A three-dimensional ponderomotive guiding center solver in Osiris

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Scale disparities in LWFA modeling

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

- **sample problem: 50 GeV LWFA stage**
  - $\lambda_0 \sim 1 \mu m$, $\lambda_p \sim 17 \mu m$
  - $L \sim 1.5 m$

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

*requirement for reduced models*
Envelope approximation reduces spatial resolution

**particle-in-cell (PIC)**

- **spatial resolution:**
  - laser wavelength

  ✦ resolve laser wavelength over propagation distance
  ✦ particle advancing is based on Lorentz force

**ponderomotive guiding center (PGC)**

\[
\frac{\partial E}{\partial \tau} = c \nabla \times B - 4\pi j
\]
\[
\frac{\partial B}{\partial \tau} = -c \nabla \times E
\]

- **spatial resolution:**
  - plasma skin depth

  ✦ requires model for laser envelope propagation
  ✦ push particles using self consistent plasma fields and ponderomotive force

**speedup** \[\sim (\lambda_p/\lambda_0)^2\]
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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Major features of PGC in OSIRIS

**Physical features:**
- moving window frame
- 2d cartesian
- 2d cylindrical cartesian
- 3d cartesian
- different laser pulse shapes
- different boundary conditions for transversal direction
- field ionization based on ADK model

**Numerical stability and stability control:**
- stability condition for envelope equation
- up to 4th order interpolation and deposition schemes
- smoothing for stability control

**Parallel performance:**
- shared memory parallelization
- distributed memory parallelization
- scalable up to $10^5$ cores
Outline

- **Incorporation of PGC into Osiris**
  numerical stability and control of numerical noise

- **Parallel scalability of PGC**
  incorporation of shared and distributed memory parallelization

- **Physical applicability for PGC**
  down-ramp injection with PGC and full scale modeling of self-modulation instability
Incorporation of PGC into PIC cycle

**PGC extension**

- time-averaged equation for laser evolution* in a co-moving frame

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

laser frequency laser envelope

- particle advancing

\[ F_p = -\frac{1}{4} q^2 \frac{1}{\langle m \rangle} \nabla |a|^2 \]

- coupling parameters

\[ \chi = -\sum_i \frac{q_i \rho_i}{\langle m_i \rangle} \]

\[ \langle m \rangle = \sqrt{m_0^2 + p^2 + (q|a|)^2} / 2 \]

**extended PIC algorithm**

extend equation of motion to include ponderomotive force

integration of equation of motion, moving particles

\[ F_i \rightarrow p_i \rightarrow x_i \]

weighting

\[ (E, B)_j \rightarrow F_i \]

integration of field equations on the grid

\[ J_j \rightarrow (E, B)_j \]

weighting

\[ (x, p)_i \rightarrow J_j \]

advance envelope

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** P. Mora and T. M. Antonsen, AIP 4, 217 (1997)
Incorporation of PGC into PIC cycle

**PGC extension**

- time-averaged equation for laser evolution* in a co-moving frame

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

\( \omega \) - laser frequency  
\( a \) - laser envelope

- particle advancing

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

- coupling parameters

\[ \chi = -\sum_i \frac{q_i \rho_i}{\langle m_i \rangle} \]

\[ \langle m \rangle = \sqrt{m_0^2 + p^2 + (q|a|)^2 / 2} \]

** P. Mora and T. M. Antonsen, AIP 4, 217 (1997)
Stability of the envelope solver depends on laser frequency

**Courant-Friedrichs-Lewy (CFL)**

\[ \Delta t \leq \sqrt{\frac{1}{(1/\Delta x)^2} + (1/\Delta y)^2 + (1/\Delta z)^2} \]

- necessary condition for stability of Maxwell solver
- does not depend on physical parameters

**vacuum stability condition**

- implicit solver for advancing of the envelope
- von-Neumann analysis for stability condition
- stability condition for the vacuum case

