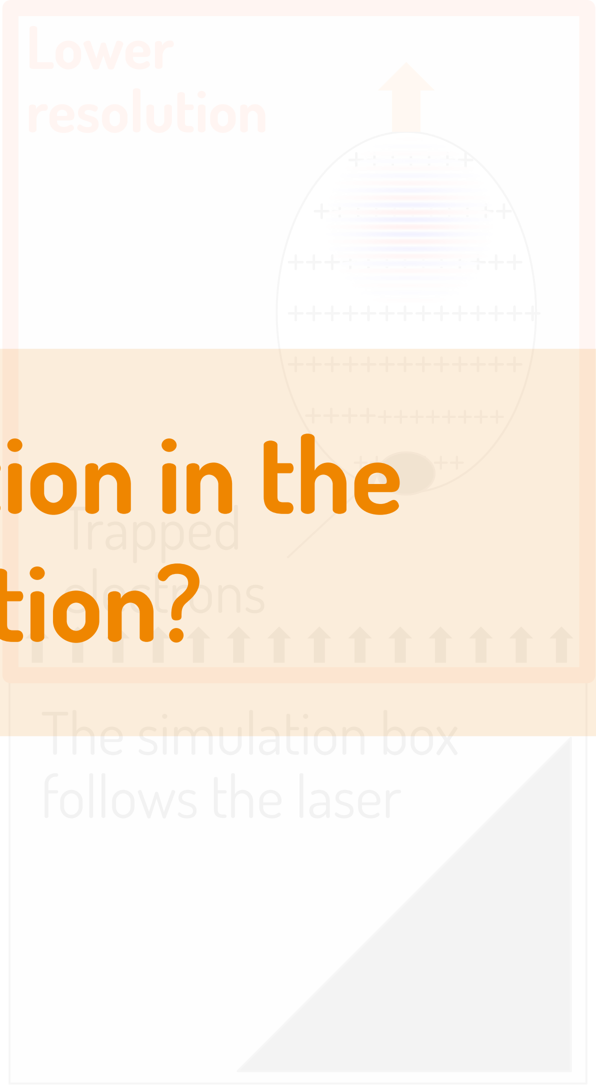


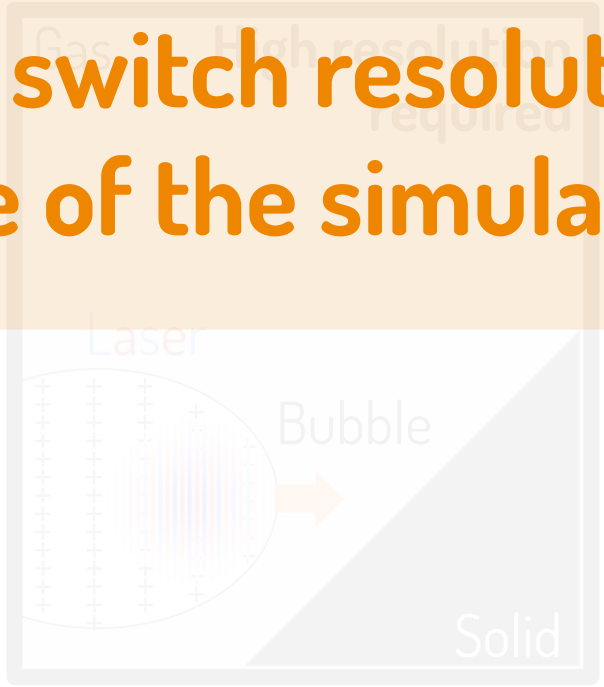
The main challenge concerns laser-solid interaction

Enabled by **very good strong scaling** →



How do we switch resolution in the middle of the simulation?

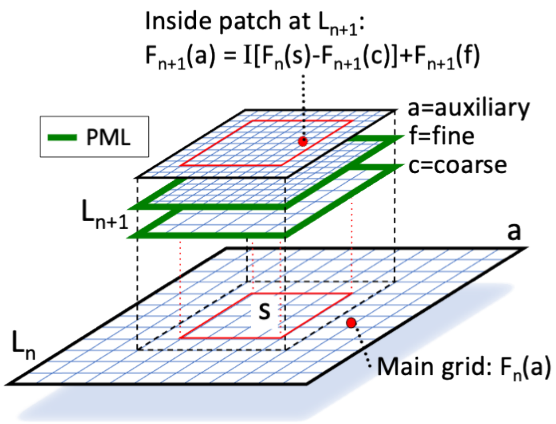
Enabled by **very good weak scaling** →

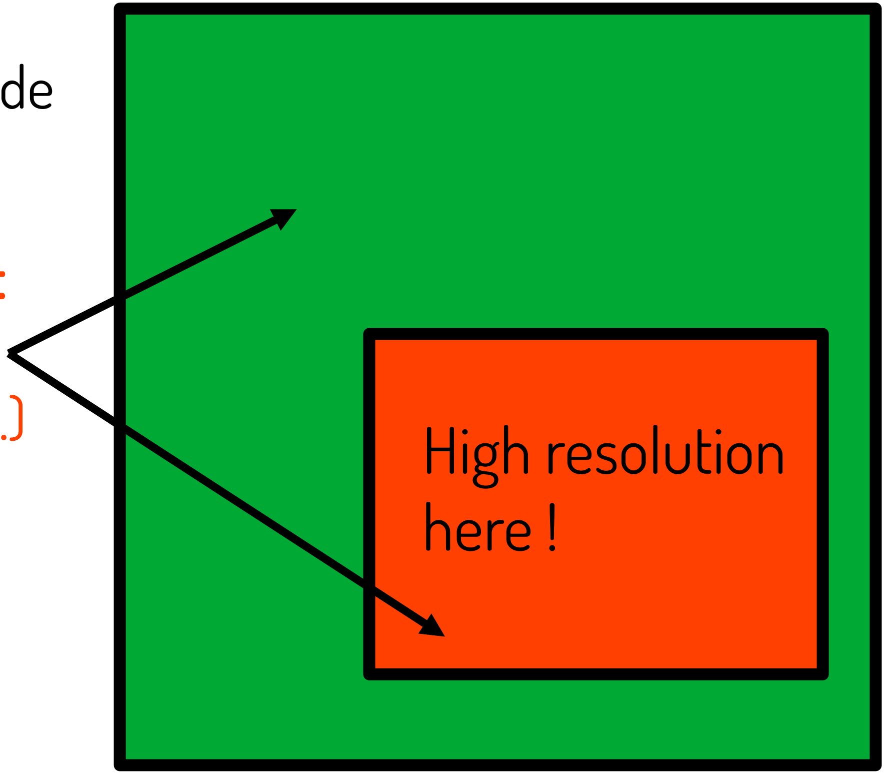


Mesh refinement, one of the most advanced WarpX features, comes to help

Mesh refinement in a Particle-In-Cell code is **a nightmare!**

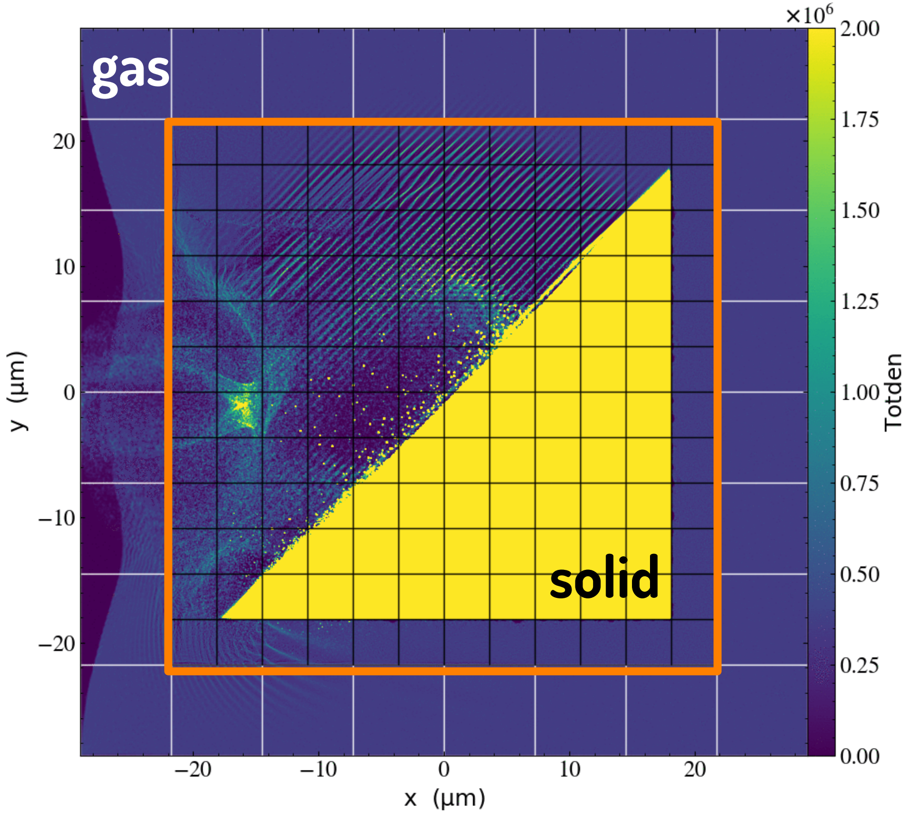
Electromagnetic waves have different dispersion relations in the two areas!
(spurious reflections, unphysical effects...)



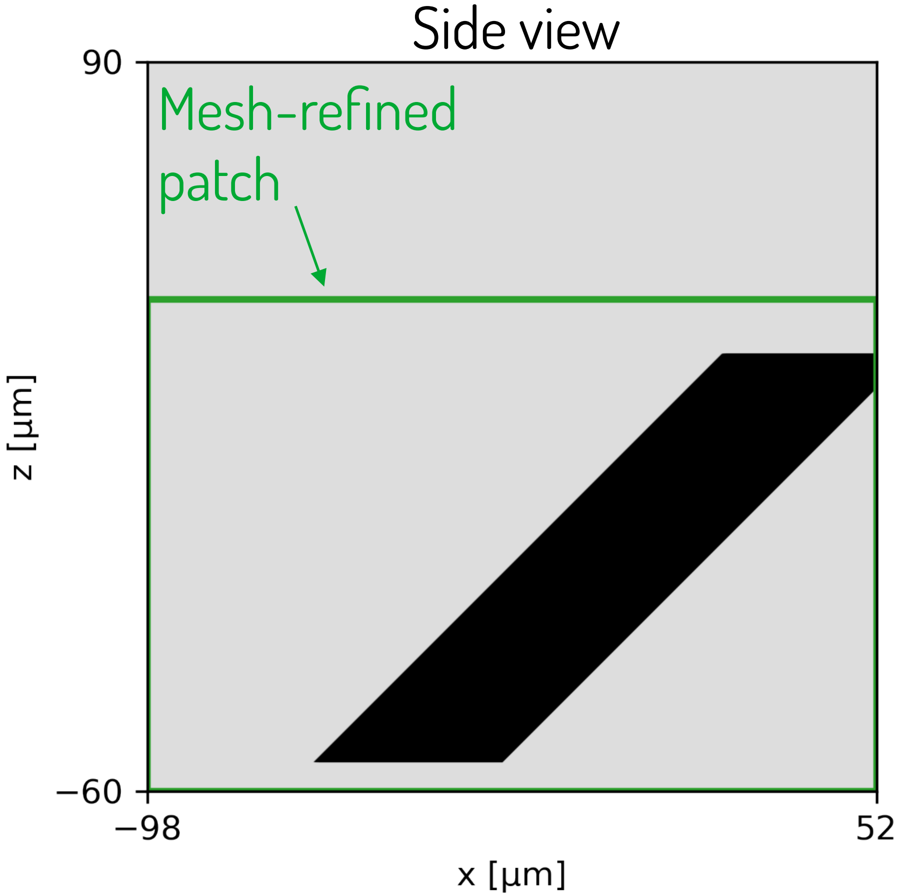


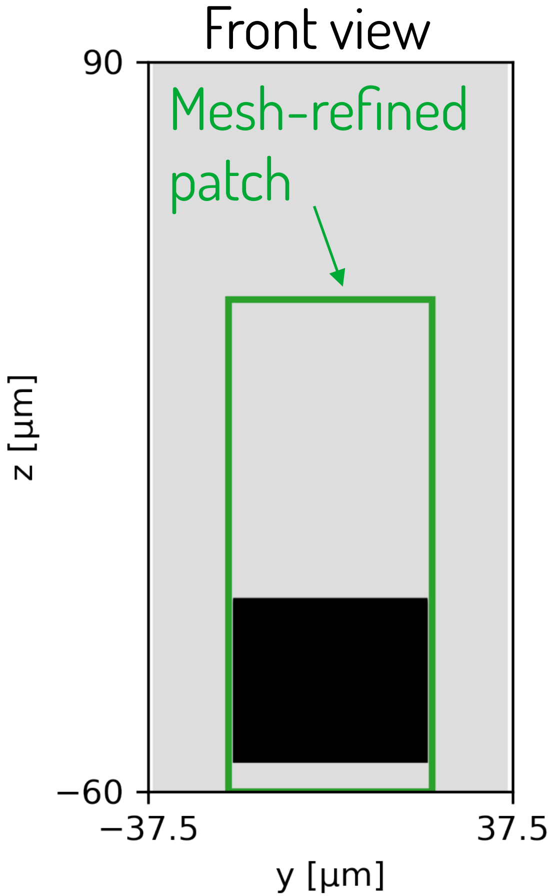
J.-L. Vay et al, Phys. Plasmas 11, 2928 (2004)
R. Lehe et al, Phys. Rev. E 106, 045306 (2022)

