LCODE: a code for fast simulations of plasma wakefield acceleration

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AWAKE Collaboration
Goals defined by plasma-based accelerators

Collider-oriented simulation tasks are order of magnitude “heavier” than those related to proof-of-principle experiments.
These goals are difficult to reach with general-purpose PIC codes:

Nils Moschuring, Hartmut Ruhl (LMU Munich)
Presented at AWAKE Collaboration Meeting, CERN, March 13, 2015

Time and cost estimates for 3D PIC simulation of AWAKE baseline scenario (16 cm long proton bunch, 10 m plasma, 7 \times 10^{14} \text{cm}^{-3}, proton-driven plasma wakefield acceleration experiment)

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

- Volume filled with plasma
  \[ V = \frac{L_{\text{max}} \pi}{3} \left( r_0^2 + r_0 r_1 + r_1^2 \right) \]
  \[ \Rightarrow V = 5 \cdot 10^{-5} \text{m}^3 \]
- \( \Delta x = \frac{\lambda_p}{N_{\text{per}\lambda_p}} \)
- \( \Delta t = k_{\text{cfl}} \sqrt{\frac{1}{3 c_0^2 \Delta x^2}} \)
- \( f_{\text{pps}} = 1.2 \cdot 10^6 \) (particles pushed per second)

\[
t_{\text{percore}} = \frac{VN_{\text{ppc}}}{\Delta x^3 f_{\text{pps}}} \frac{L_{\text{max}}}{c \Delta t} \frac{L_{\text{window}}}{L_{\text{max}}} = \frac{\sqrt{3 VN_{\text{ppc}} N_{\text{per}\lambda_p}^4 N_{\text{ppc}}}}{\lambda_p^4 f_{\text{pps}} k_{\text{cfl}}} \]
\[ \Rightarrow t_{\text{percore}} = 3.15 \cdot 10^{-3} \cdot N_{\text{per}\lambda_p}^4 N_{\text{ppc}} \text{ch} = 2.7 \text{Mch} \]

- Using 4 islands totaling 32768 nodes on Supermuc
  \[ Wt = 2.7 \cdot 10^6 / 32768 \approx 82 \text{cpu}h \] total Walltime
- All output, management and grid overhead is omitted (but is comparatively small).
- Beam and witness beam are four orders of magnitude less particles than the plasma, also omitted.
- 1 ch costs approximately 0.01 - 0.013 €, total cost = 27000 - 35000 € per Simulation
- Memory: less than 2 TB out of the available 50 TB

Time efficient specialized codes are needed.
What is AWAKE? Experiment under preparation at CERN

>50 mJ, 100 fsec, 810 nm

Beam portrait (2nd half)

Excited field ($\Phi$)

rubidium vapor

modulated proton bunch

intact part of the proton bunch

trapped electrons

laser pulse
Ways to speed-up simulations

• Cylindrical 2D or quasi-2D (azimuthal harmonics)

• Boosted frame: helps to resolve laser fields, most physics retained

• Fluid model: applicable to low-amplitude waves with no wavebreaking

• Quasistatic approximation: good for slowly evolving drivers and slowly changing plasma density (along the beam path)

When we calculate the plasma response, the driver is “rigid” (not evolving in time).

The fields depend on $\xi = z - ct$ and can be found layer-by-layer starting from the driver head, because all particles started from some $r_0$ copy the motion of each other, their parameters are functions of $\xi$.

A plasma “macroparticle” is a particle tube, i.e., a group of real particles started from $r_0$ with a given momentum.

This greatly reduces the memory required for storing plasma particles (dimension – 1).

The fields are used to modify the driver. The time step $\Delta t$ can be large (several orders of magnitude speed-up).
Quasi-static codes

widely used for LWFA, includes particle trapping,
recently adopted for PWFA

originally developed for PWFA, tuned for long beams and propagation distances,
recently adopted for LWFA

QUICKPIC [C. Huang et al., Journal of Computational Physics 217, 658 (2006)]:
workhorse for SLAC PWFA experiments, first 3d code

recently joined the family
Unique features of LCODE

- Two plasma solvers (fluid and PIC), two 2d3v geometries (plane and cylindrical)

![Fluid solver](image1)
![PIC solver](image2)

The fluid solver is unique; it is ~10 times faster than PIC and more precise at the same resolution.

