Large Scale Fully Kinetic 3D PIC Simulation for the Awake Collaboration

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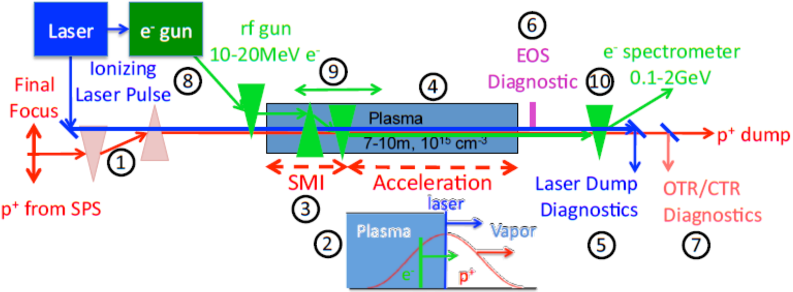
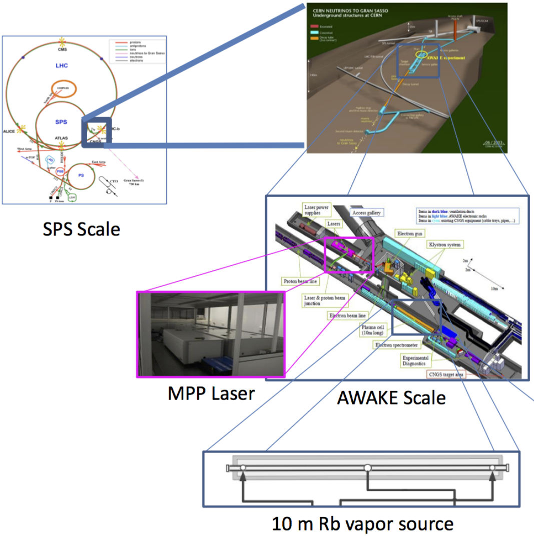
CCP2016, Johannesburg, July 13, 2016

What is AWAKE?

- AWAKE stands for Advanced WAKefield Experiment (advanced accelerator concept)
- 400 GeV SPS proton beam drives wakefields in a 10 meter plasma through a self modulation instability
- According to simulations the wakefields can can accelerate electrons from 16 MeV to 2 GeV
- Using the easier to perform hadron acceleration to perform lepton acceleration



AWAKE at CERN

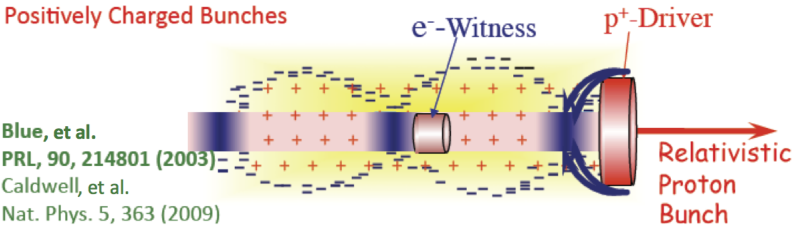


Diagnostics:

- OTR/CTR proton beam diagnostics
- Electron Spectrometer

Quick Overview of Plasma Wakefield Acceleration

- Fields from a charged particle beam or a laser drive wakefields inside the plasma
- Witness beam can be trapped within wakefield's accelerating and focusing phase
- Achievable accelerating gradient: $E_{\mathrm{z,linear}} \approx \mu \frac{N}{\sigma_z^2}$



The 3 "D's" of PWFA vs SPS ion beam

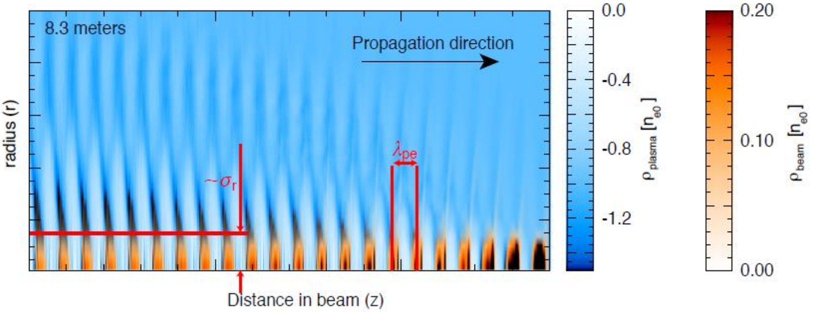
- Diffraction (Increase of the transverse size of the driver)
  $\Leftrightarrow$ SPS beam has a long beta function
- Dephasing (Dephasing of the wakefield with respect to the witness beam)
  $\Leftrightarrow$SPS beam has a very high γ
- Depletion (Driver energy gets depleted)
  $\Leftrightarrow$SPS beam has a very high energy content

Problem:

