Full-scale modeling of plasma-based accelerators using ponderomotive guiding center solver in OSIRIS

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LWFA is an Exascale problem

scale disparity in modeling

- multi-scale problems
  - large disparity of spatial/temporal scales

sample problem: 50 GeV LWFA stage
  - $\lambda_0 \sim 1\mu m / \lambda_p \sim 17\mu m$
  - $L \sim 1.5 \text{ m}$

computational requirements (moving window)
  - $\sim 10^9$ grid cells
  - $\sim 10^{10}$ particles
  - $\sim 10^6 - 10^7$ iterations
  - $\sim 10^{18} - 10^{19}$ operations

requirement for reduced models
Outline

- **Implementation of PGC into Osiris**
  parallel scalability, numerical stability and control of numerical noise

- **Reduced modeling of down-ramp injection**
  one-to-one comparison of PGC and PIC simulations

- **Reduced modeling in the realm of AWAKE**
  ionization seeding for self-modulation of a long proton bunch
Committed to open science

Open-access model
- 40+ research groups worldwide are using OSIRIS
- 300+ publications in leading scientific journals
- Large developer and user community
- Detailed documentation and sample inputs files available

Using OSIRIS 4.0
- The code can be used freely by research institutions after signing an MoU
- Find out more at:
  http://epp.tecnico.ulisboa.pt/osiris

OSIRIS framework
- Massively Parallel, Fully Relativistic Particle-in-Cell Code
- Parallel scalability to 2 M cores
- Explicit SSE / AVX / QPX / Xeon Phi / CUDA support
- Extended simulation/physics models

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Extensions to PIC cycle

- time-averaged equation for laser evolution in a co-moving frame
  \[ 2i\omega_0 \partial_\tau a = \left( 1 + \frac{\partial_\xi}{i\omega_0} \right) \left( \chi a + \nabla^2_{\perp} a \right) \]

- particle advancing
  \[ \mathbf{F}_p = -\frac{1}{4} \frac{q^2}{\langle m \rangle} \nabla |a|^2 \]

- coupling parameters
  \[ \chi = -\sum_i \frac{q_i \rho_i}{\langle m_i \rangle} \]
  \[ \langle m \rangle = \sqrt{m_0^2 + p^2 + (q|a|)^2} / 2 \]

Scale disparity can be overcome by modeling the envelope evolution

Extensions to PIC cycle

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Scale disparity can be overcome by modeling the envelope evolution


Plasma gradients lead to numerical instabilities*

\[ \Delta \tau^2 \leq \frac{\Delta y^4 \Delta z^4 \Delta \xi^2 \omega_0^4}{4 \left( \Delta z^2 + \Delta y^2 \left( 1 + \Delta \xi \omega_0 \right) \right)^2 - \Delta y^4 \Delta \xi^2 \omega_0^2} \]

\[ \Delta y = \Delta z = 0.2 \]

error at time step n: \( e^n \)

error growth rate: \( g = \frac{e^{n+1}}{e^n} \)

stability condition: \( |g| \leq 1 \)

* A. Helm et al., to be submitted (2019)
Plasma gradients lead to numerical instabilities*

Δy = Δz = 0.2

Δτ = 0.15, Δξ = Δy = Δz = 0.2

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\[ \Delta y = \Delta z = 0.2 \]

\[ \Delta \tau = 0.15, \Delta \xi = \Delta y = \Delta z = 0.2 \]

\[ \Delta \chi = \chi_{i+1,j,k} - \chi_{i-1,j,k} \]

\[ |\chi| = 1.0, |\Delta \chi| = 1.0 \]

\[ |\chi| = 1.0, |\Delta \chi| = 0.01 \]

\[ \omega_0/\tilde{\omega} = 15 \]

\[ \omega_0/\tilde{\omega} = 7.5 \]
Stability control for PGC

**particle interpolation order**
- current implementation matches interpolation order of PIC cycle (up to 4th order)
- field interpolation increases preciseness of ponderomotive force influence
- chi deposition increases stability especially in longitudinal direction