WarpX allows us to define a region with twice the resolution of the main grid



2D slices of our 3D simulations highlight the acceleration process





← 3D simulation on 4096 Summit nodes

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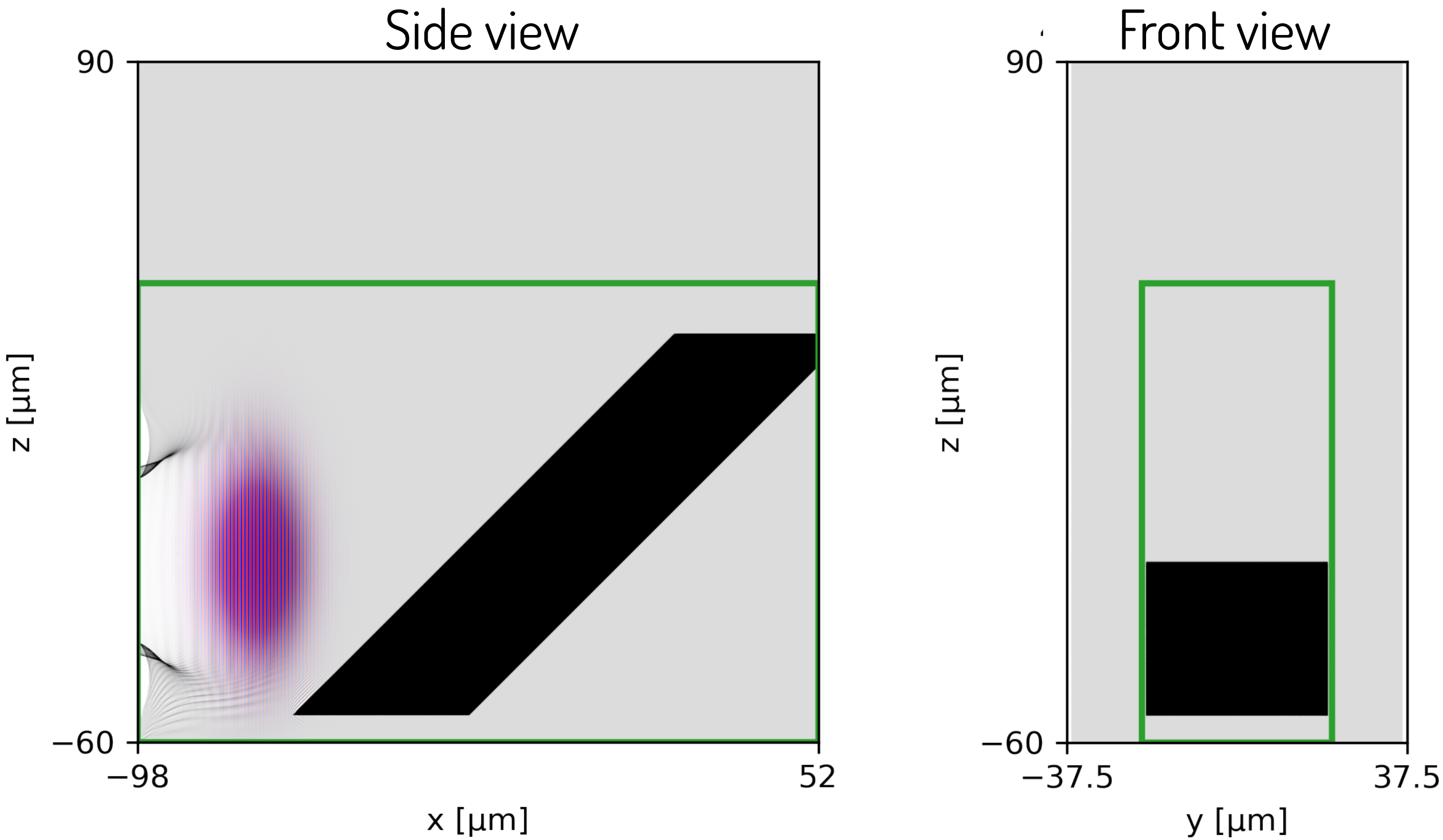

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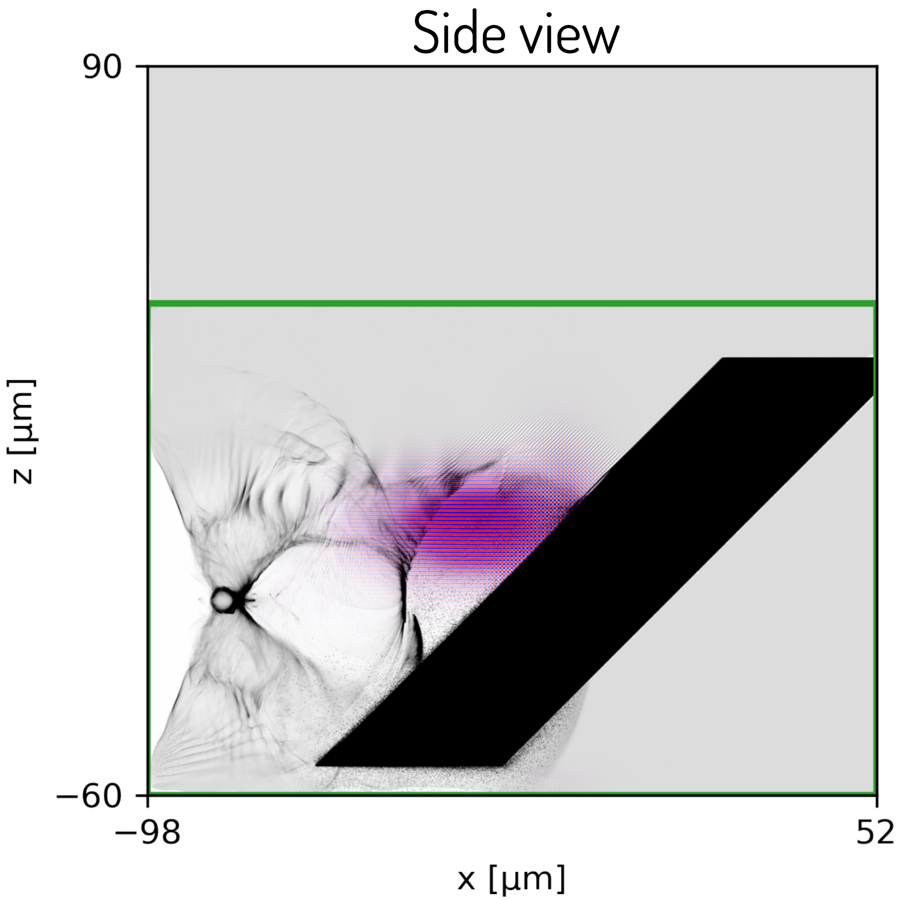

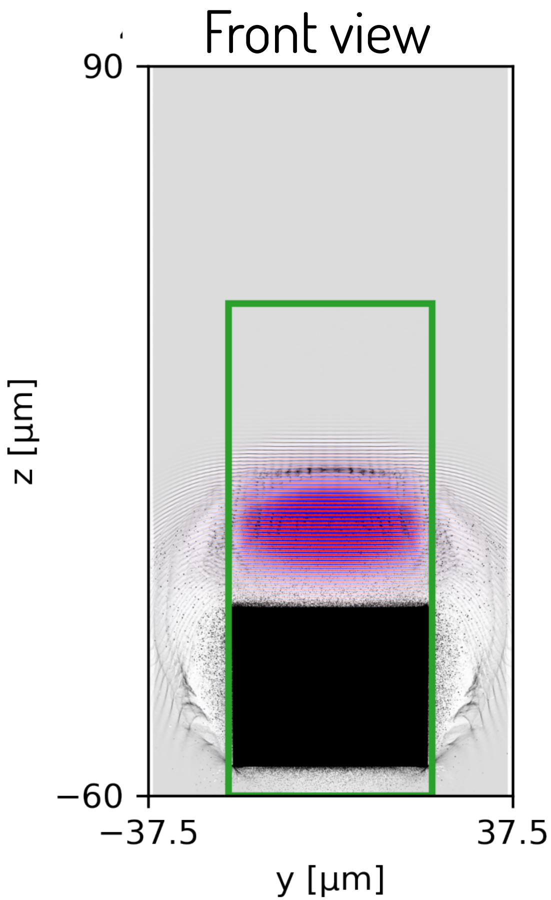

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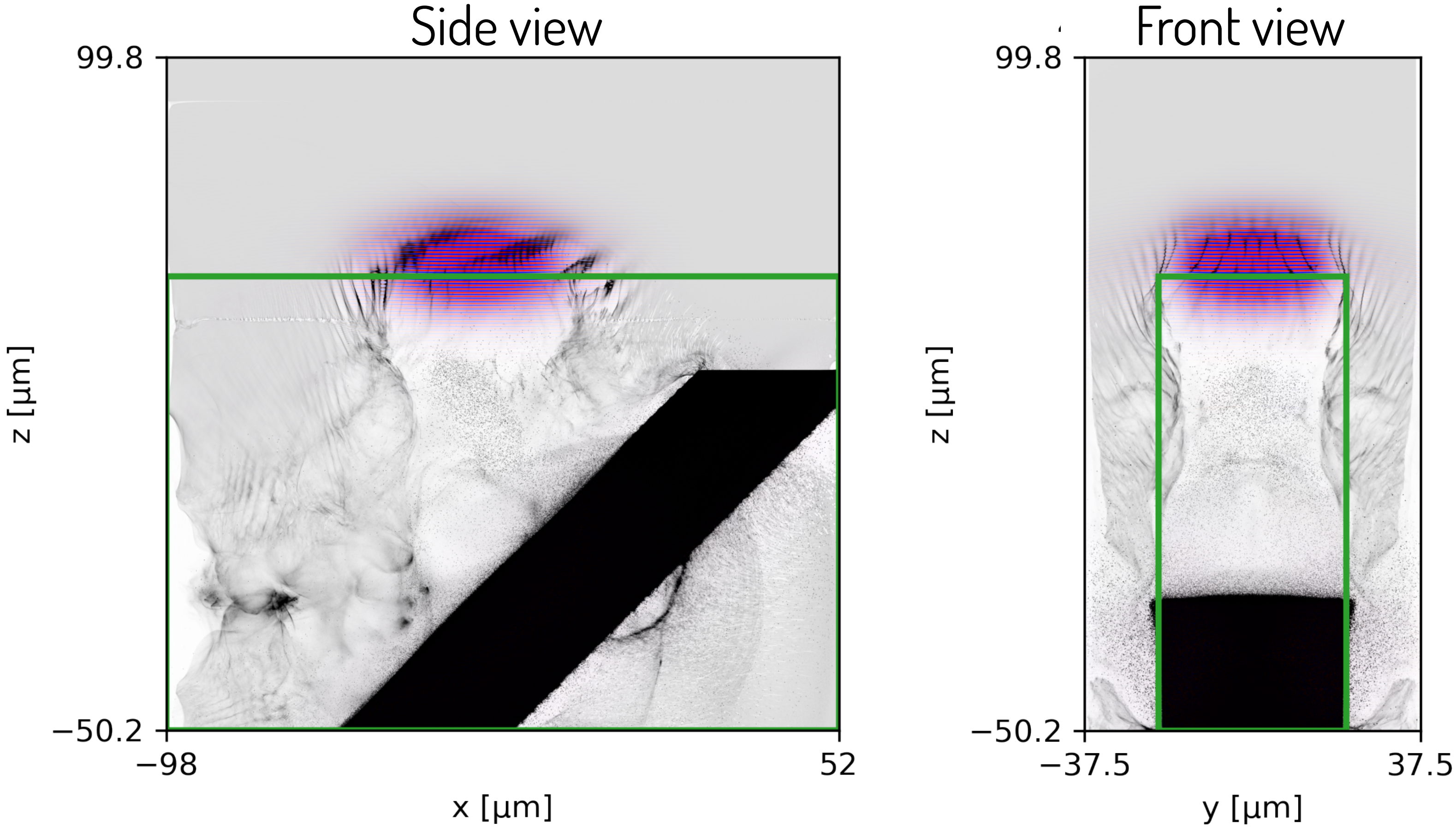
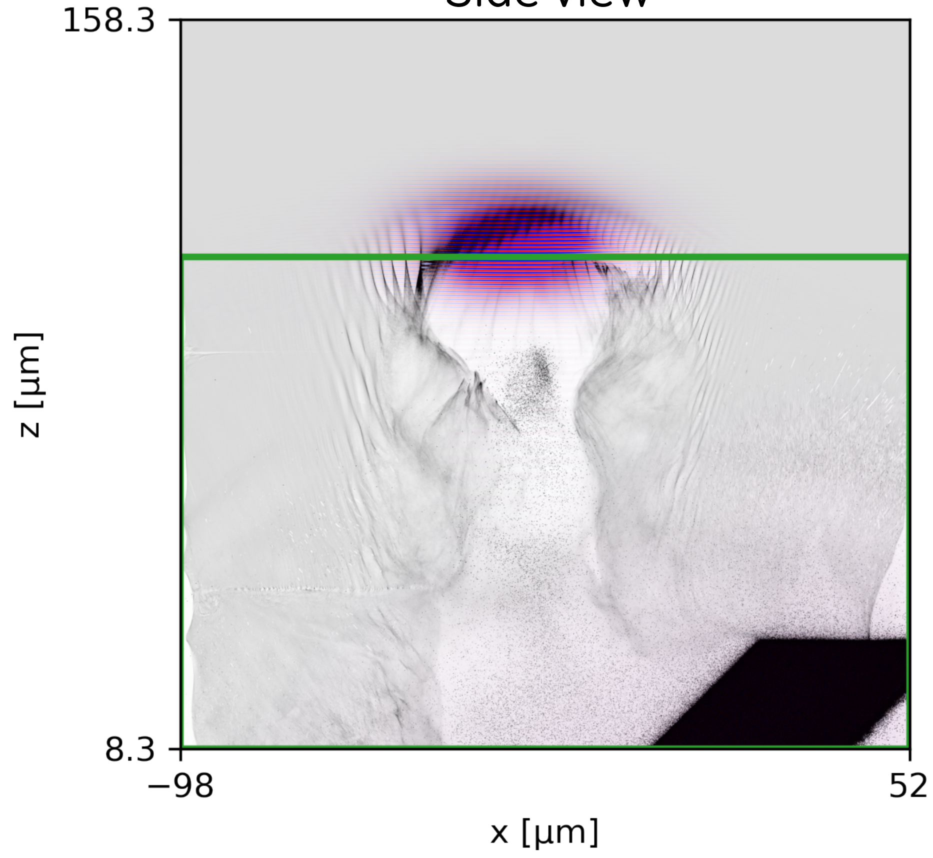