Very hard to make the driver short enough to resonantly drive the plasma

Solution: Self-Modulation Instability

- Transverse Modulation of the proton beam by the generated wakefield
- Competes with hosing instability ⇒ Seeding needed



Kumar, Pukhov and Lotov, Phys. Rev. Lett. 104, 255003 (2010)

Lotov, Physics of beam self-modulation in plasma wakefield accelerators Phys. Plasmas 22 (2015)

Awake: Overview

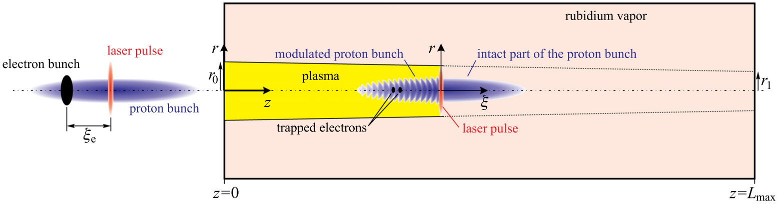


FIG. 1. Geometry of the problem (not to scale). The beams are shown at two times.

Lotov et al., Electron trapping and acceleration by the plasma wakefield of a self-modulating proton beam, Phys. Plasmas 21 123116 (2014)

Awake: Overview

TABLE I. Baseline AWAKE parameters and notation.

Parameter, notation	Value
Plasma density, n_0	7×10^{14} cm^{-3}
Plasma length, $L_{\max}$	10 m
Atomic weight of plasma ions, M_i	85.5
Plasma skin depth, $c/\omega_p \equiv k_p^{-1}$,	0.2 mm
Initial plasma radius, r_0,	1.5 mm
Final plasma radius, r_1,	1 mm
Wavebreaking field, $E_0 = mc\omega_p/e$,	2.54 GV/m
Proton bunch population, N_b	3×10^{11}
Proton bunch length, σ_{zb}	12 cm
Proton bunch radius, σ_{rb}	0.2 mm
Proton bunch energy, W_b	400 GeV
Proton bunch energy spread, δW_b	0.35%
Proton bunch normalized emittance, ϵ_{nb}	3.6 mm mrad
Proton bunch maximum density, n_{b0}	4×10^{12} cm^{-3}
Electron bunch population, N_e	1.25×10^9
Electron bunch length, σ_{ze}	1.2 mm
Electron bunch radius, σ_{re}	0.25 mm
Electron bunch energy, W_e	16 MeV
Electron bunch energy spread, δW_e	0.5%
Electron bunch normalized emittance, ϵ_{ne}	2 mm mrad
Electron bunch delay, ξ_e	16.4 cm

Quick look at the PIC scheme

$$\vec{\nabla} \cdot \vec{E} = \frac{q}{e} n$$

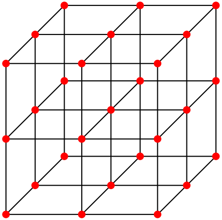
$$\vec{\nabla} \cdot \vec{B} = 0$$

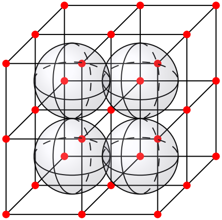
$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \frac{q}{e} n \vec{v} + \frac{\partial \vec{E}}{\partial t}$$

$$\left(\partial_t + \vec{v} \cdot \partial_{\vec{r}} + q \left[\vec{E} + \vec{v} \times \vec{B}\right] \cdot \partial_{\vec{p}}\right) f = 0.$$

$$\frac{\partial}{\partial t} \rho + \vec{\nabla} \cdot \vec{j} = 0$$





Basic features of the PSC

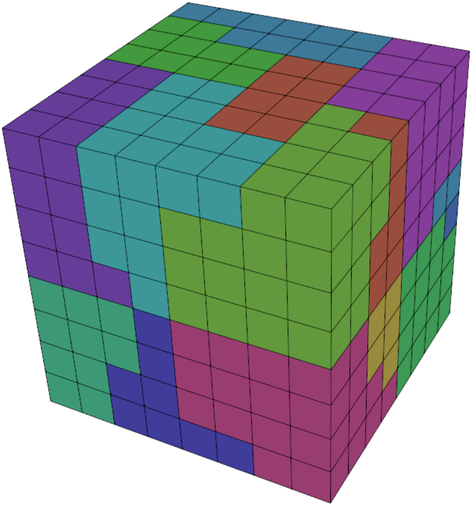
- Full 3D PIC simulation code
- Fully parallelized, great scaling properties (MPI, OpenMP)
- Written in C
- Modular framework, easily extendable (simplified polymorphism)
- Advanced memory management system, supports multiple architectures
- Data analysis and efficient parallel output (xdmf + hdf5)
- Nearly fully customizable by CLI (essential for automated test system)