- On-flight graphic diagnostics (tool for fast view of results without dumping huge amounts of data)

Example: hosing of electron beam (plane geometry)
Unique features of LCODE

- PIC solver solves equations for fields (not potentials, unique feature) and makes no use of constants of motion

This makes easier simulations of plasmas with arbitrary initial distributions of particles (transversely nonuniform, heated, non-neutral, moving, excited etc.)

Example: wakefield of a positron bunch in cold and heated plasma channels
PIC plasma solver

Maxwell equations in the co-moving frame are

\[
\frac{1}{r} \frac{\partial}{\partial r} r E_r = \rho + \rho_b - \frac{\partial E_z}{\partial \xi}, \quad \frac{1}{r} \frac{\partial}{\partial r} r B_r = -\frac{\partial B_z}{\partial \xi},
\]

\[
\frac{1}{r} \frac{\partial}{\partial r} r (E_r - B_\phi) = \rho - j_z, \quad \frac{\partial E_z}{\partial r} = j_r, \quad \frac{\partial B_z}{\partial r} = -j_\phi, \quad E_\phi = -B_r.
\]

but we solve, instead of the first two,

\[
\frac{\partial}{\partial r} \frac{1}{r} \frac{\partial}{\partial r} r E_r - E_r = \frac{\partial (\rho + \rho_b)}{\partial r} - \frac{\partial j_r}{\partial \xi} - \tilde{E}_r, \quad \frac{\partial}{\partial r} \frac{1}{r} \frac{\partial}{\partial r} r B_r - B_r = \frac{\partial j_\phi}{\partial \xi} - \tilde{B}_r,
\]

with boundary conditions (perfectly conducting tube)

\[
E_r(0) = B_r(0) = B_\phi(0) = E_z(r_{\text{max}}) = B_r(r_{\text{max}}) = 0, \quad \int_0^{r_{\text{max}}} 2\pi r B_z \, dr = \pi r_{\text{max}}^2 B_0.
\]

Plasma particles are pushed as usual

\[
\frac{d\tilde{p}}{d\xi} = \frac{d\tilde{p}}{dt} \frac{dt}{d\xi} = \frac{q}{v_z - 1} \left( \tilde{E} + [\tilde{v} \times \tilde{B}] \right), \quad \frac{dr}{d\xi} = \frac{v_r}{v_z - 1}, \quad \tilde{v} = \frac{\tilde{p}}{\sqrt{M^2 + p^2}}.
\]

\[
\tilde{j} = A \sum_i \frac{q_i \tilde{v}_i}{1 - v_{z,i}}, \quad \rho = A \sum_i \frac{q_i}{1 - v_{z,i}}.
\]
Fluid plasma solver

Equation of motion for electron fluid:
\[
\frac{\partial \vec{p}}{\partial t} + (\vec{v} \nabla) \vec{p} = -\vec{E} - [\vec{v} \times \vec{B}],
\]

Integrals of motion:
\[
\vec{B} = \text{rot} \, \vec{p} + n_e B_0 (\vec{e}_z - \vec{v}), \quad \Phi = \gamma - p_z;
\]

Final set of equations:
\[
\frac{\partial \Phi}{\partial \xi} = -E_z, \quad \frac{\partial \rho_r}{\partial \xi} = \frac{\partial \rho_z}{\partial r} + B_\varphi + \frac{N p_\varphi B_0}{\Phi}, \quad N = 1 + \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial \Phi}{\partial r},
\]
\[
\frac{\partial}{\partial r} \frac{1}{r} \frac{\partial}{\partial r} r p_\varphi - \frac{N p_\varphi}{\Phi} = -B_0 \frac{\partial N}{\partial r}, \quad p_z = \frac{1 + p_r^2 + p_\varphi^2 - \Phi^2}{2\Phi}, \quad \frac{\partial E_z}{\partial r} = -\frac{N p_r}{\Phi};
\]
\[
B_r = -E_\varphi = -\frac{N p_r B_0}{\Phi} - \frac{\partial p_\varphi}{\partial \xi}, \quad B_z = \frac{1}{r} \frac{\partial}{\partial r} r p_\varphi + B_0 N,
\]
\[
\frac{\partial}{\partial r} \frac{1}{r} \frac{\partial}{\partial r} r B_\varphi - \frac{N}{\Phi} B_\varphi = \frac{\partial j_b}{\partial r} - p_z \frac{\partial N}{\partial r} + \frac{p_r}{\Phi} \frac{\partial}{\partial r} r N p_r + \frac{N p_r E_z}{\Phi^2} + \frac{N^2 p_\varphi B_0}{\Phi^2}.
\]
\[
N = n_e (1 - v_z) \quad E_z = -\frac{\partial \Phi}{\partial \xi}, \quad E_r - B_\varphi = -\frac{\partial \Phi}{\partial r}.
\]
Unique features of LCODE