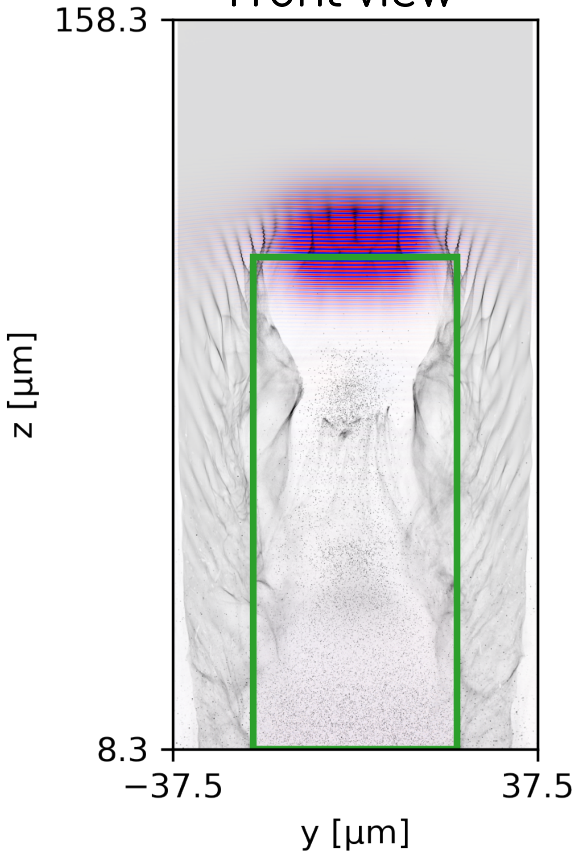
← 3D simulation on 4096 Summit nodes

2D slices of our 3D simulations highlight the acceleration process

Side view



Front view



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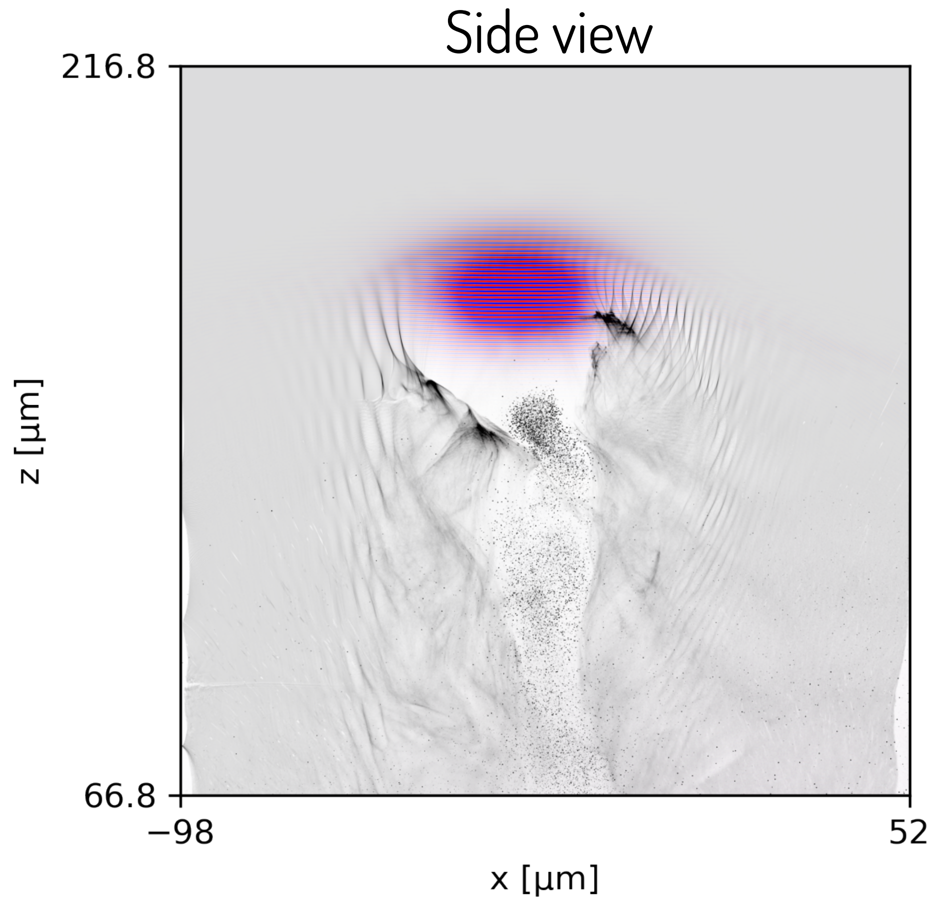

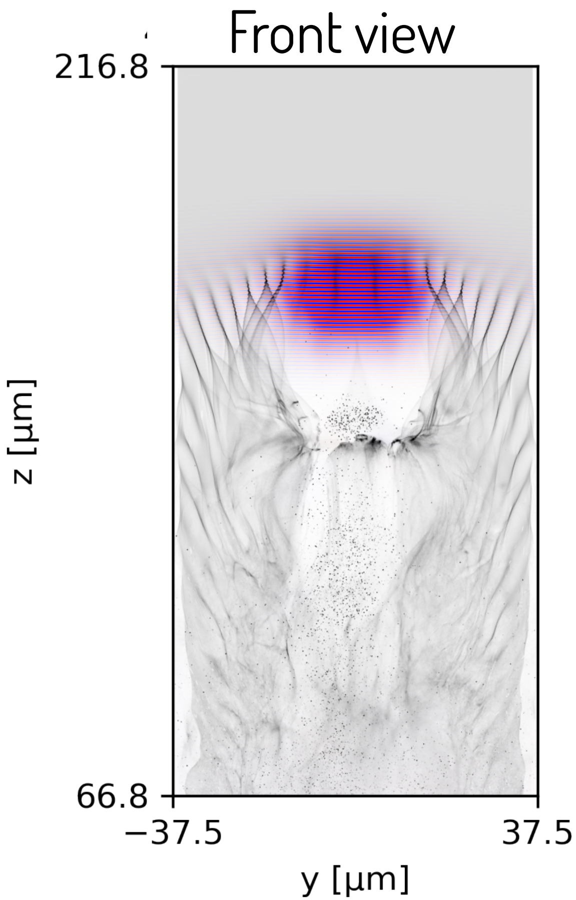

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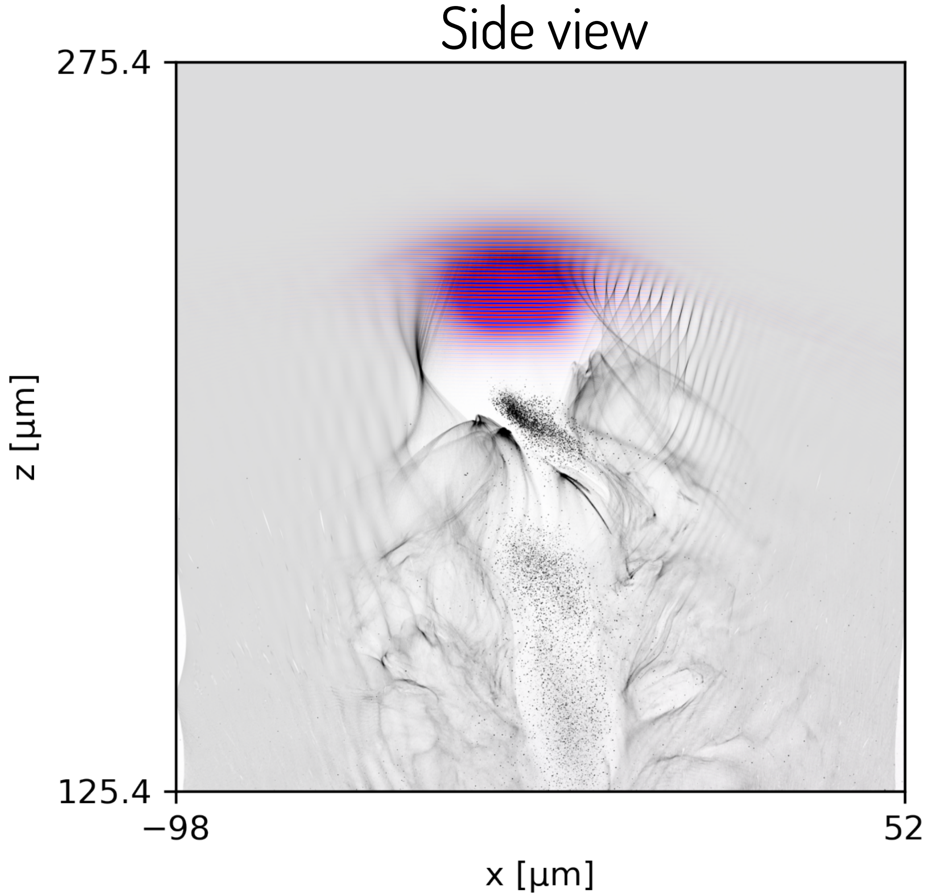

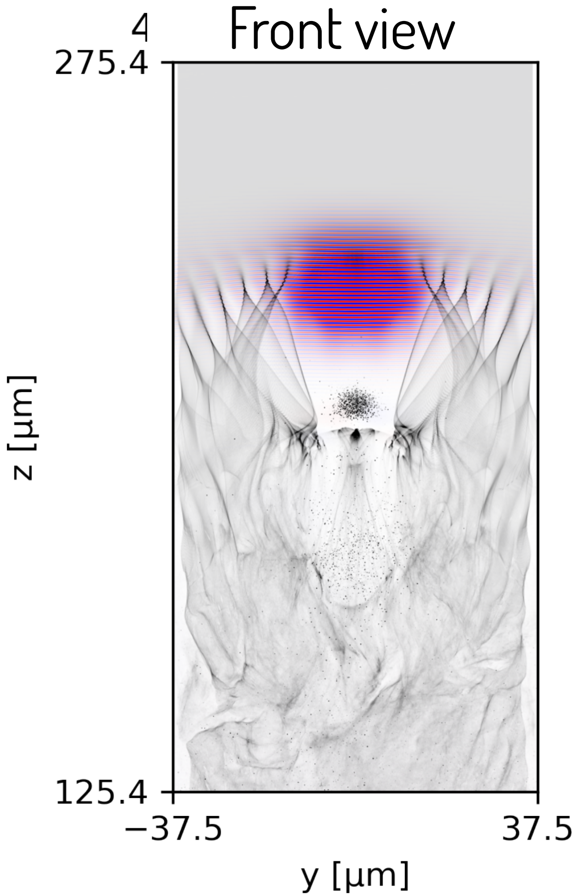

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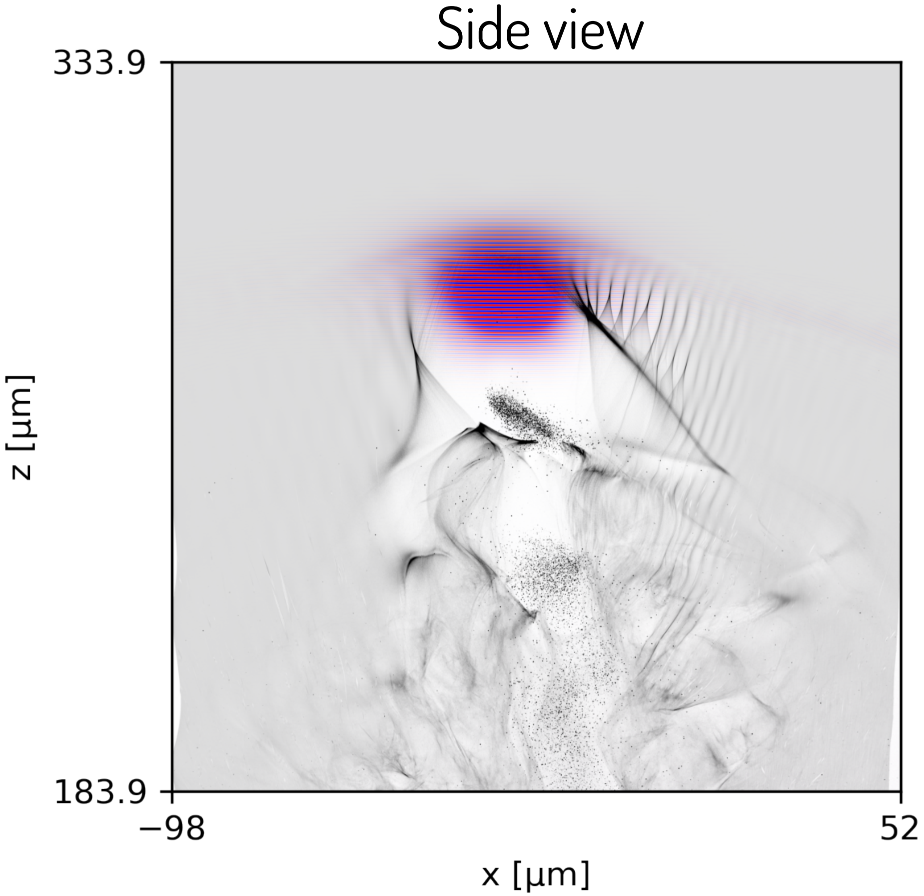