Advanced features of the PSC

These provide important techniques to speed up calculation

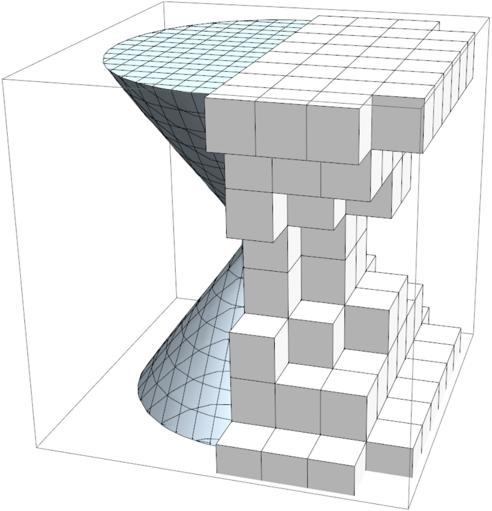
- Patch based approach
- Enables moving frame and boost frame
- Enables dynamical load balancing
- Enables AMR (Adaptive Mesh refinement) and APR (Adaptive particle refinement)
- GPU particle pushing, eg. Jaguar with 900 GPUs pushes 215 billion particles/sec
- Event generator module (allows particle injection)
- Background field module allows for external magnetic (and electric) field configurations
- Features multiple maxwell solvers (4th order, friedman filter)

Patch based approach, dynamical load balancing



(image provided by F. Deutschmann)

Patch based approach, complex frame



(image provided by F. Deutschmann)

Overview

- Fully 3D. Size: $3 \cdot 10^{10}$ cells, $3 \cdot 10^{10}$ particles, $2.5 \cdot 10^{6}$ timesteps
- Fully kinetic
- Non quasi-static

Computing resources: 35 Mch on SuperMUC.

Why?

- PIC can be seen as the only available theory fully describing this experiment.
- Justify the assumptions in baseline parameter simulations done up to now:
  - Quasistatic
  - Cylindrically symmetrical 2D
- Study of transversal beam filamentation
- Benchmarks and code comparison
- Large scale PIC simulations are challenging
- Possibility of a direct comparison between measurement and simulation

Cost

Using $N_{\text{per}\lambda_p} = 130$, $N_{ppc} = 3$, no plasma ions:

- Volume filled with plasma $V_p = L_{\max}\pi r_0^2 = 7 \cdot 10^{-5} m^3$
- Volume filled with ions $V_i = L_{\max}\pi \left(3\sigma_{rb}\right)^2 = 1.1 \cdot 10^{-5} m^3$
- $\Delta x = \frac{\lambda_p}{N_{\text{per}\lambda_p}}$
- $\Delta t = k_{\text{cfl}} \sqrt{\frac{1}{\frac{3c^2}{\Delta x^2}}}$
- $f_{\text{pps}} = 1.2 \cdot 10^6$ (particles pushed per second)

$$t_{\text{percore}} = \frac{\left(V_p + V_i\right) N_{\text{ppc}}}{\Delta x^3 f_{\text{pps}}} \frac{L_{\max}}{c\Delta t} \frac{L_{\text{window}}}{L_{\max}}$$

$$= \frac{\sqrt{3}\left(V_p + V_i\right) L_{\text{window}}}{\lambda_p^4 f_{\text{pps}} k_{\text{cfl}}} N_{\text{per}\lambda_p}^4 N_{\text{ppc}}$$

$$\Rightarrow t_{\text{percore}} = 5.1 \cdot 10^{-3} \cdot N_{\text{per}\lambda_p}^4 N_{\text{ppc}} ch = 4.4 Mch$$

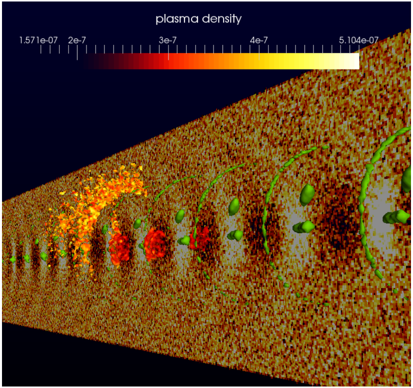
Cost

- Using 8 islands totaling 65536 nodes on Supermuc
  $Wt = 4.4 \cdot 10^6 / 65536 \approx 67 cpuh$ total Walltime
- All output, management and grid overhead is omitted in this calculation.
- Perfect Scaling is assumed
- Witness beam is one order of magnitude less particles than the ion beam, omitted.
- 1 ch costs approximately 0.01 - 0.013 €, total cost = 44000 - 57200 € per Simulation
- Memory: using about 25 TB peak memory out of the available 50 TB