- Energy flux control

The wakefield acceleration is the process of energy transfer from one beam to another:

Natural and convenient **measure** of beam-plasma and beam-beam energy exchange is

Energy flux in co-moving window = $-c \vec{e}_z \cdot (\text{Energy density}) + (\text{Usual energy flux})$

**Energy flux density:**

$$\vec{S} = -c \vec{e}_z \frac{E^2 + B^2 - B_0^2}{8\pi} + \frac{c}{4\pi} \left[ \vec{E} \times \vec{B} \right] + \sum_{\text{unit volume}} (\gamma - 1)m c^2 (\vec{v} - c \vec{e}_z)$$

- Electromagnetic energy
- Poynting vector
- Relativistic factor

**Electromagnetic energy flux density,** $\vec{S}_{em}$
Unique features of LCODE

- Energy flux control

Energy flux - measure of beam-plasma energy exchange:

\[ \Psi = - \int_{0}^{\infty} S_z 2\pi r \, dr, \quad \frac{\partial \Psi}{\partial \xi} = \int_{0}^{\infty} j_{bz} E_z 2\pi r \, dr, \quad \xi = z - ct \]

The energy flux must be constant between the beams.
Too coarse grid, too few macro-particles, too close wall, escape of fast plasma particles etc. \[ \Rightarrow \Psi \neq \text{const} \]

We (almost) always know if simulations go wrong
(especially important for long beams)

Example: The energy flux between electron driver and witness, linear plasma response
Example:

- Energy flux in blowout regime
Unique features of LCODE

- Automatic substepping in beam and PIC plasma solvers

Time step $\Delta t$ for low energy electrons is individually reduced with respect to the main driver time step $\Delta t_0$.

Grid step $\Delta \xi$ is automatically reduced in regions of abrupt field change.

Example: SLAC E-157 simulation.
Features of LCODE

- **Parallel operation**

  “Pipe-line” concept: plasma solvers move along the beam and change its state

Several time steps are made in a single pass of the simulation window by several solvers
Examples of heavy tasks

Self-modulating LHC beam:
20 cm long simulation window travelled 17 km in $3 \times 10^{15}$ cm$^{-3}$ plasma ($\lambda_p=0.6$ mm) in 6 months (single CPU)

[Phys. Plasmas 18, 103101 (2011)]

Map of density steps:
A small up-step of the plasma density during beam self-modulation results in a stronger established wakefield

2400 full length runs to produce this graph (beam length $160c/\omega_p$, propagation distance $10^4c/\omega_p$)

[Phys. Plasmas 22, 103110 (2015)]
Availability of LCODE

I invite you to use LCODE for your studies. It is free to use. We do not ask for money, but expect collaboration with users.

Executables and manual can be downloaded from http://www.inp.nsk.su/~lotov/lcode/
Degree of maturity – always young

Scientifically interesting problems need new features of the code,
hottest results are obtained during the testing stage,
after the testing stage everything works reliably, but the best results are already published

Recent advances and plans:
Highly precise plasma solver (for AWAKE)
Parallel operation
Laser solver
3d code
Plasma particle trapping
Ionization injection
LCODE team & user support

It may not be easy to start using LCODE with 30-page manual only, so we invite users to become a part of LCODE team:

Solver developer (mathematician)

Architect (computer scientist)

Solver developer (mathematician)

Experienced user (physicist)

Solver developer (mathematician)

Less experienced user (physicist, student)

Experienced user (physicist)

Less experienced user (physicist, student)

Beginning user

Our students are ready to help new users, e.g., by making a configuration file for the first run.

Discussions are very important as a quality check of simulation results.
SLAC E-157 experiment, example of the code run
Thank you

Welcome to use LCODE for your research