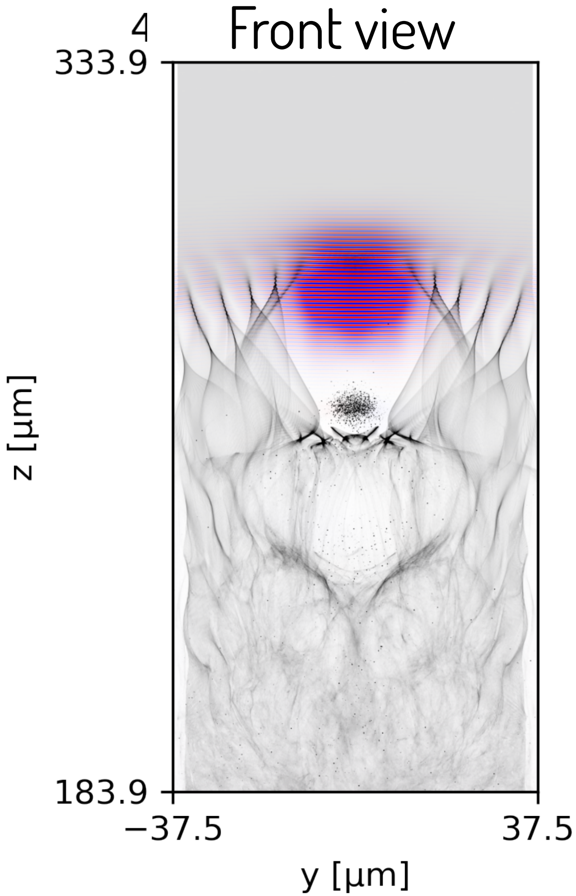

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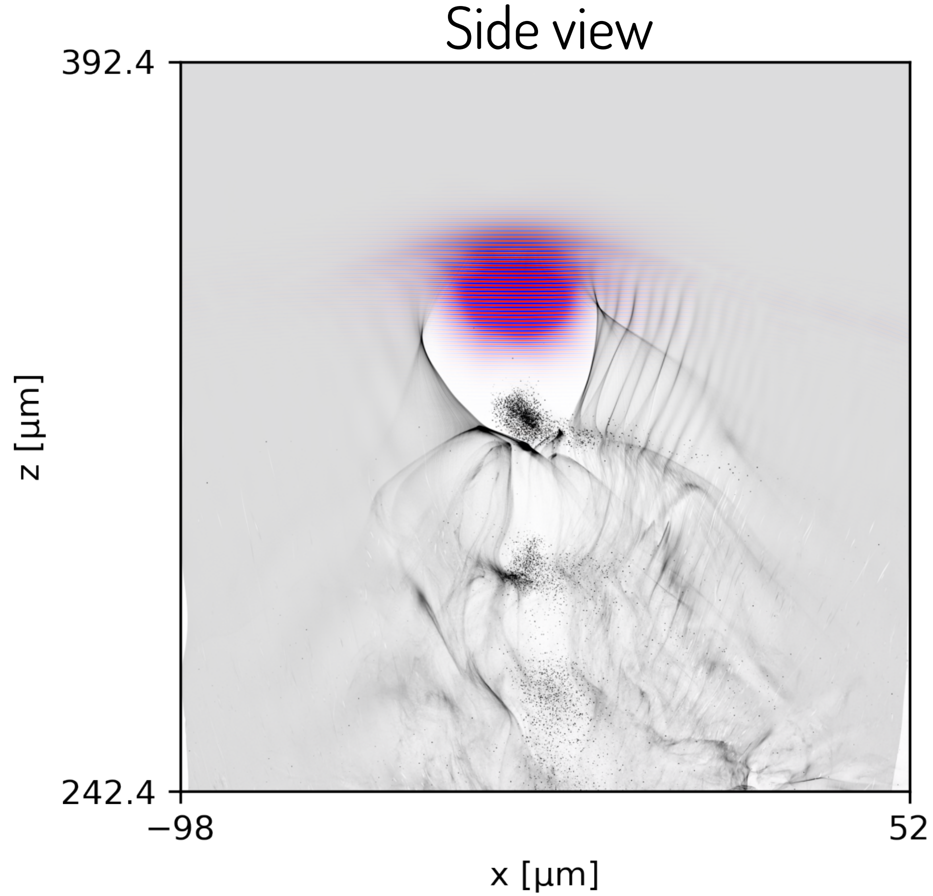

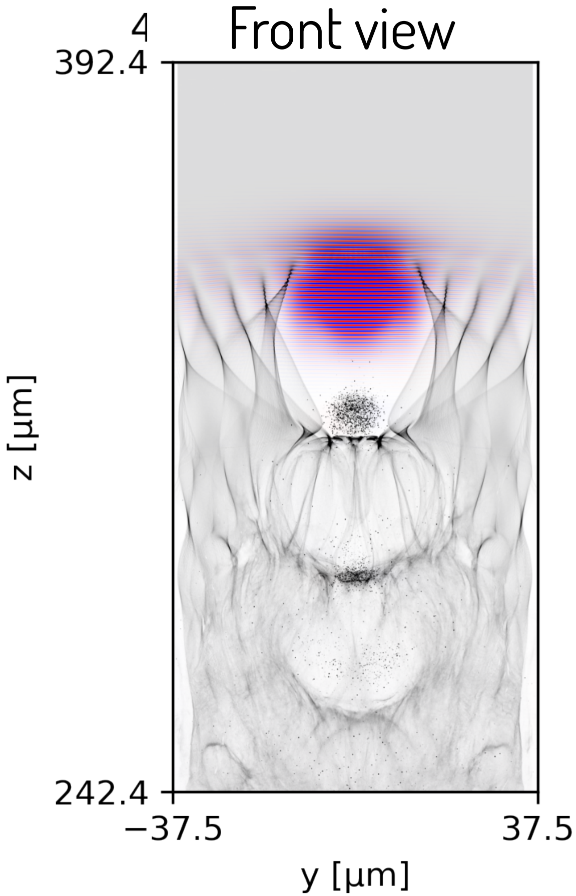

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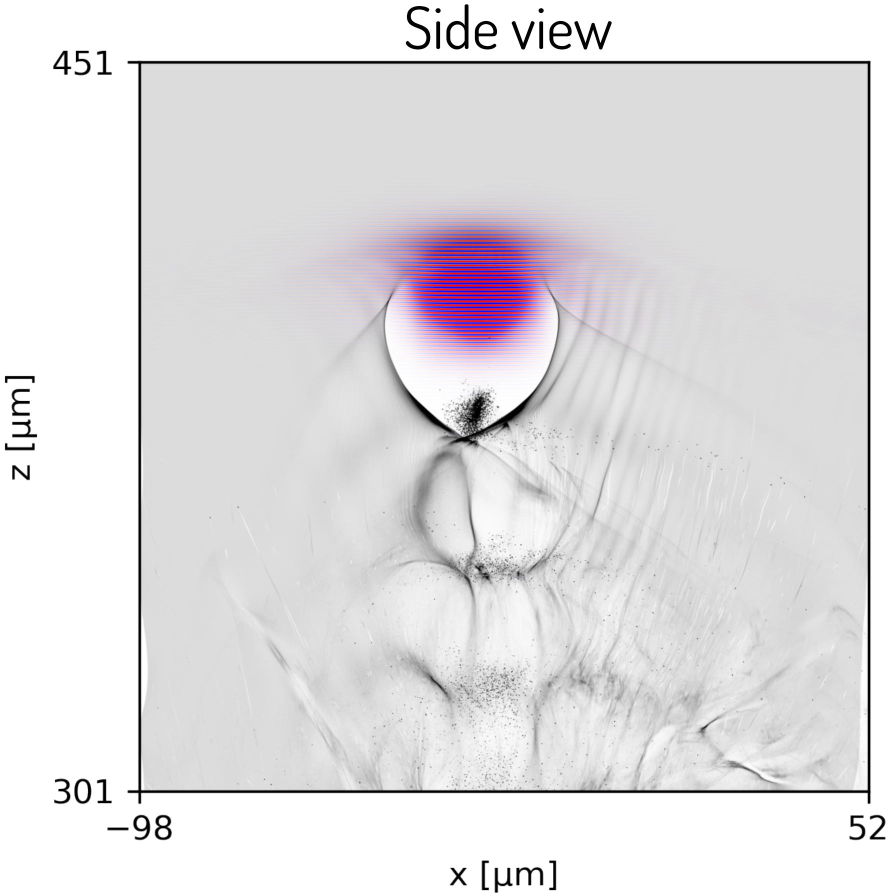

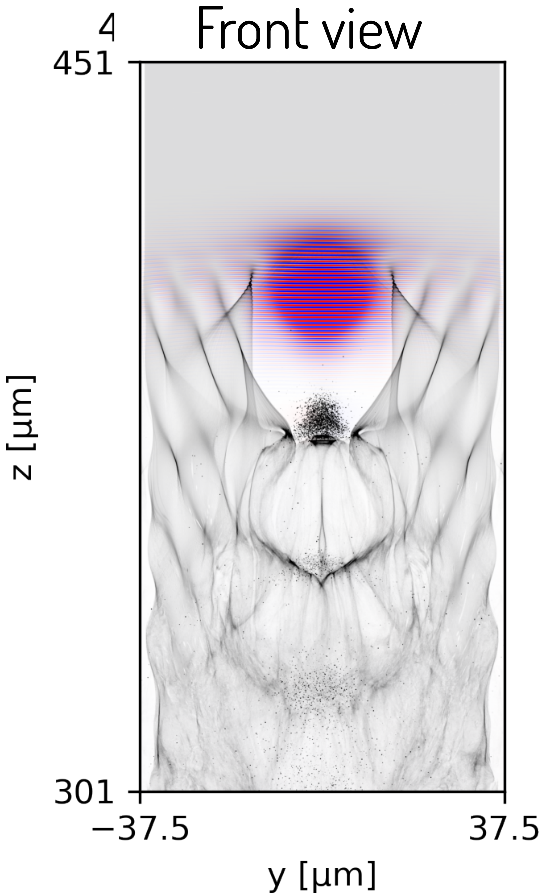

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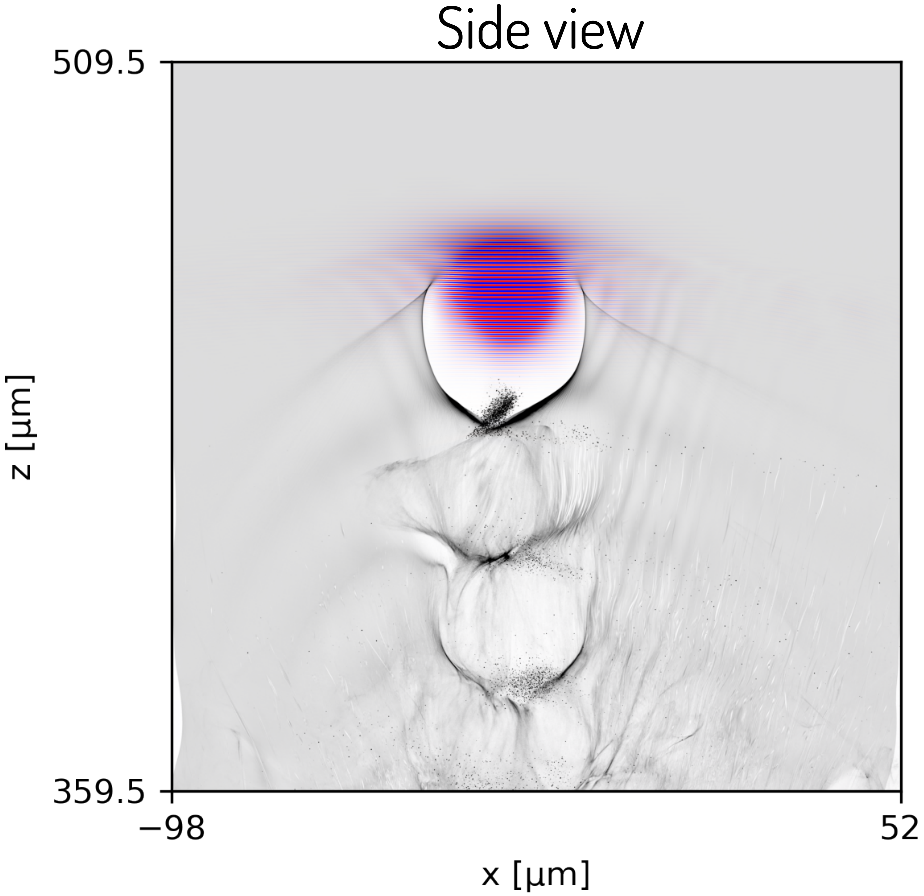