Progress

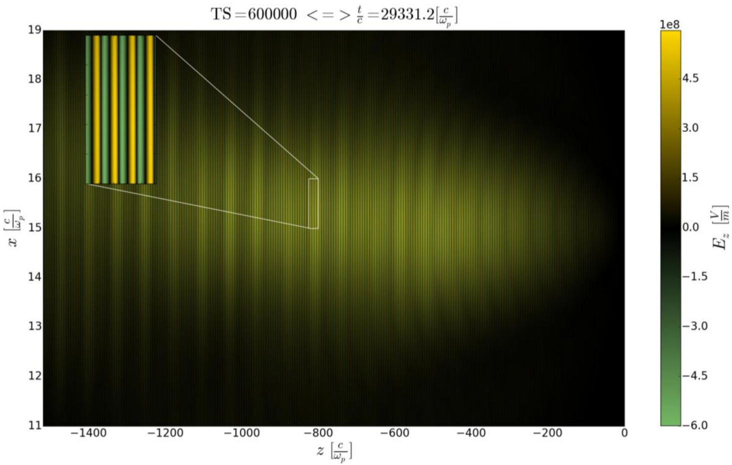
- Many new inline outputs to save hard disk space and I/O bandwidth
- Scaling to 65536 nodes on SuperMUC
  - particle injection $\rightarrow$ non-symmetric, non-homogeneous configuration
  - improvements and specializations to the load balancer
  - I/O specializations for the SuperMUC system
    - $<$ 1000 concurrent filestreams
    - $<$ 1000 files per directory
    - Don't write into a directory from multiple nodes or multiple islands
    - Serialization in very specific, optimal patterns using subdirectories
    - No parallel mpi io since we have large chunks of unscattered data
    - We achieve 105 Gbyte/s out of 125 Gbyte/s technical maximum
  - rigorous scalability analysis
    - Eradication of all unnecessary duplications in memory and output files
    - Example: checkpointing went from 120 TB files written out in 2.5h to 30 TB written out in 6 min (in memory compression, less file entries in hdf5 file)
  - Since computation is only performed in 48h chunks a lot of restarts are necessary (with a lot of waiting in between)

Results, 65 points per λ_p



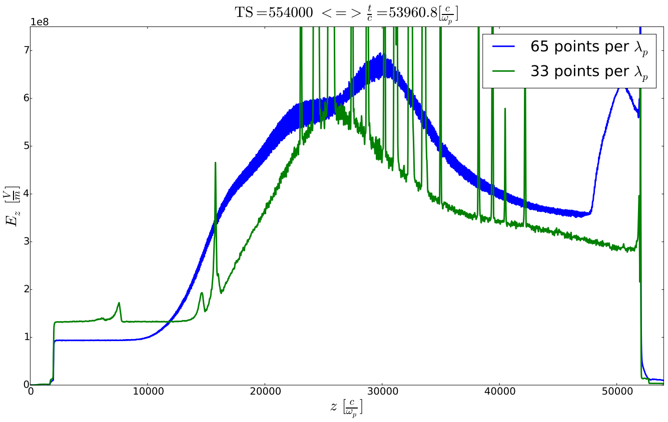
Simulation state after 5m.
Green: ion beam micro-bunches at density $1.9 \cdot 10^{12} \frac{1}{cm^3}$.
Red and orange: trapped electron witness beam at density $1.9 \cdot 10^{10} \frac{1}{cm^3}$.
Color legend: density in units of $1.9 \cdot 10^{21} \frac{1}{cm^3}$.

Results, 65 points per λ_p



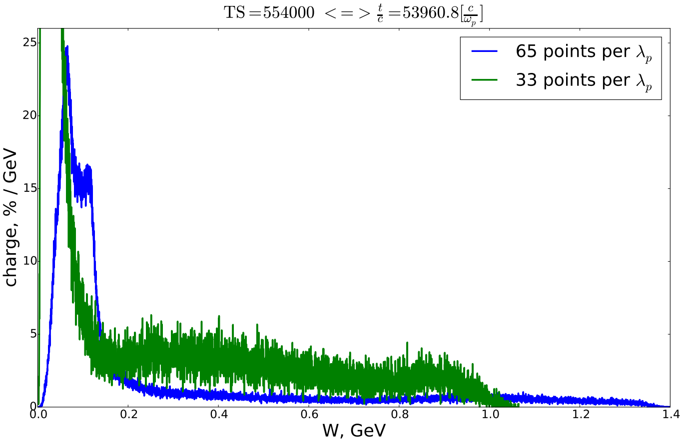
Maximum of the E_z field amplitude averaged over 1000 time steps at each x-z-position of simulation space after 5m of beam propagation inside the plasma.

Results, Resolution comparison



Maximum electric field in z-direction over the whole 10m simulation.

Results, Resolution comparison



Percentage, in relation to initial beam, of charge per GeV in the electron witness beam over energy after traversing 10m in plasma.