**smoothing of PGC quantities**
- allows explicit control of numerical noise
- includes several filters to control the noise level and cutoff of the noise
- smoothable quantities:
  - plasma parameter chi
  - ponderomotive force
  - laser envelope
Shared memory parallelization

\[ 2i\omega_0 \partial_\tau a = \left( 1 + \frac{\partial_\xi}{i\omega_0} \right) (\chi a + \nabla_\perp^2 a) \]

enforces data locality in transverse plane

- JUQUEEN (IBM BlueGene/Q) - 16 cores per node
- number of cores: 32 / 64 / 128 / 256 / 512
- 500 time steps - 608x152x152 cells and 8 ppc
- using distributed parallelization in longitudinal direction
- ✔ scaling over one order of cores using shared memory parallelization

**thread-based strong scaling**

\[ \text{speed-up} \]

\[ \text{number of threads} \]

efficiency: 68%
Shared memory parallelization for PGC

**Strong scaling**

- Ideal: -
- Partitions: $x \times 8 \times 8$
- Partitions: $4x \times x \times x$

Efficiency: $\sim 70\%$

**Weak scaling**

- Efficiency [%]

128 partitions

- Nodes: $32/2^x/1$
- Nodes: $32/1/2^x$
Reduced modeling of down-ramp injection

**short down-ramp transition**

<table>
<thead>
<tr>
<th>Density [10^{18} cm^{-3}]</th>
<th>3</th>
<th>2</th>
<th>1</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>z [μm]</td>
<td>0</td>
<td>100</td>
<td>200</td>
<td>300</td>
</tr>
</tbody>
</table>

\[ L_{\text{ramp}} = 19.2 \text{ μm} \]

- Laser parameters:
  - laser wavelength: \( \lambda_0 = 800 \text{ nm} \)
  - pulse duration: \( \tau_l = 57.2 \text{ fs} \)
  - normalized vector potential: \( a_0 = 2.82 \)
  - beam waist: \( w_0 = 17.2 \text{ μm} \)

**long down-ramp transition**

<table>
<thead>
<tr>
<th>Density [10^{18} cm^{-3}]</th>
<th>6</th>
<th>4</th>
<th>2</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>z [mm]</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
</tbody>
</table>

\[ L_{\text{ramp}} = 150 \text{ μm} \]

- Laser parameters:
  - laser wavelength: \( \lambda_0 = 800 \text{ nm} \)
  - pulse duration: \( \tau_l = 30.0 \text{ fs} \)
  - normalized vector potential: \( a_0 = 1.8 \)
  - beam waist: \( w_0 = 18 \text{ μm} \)

* S. Kalmykov et al., PRL 103, 135004 (2009)
Reduced time-step affects impacts on beam emittance

- charge and mean energy are in good agreement
- emittance is 5x higher for PGC case
- discrepancy in emittance arises from poor injection
- higher order pusher could lead to reduced emittance
Reduced modeling for injector stage in the context of EuPRAXIA*

- comparison of full PIC and PGC
- strong agreement for laser evolution and plasma fields
- PGC does not model injection properly
- mitigation of numerical Cherenkov instability through Lehe-solver**
- PGC can be used for grasping laser evolution and the plasma response with the wakefield structure

* T. Silva et al., submitted (2019)
** R. Lehe et al., *PRE*, 94 (5), 053305–16 (2016)
Acceleration of electrons in the plasma wakefield of a proton bunch*

Accelerated electron plasma

Electron source system

20-MeV radio-frequency gun

Radio-frequency gun

Proton beam

Laser beam

Dipole

Dipole

Electron beam

10-m Rb plasma

Rb flask

Scintillator screen

Scintillator screen

Imaging station 1

OTR, CTR screens

Quadrupoles

Dipole

Scintillator screen

Electron spectrometer

Laser dump

Imaging station 2

Electron plasma

ionizing laser pulse

proton beam

proton micro bunches

Ionization seeding with PGC for self-modulation instability

- Simulation box: 75 mm x 13 mm x 13 mm
- 10 m propagation distance
- $10^6$ time steps
- 17,664 cores (92% of Marenostrum)
- ~3M CPUh
Conclusions & acknowledgement

**Reduced modeling on the plasma scale**
- control of numerical instability is crucial for PGC
- parallelisation of envelope equation over thousands of cores

**Reduced modeling of down-ramp injection**
- PGC can be used to grasp the laser evolution and generated plasma fields
- higher order particle pusher for better modeling the particle injection

**Self-consistent modeling of self-modulation instability**
- ionization injection incorporated into PGC
- full 10 m AWAKE runs can be modeled with PGC

Simulation results obtained on IST-cluster (IST), JUQUEEN (JSC), Cori (NERSC/LBNL) and Marenosrmm (BSC)

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