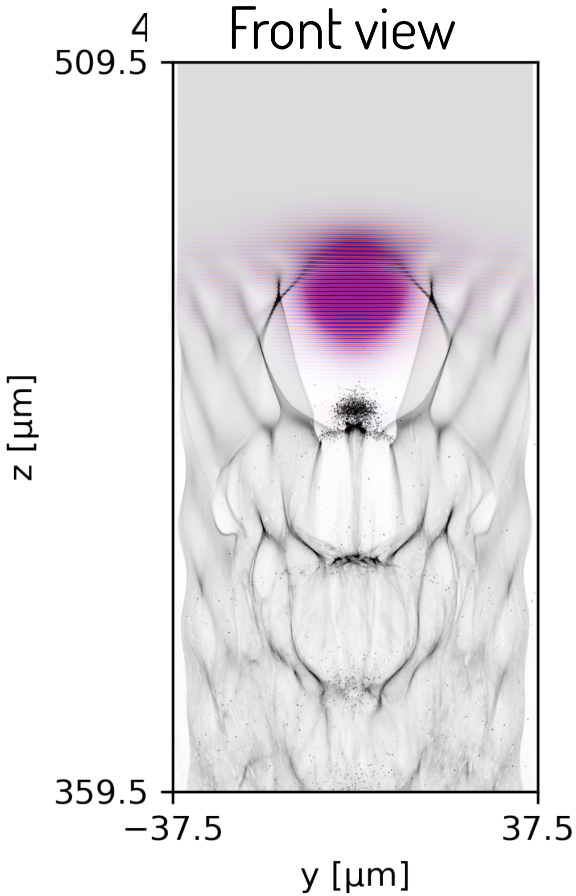

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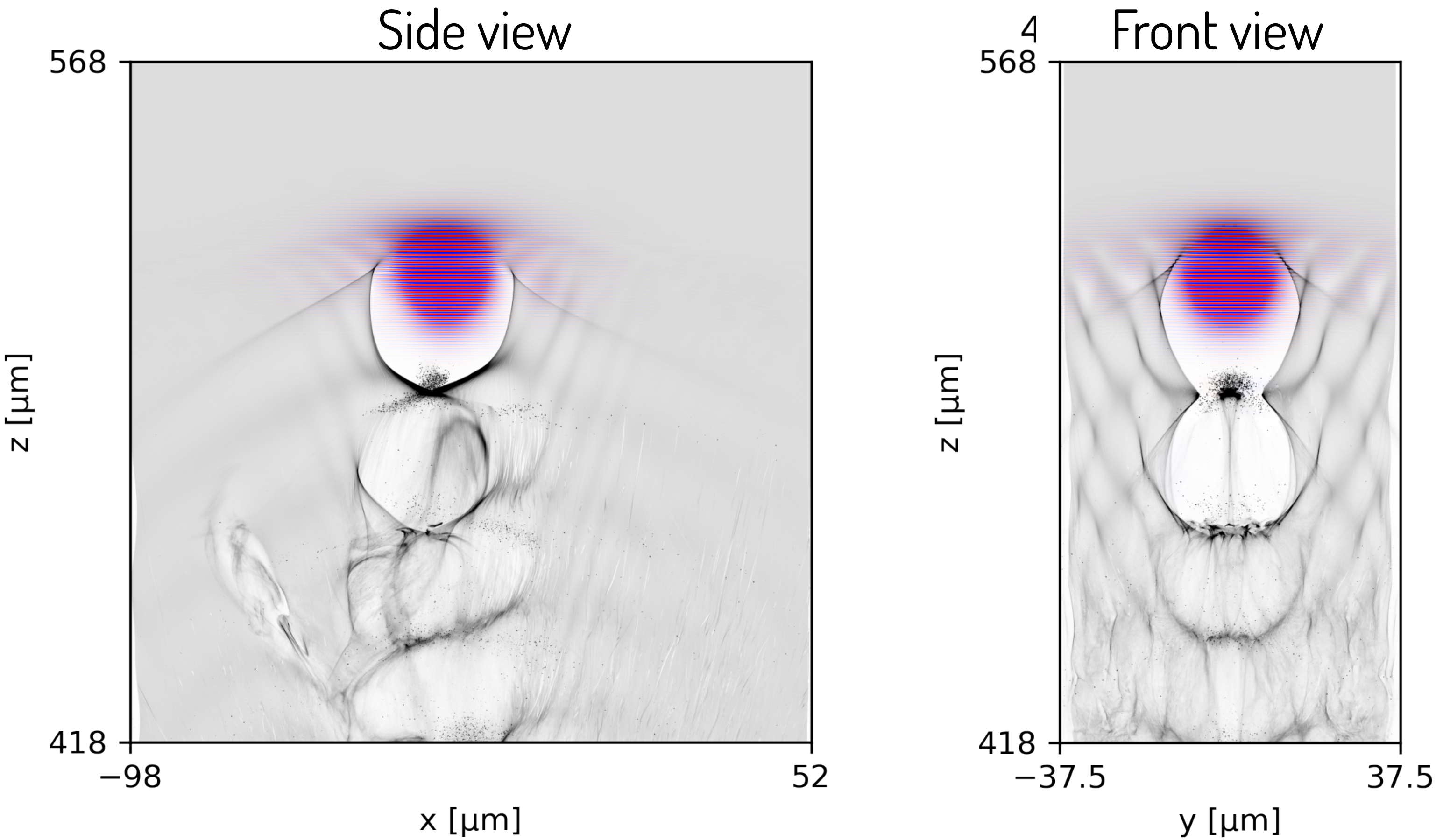

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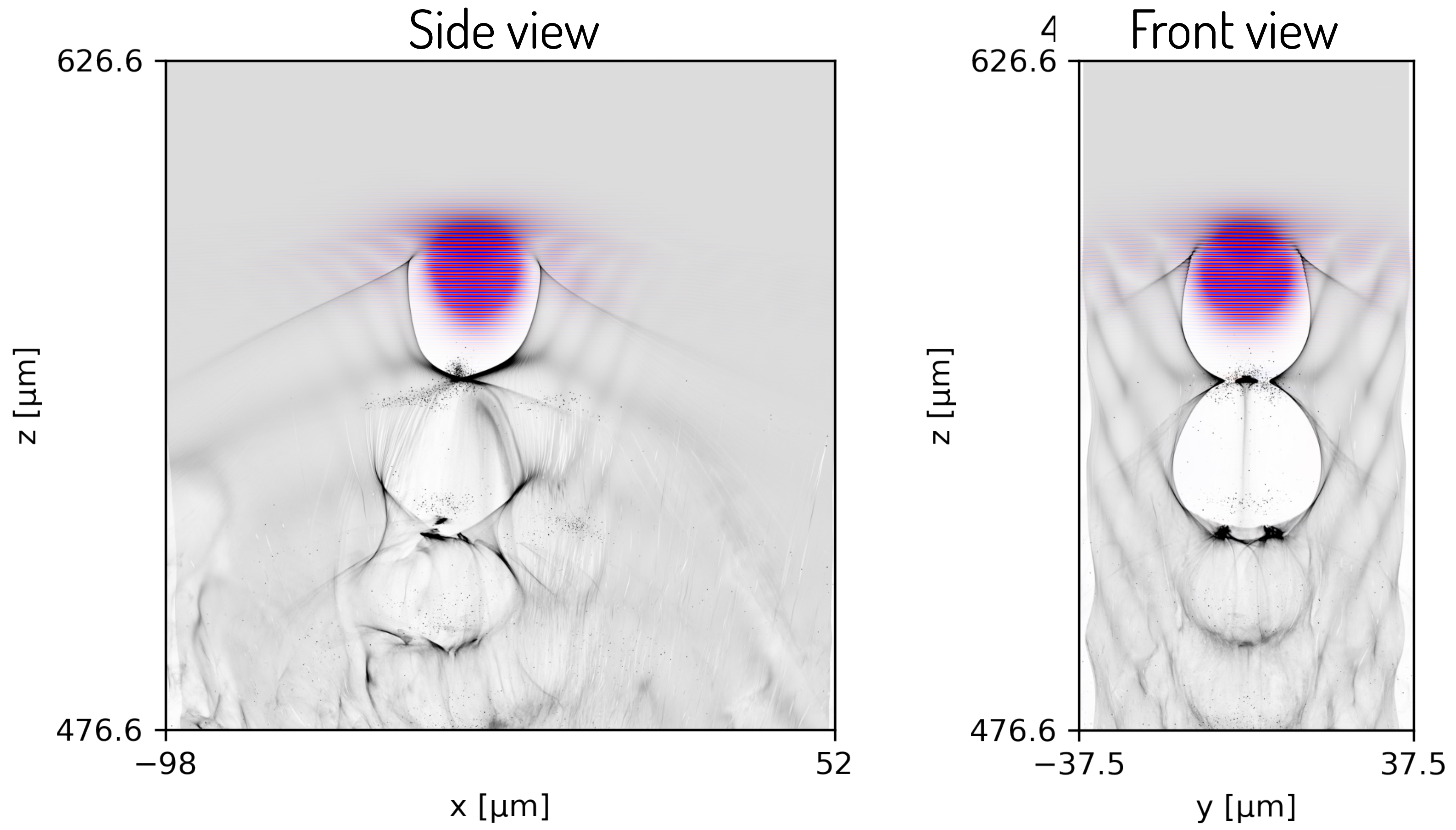

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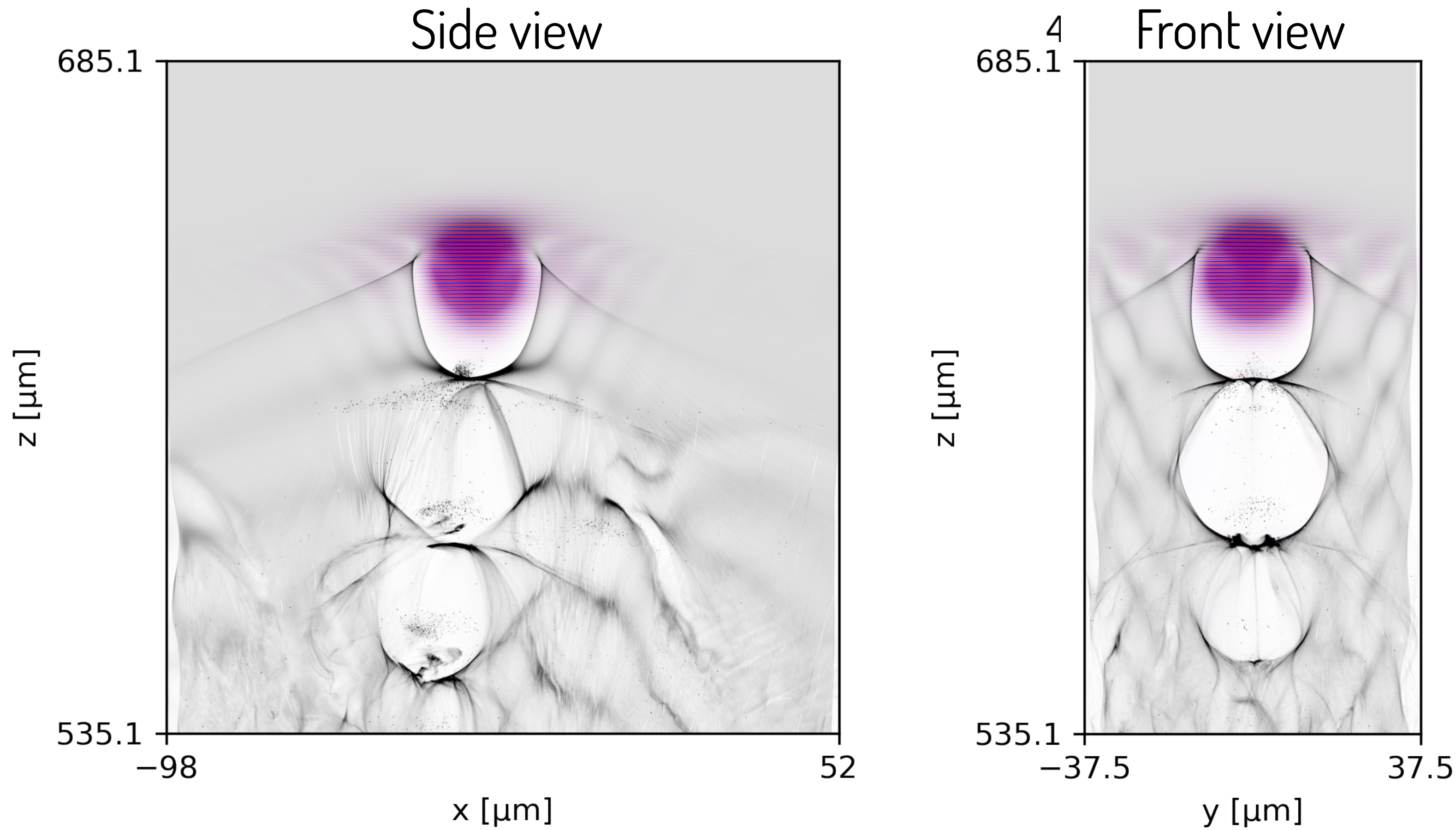

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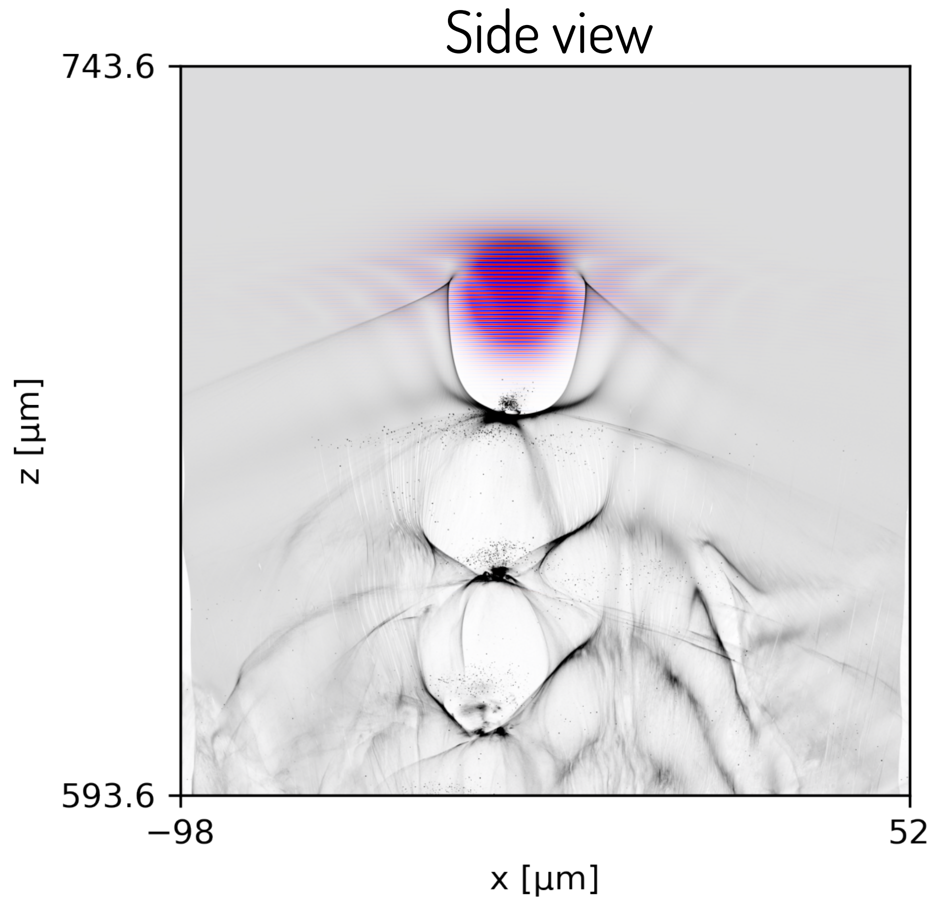