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

- stability depends on the laser frequency
- for higher frequencies the envelope equation becomes “more stable"
Plasma gradients lead to numerical instabilities

\[ 2i\omega_0 \partial_\tau e^n_{ijk} = \left( 1 + \frac{\partial_\tau}{i\omega_0} \right) \left( \chi e^n_{ijk} + \nabla^2 e^n_{ijk} \right) \]

- numerical stable:
  \[ |g| = |e^{n+1}/e^n| \leq 1 \]

- plasma parameter:
  \[ \chi \equiv \chi_{ijk} \sim \mathcal{O}(\rho) \]

- plasma gradients:
  \[ \delta\chi \equiv \chi_{(i+1),j,k} - \chi_{(i-1),j,k} \]

**numerical error growth rate for PGC**

- vacuum: \( \Delta\tau = 0.1\omega_p^{-1} \)
- \( \chi = 5.0 \):
  - \( \Delta x = 0.2 c/\omega_p \)
  - \( \Delta y = 0.2 c/\omega_p \)
  - \( \Delta z = 0.2 c/\omega_p \)

* A. Helm et al., to be submitted (2019)
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 for PGC

**thread-based particle advancing**

- ✔ data sharing between threads is fast
- ✔ envelope solver can be parallelized easily
- ❌ lack of scalability between memory and cores
- ❌ memory is limited to cores and does not scale

**thread-based strong scaling**

- ✦ 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

speedup: 10.9×
Parallelization is scalable over thousands of cores

**distributed memory parallelization**

- advancing the envelope requires data locality in transversal direction due to implicit finite difference scheme
- data locality can be achieved through a transpose operation
- scaling tests were carried out on JUQUEEN
  - 16 cores per node / no threading (IBM BlueGene/Q)
  - strong scaling: $15360 \times 240 \times 240$ with 8 ppc and 500 steps
  - weak scaling: 10 cells in $x_2$ and 50 cells in $x_3$
- PGC scales from 1536 to 216000 with >70% efficiency

**strong scaling**

- ideal
- $\text{partitions: } x|8|8$
- $\text{partitions: } 4|x|x$

efficiency: ~70%

**weak scaling**

- $128$ partitions

- nodes: $32/2^x/1$
- nodes: $32/1/2^x$
PGC for parametric studies for down ramp injection

**down ramp injection case**

**density profile:**

- PGC allows to perform parametric studies with a fraction of computational costs compared to PIC
- attractive tool for design studies like EuPRAxia
- comparison of PGC vs. PIC:
  - identical transversal resolution
  - longitudinal resolution: $\Delta\xi_{\text{PIC}}|_{\text{PGC}} = \lambda_{0p} / 62$
  - injected electron bunch with $\gamma > 50$
  - mean energy and charge are in agreement
  - emittance 5x higher for PGC

**injected beam properties**

- mean energy $[m_ec^2]$
- charge $[c^3/m_e]$ (with $p_e$)
- trans. norm. rms emittance $[c/\omega_p]$
Temporal resolution leads to higher emittance

- Fields structure is described on long scales associated to plasma scales.
- Plasma scales are resolved by PGC.
- Temporal resolution for PGC case is reduced by $\frac{\lambda_p}{\lambda_0}$.
Acceleration of electrons in the plasma wakefield of a proton bunch*

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

Propagation distance = 10.00 m

- Ionized electrons
- Proton beam
- Laser pulse
Conclusions & acknowledgement

**Numerical stability and control**
- in general PGC is unconditionally unstable if plasma gradients are present
- control can be provided by applying smoothing filters

**Scale disparity can be overcome with reduced models for LWFA**
- important for parametric studies of LWFA
- for cases where $\frac{\omega_0}{\omega_p} \gg 1$

**Parallel scalability**
- using shared memory parallelization, PGC can scaled over one order of magnitude
- using distributed memory parallelization, PGC can be scaled over $10^5$ cores
- PGC and parallel scalability is required for full study of experiments like AWAKE

Simulation results obtained on JUQUEEN (JSC), Cori (NERSC/LBNL) and Marenostrum (BSC)

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