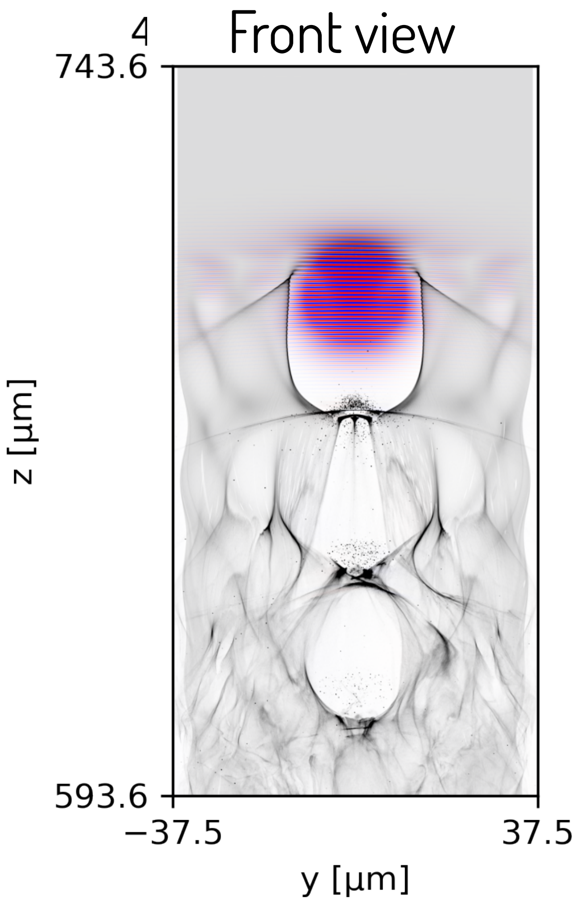

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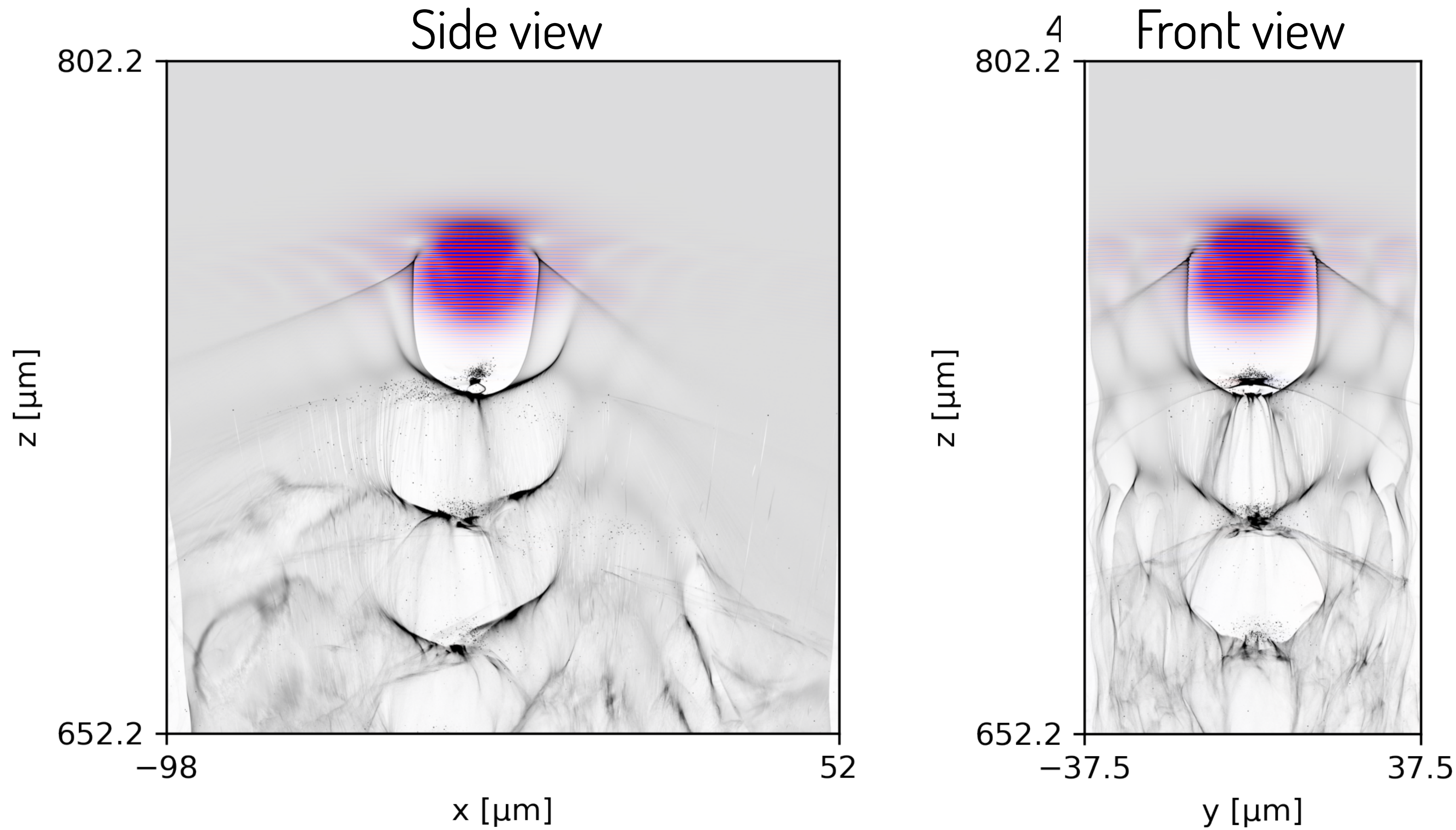

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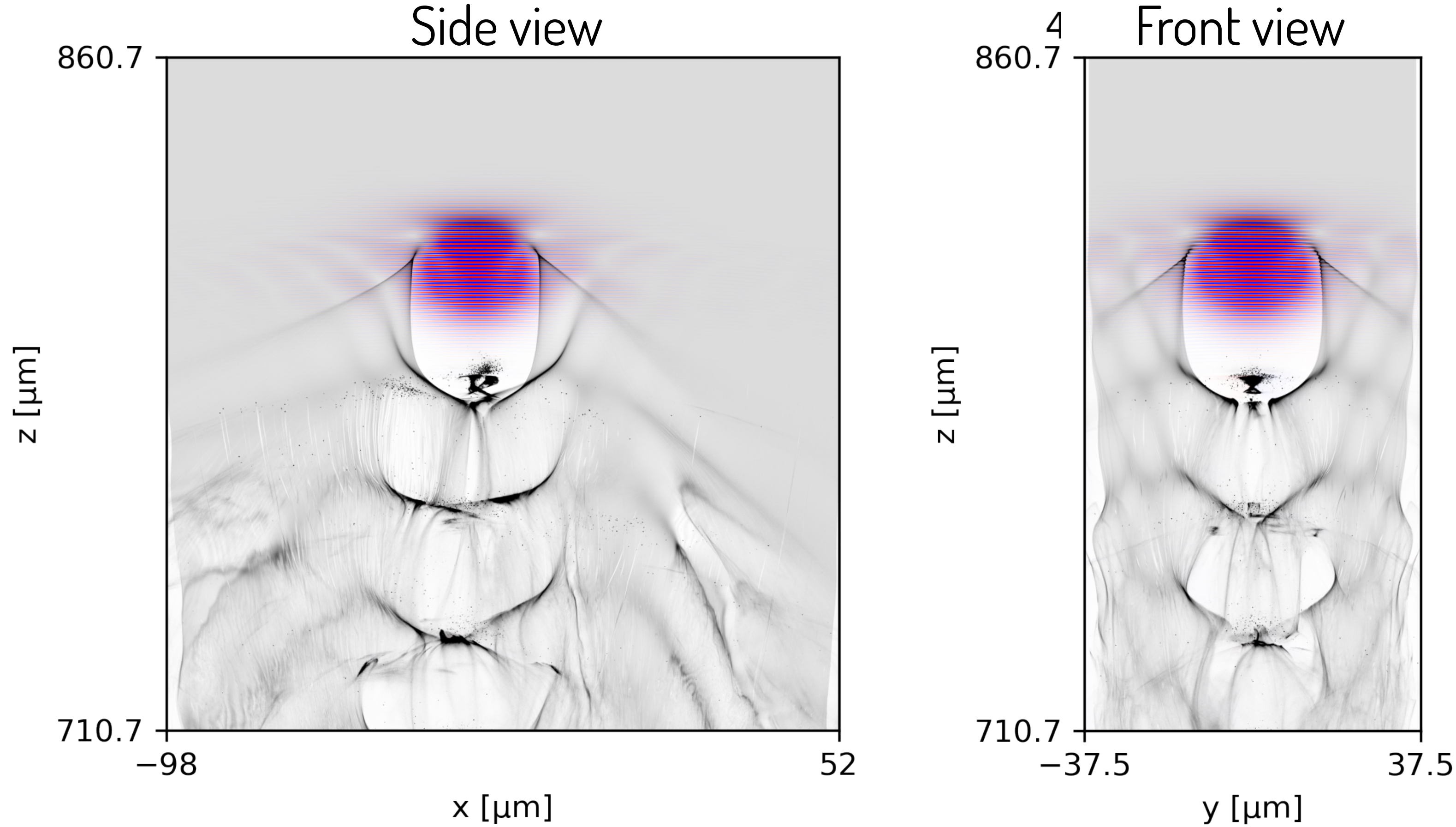

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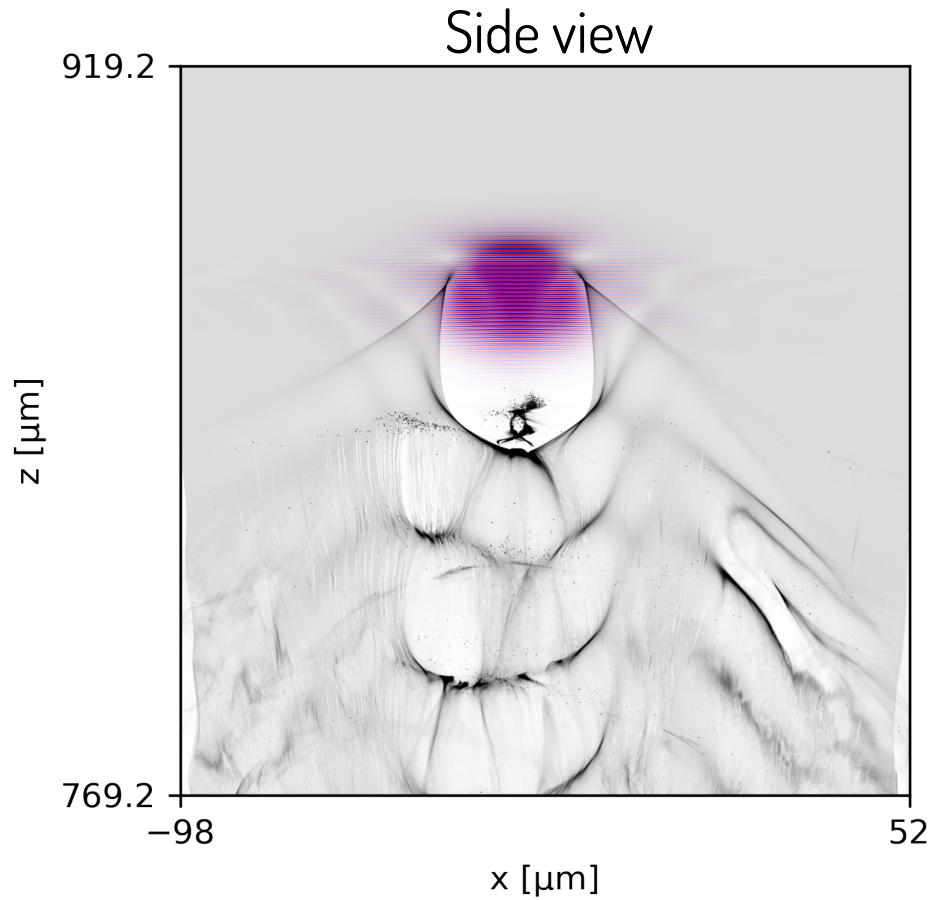

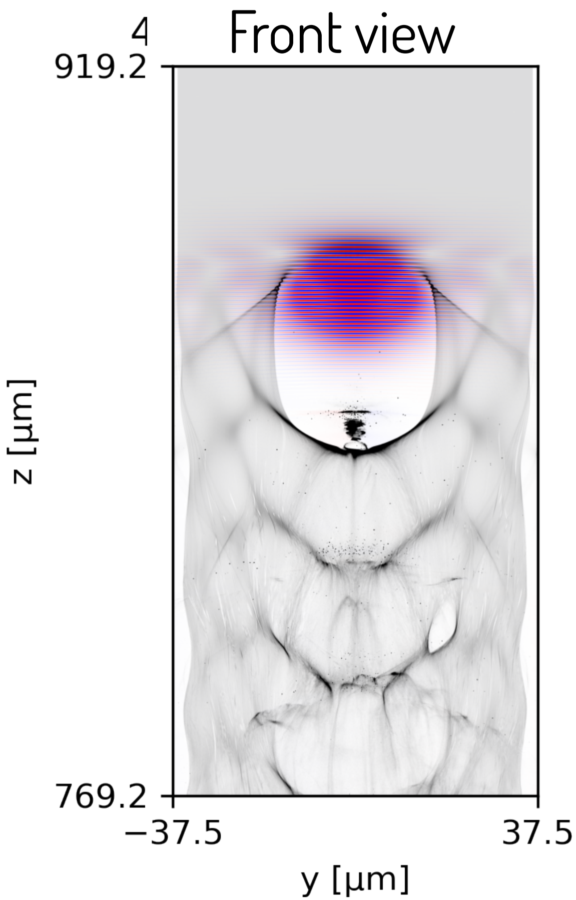

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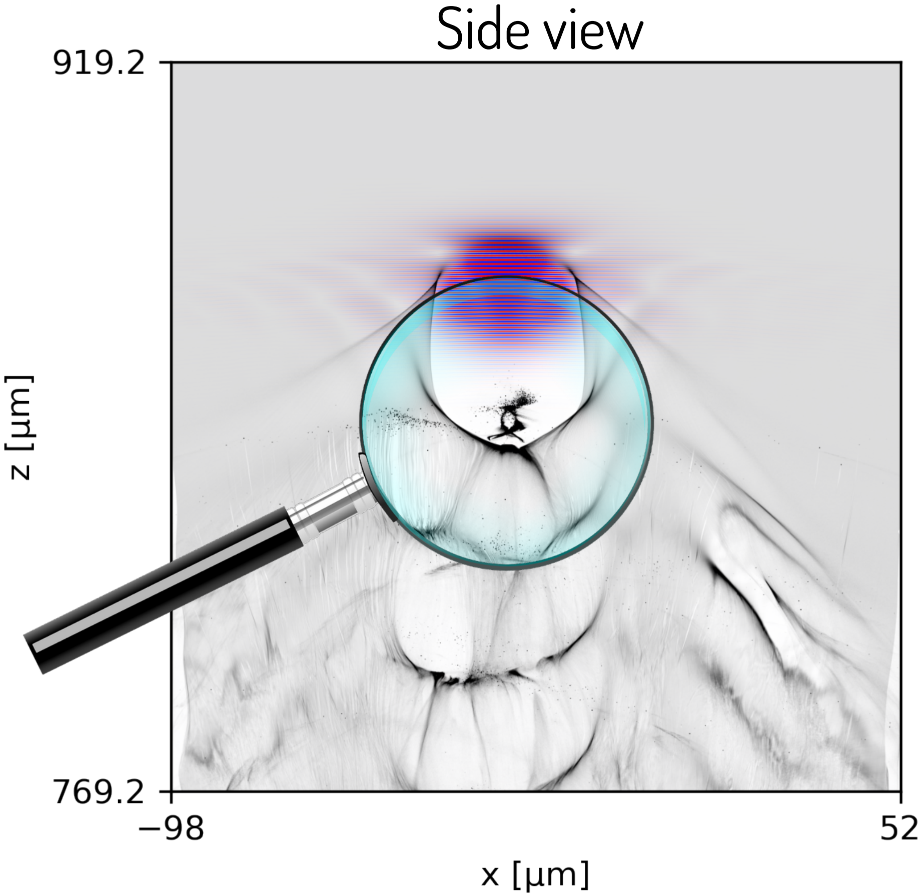
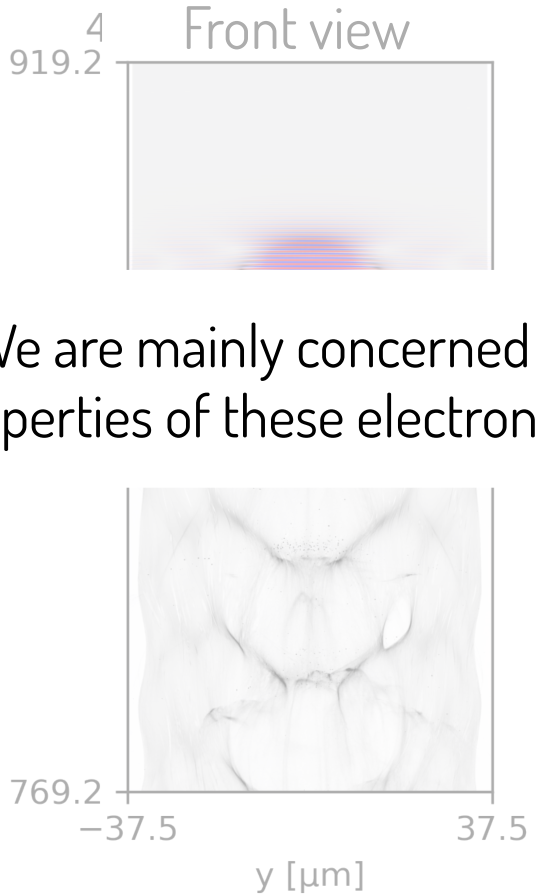
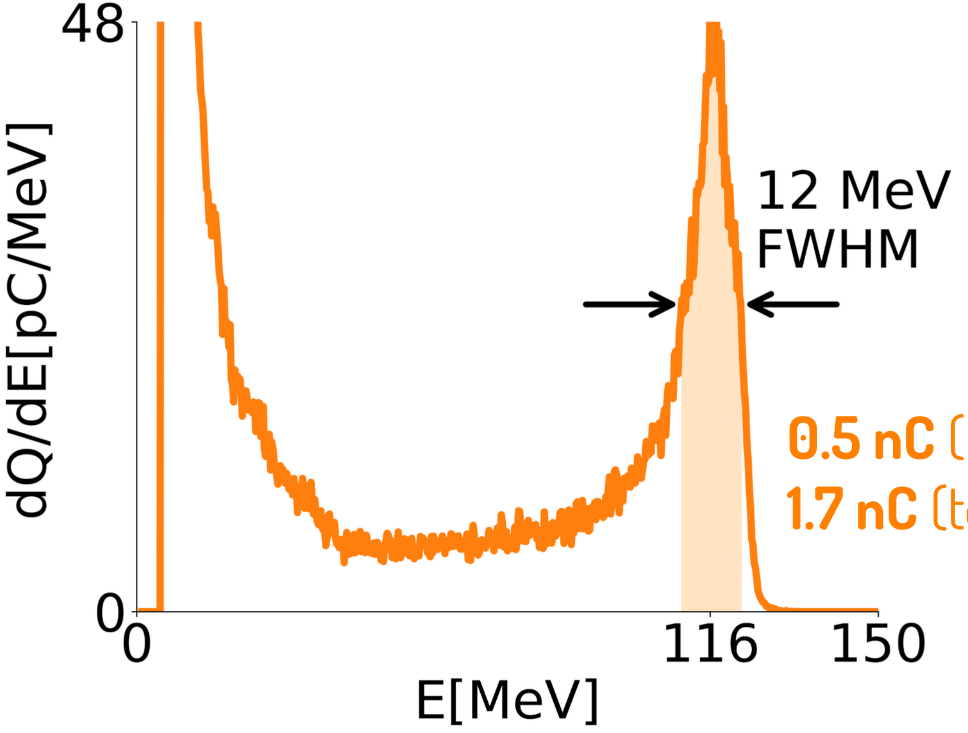




←We are mainly concerned with the properties of these electrons

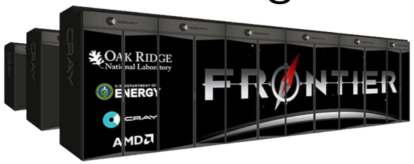
Our simulations with a PW-class laser show that we can accelerate a substantial amount of charge with high quality

After ~ 1mm
(acceleration still in progress)

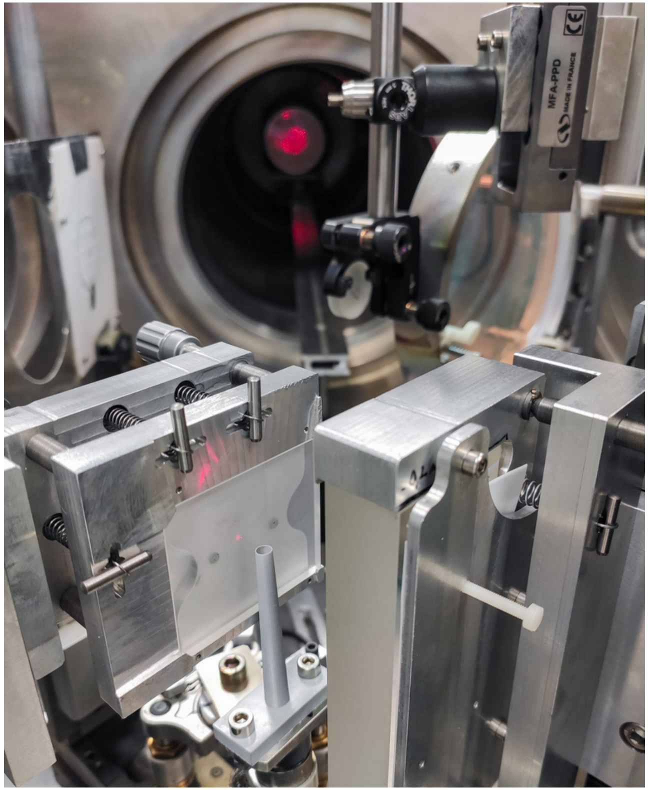


0.5 nC (peak)
1.7 nC (total)
for a **PW laser**

Production runs on
Frontier, Fugaku and Summit



Exascale simulations informed the design of the first experimental validation of our concept (at LOA, France)



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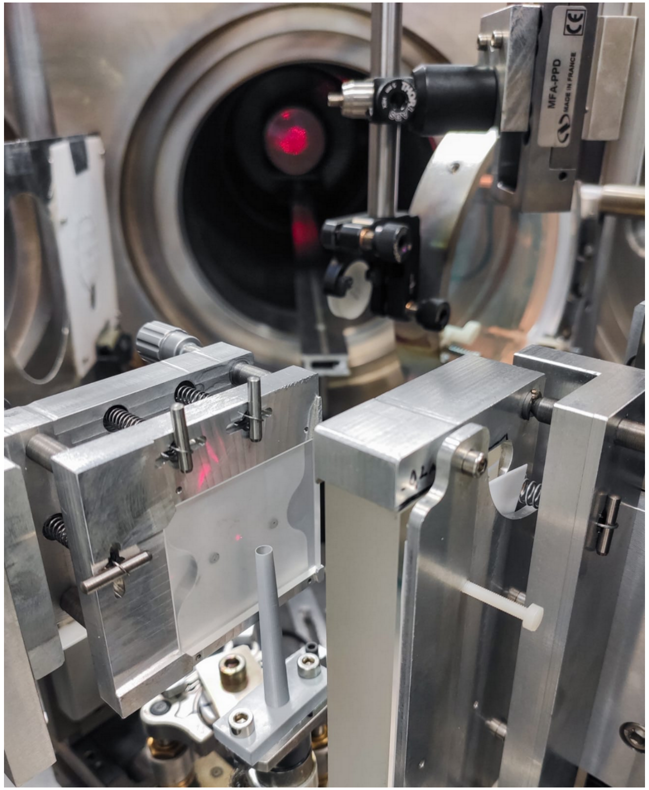
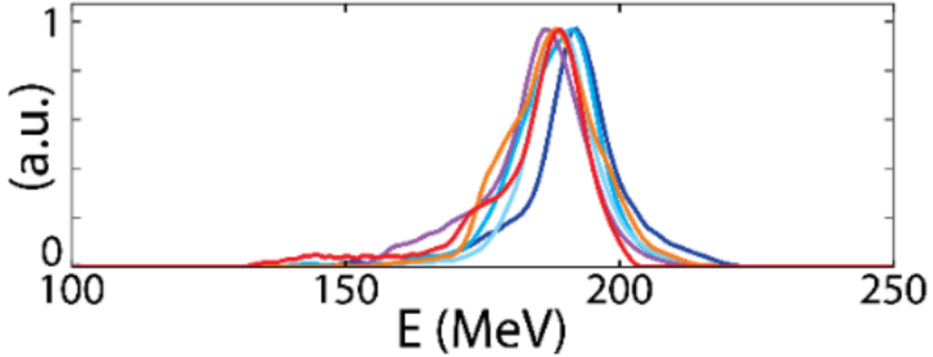


Electron energy spectrum



Laser parameters

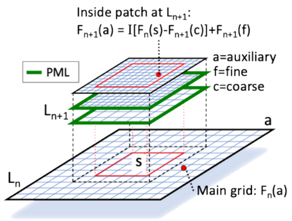
E = 400 mJ
waist = 15 µm
P_{peak} = 10 TW

Results

Q= 17 pC (at least)
dE/E_{peak} = 8%

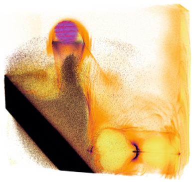
4X increase of accelerated charge with respect to conventional techniques for the same laser energy!

Conclusions and perspectives



- WarpX is a state-of-the-art open-source Particle-In-Cell code implementing sophisticated numerical algorithms

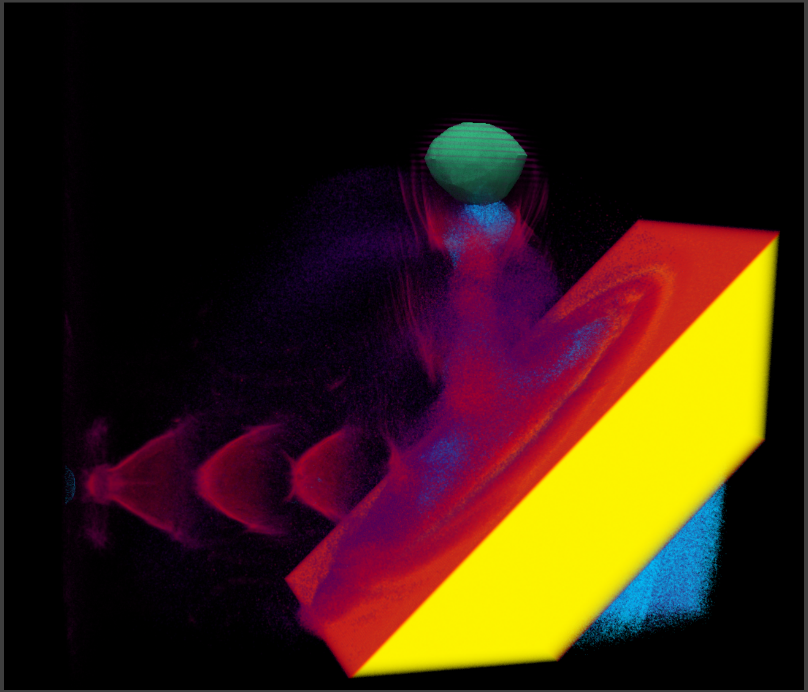
- WarpX is portable across different architectures and scales well on top machines, including the first exascale supercomputer



- WarpX allows us to simulate novel electron acceleration strategies that could find application for e.g. FLASH radiobiology experiments

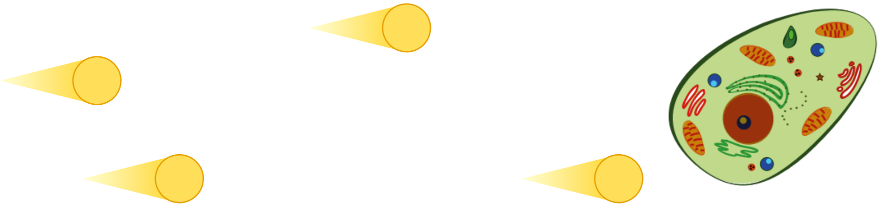
Modeling a novel laser-driven electron accelerator concept: Particle-In-Cell simulations at the exascale.

Luca Fedeli, Axel Huebl, France Boillod-Cerneux, Thomas Clark, Kevin Gott, Conrad Hillairet, Stephan Jaure, Adrien Leblanc, Rémi Lehe, Andrew Myers, Christelle Piechurski, Mitsuhisa Sato, Neïl Zaim, Weiqun Zhang, Jean-Luc Vay, Henri Vincenti

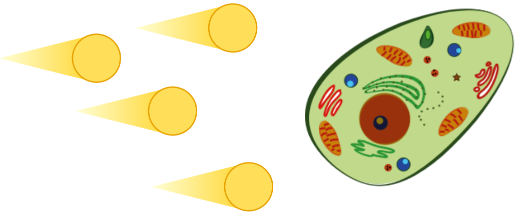


The End

FLASH effect : cells react differently to irradiation if it is administered very fast



$\neq$

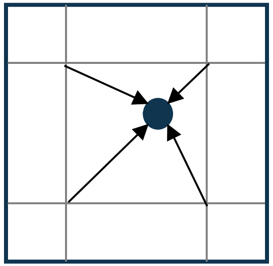


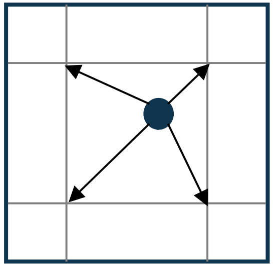
promising for **cancer treatment** , but still not well understood

Favaudon et al, Science. Trans. Med., 2014
Bourhis et al, Radiotherapy and Oncology, 2019

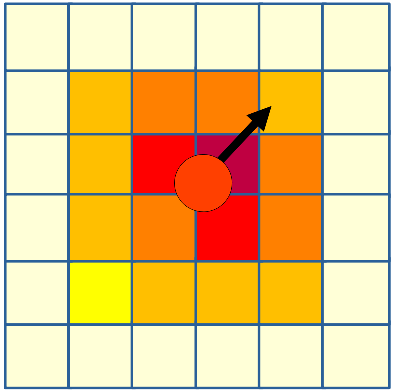
With the help of Atos

we optimized the most expensive kernels for A64FX (single precision only)





Current deposition and field gather require to sample a lot of points per particle



Particles have a shape function

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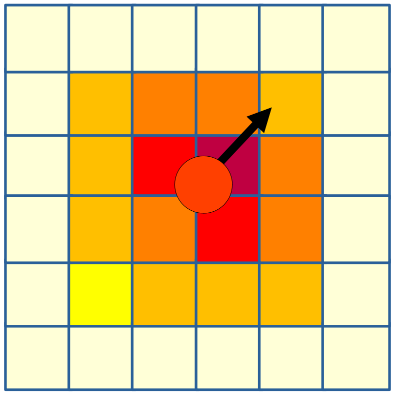

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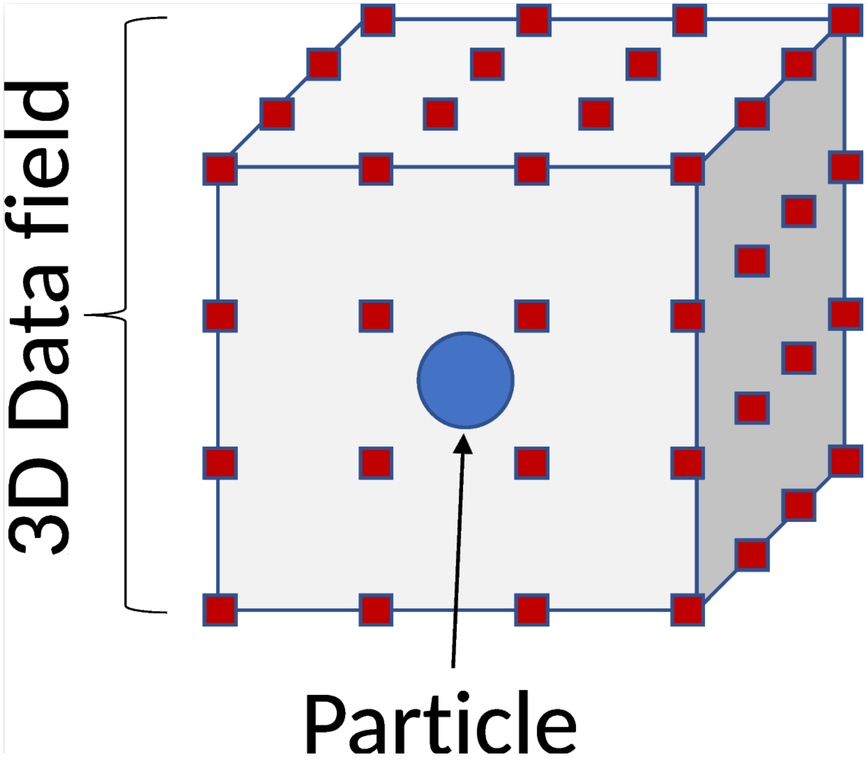
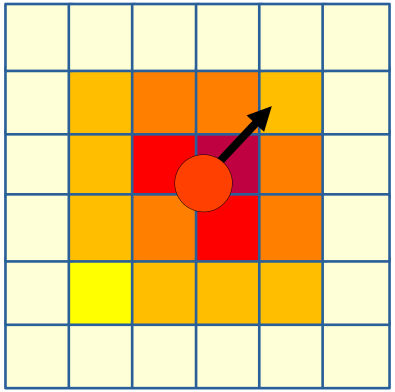


64 points per particle!

Vectorization is key to achieve good performances



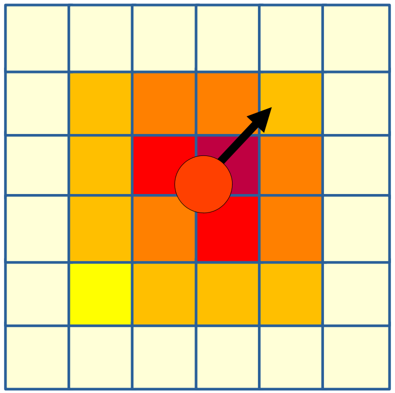
```
for p : particle
{
  for i : x_indices
    for j : y_indices
      for k : z_indices
      {
        compute n_ijk
      }

}
```

Very small loops (4x4x4)

→ Inefficient vectorization

Vectorization is key to achieve good performances



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Very small loops (4x4x4)

→ **Inefficient vectorization**

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```

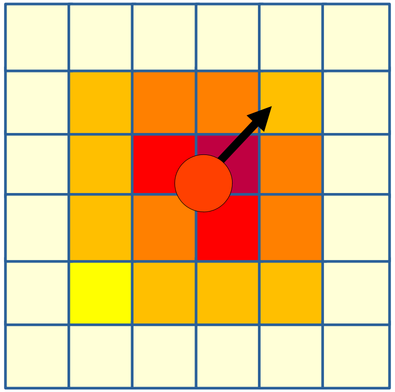
Longer inner loop

→ **Efficient vectorization**

→ **Data reorganization**

Vectorization is key to achieve good performances

* Particles are grouped (N = 32-128) to keep data in CPU cache.



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```
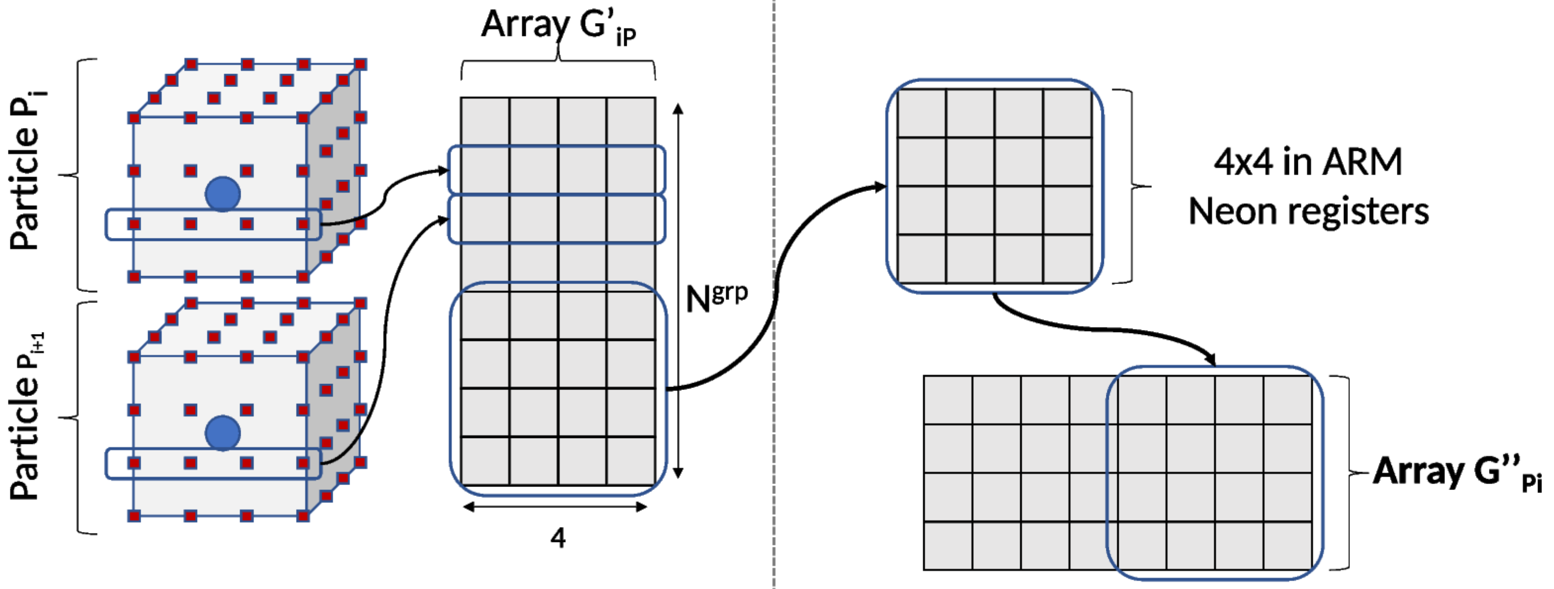

Longer inner loop

→ **Efficient vectorization**

→ **Data reorganization**

Data re-organization makes heavy use of NEON intrinsics



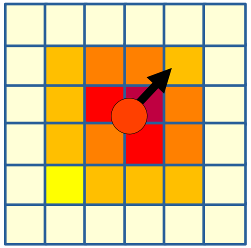
For each j,k:

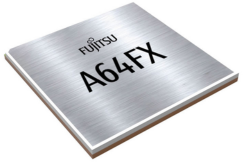
For each particle in batch:

Gather 4 contiguous sampling points using ARM Neon intrisinc

Transpose array **4xN^{grp} ⇒ N^{grp}x4** using ARM Neon intrisincs

Optimized field gather and current deposition lead to very significant speed-ups!





Routine	Speed up
Gather	2.63X
Deposition	4.60X

fipp profiling (whole code):

SIMD inst. rate: 2.2% → 27 %

SVE operation rate: 3.6% → 70 %