OPAL for Self-Consistent Start-to-End Simulation of Undulator-Based Facilities

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Object Oriented Parallel Particle Library (OPAL)

https://gitlab.psi.ch/OPAL/src/wikis/home

OPAL is a versatile open-source tool for charged-particle optics in large accelerator structures and beam lines including 3D EM field calculation, collisions, radiation, particle-matter interaction, and multi-objective optimisation

- OPAL is built from the ground up as an HPC application
- OPAL runs on your laptop as well as on the largest HPC clusters
- OPAL uses the MAD language with extensions
- OPAL is written in C++, uses design patterns, easy to extend
- The OPAL Discussion Forum: https://psilists.ethz.ch/sympa/info/opal
- International team of 11 active developers and a user base of $\mathcal{O}(100)$
- The OPAL **sampler** command can generate labeled data sets using the largest computing resources and allocations available

The Active OPAL Developer Team

UKRI Science and Technology Facilities Council | ISIS Neutron and Muon Source

SLAC NATIONAL ACCELERATOR LABORATORY

PAUL SCHERRER INSTITUT PSI

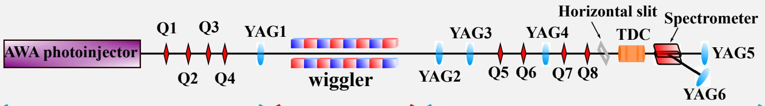
MIT

Ciemat
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

University of St Andrews

The Need for a Full EM Solver

AWA Wiggler Experiment



Only space charge

(electrostatic approximation okay)

Space charge and radiation

(requires full EM)

Only space charge

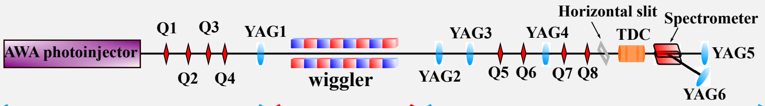
(electrostatic approximation okay)

To the best of our knowledge, there are currently no single particle-tracking codes that can model this beamline start-to-end.

Spoiler: OPAL can now do it!

The Need for a Full EM Solver

AWA Wiggler Experiment



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Space charge and radiation
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Only space charge
(electrostatic approximation okay)

OPAL electrostatic solver:

$$\begin{cases} \boldsymbol{\nabla}\cdot\boldsymbol{E} = \dfrac{\rho}{\varepsilon_0}, \quad \boldsymbol{\nabla}\wedge\boldsymbol{E} = -\cancelto{0}{\dfrac{\partial \boldsymbol{B}}{\partial t}}\,, \\ \boldsymbol{\nabla}\cdot\boldsymbol{B} = 0, \quad \boldsymbol{\nabla}\wedge\boldsymbol{B} = \mu_0\boldsymbol{j} + \cancelto{0}{\dfrac{1}{c^2}\dfrac{\partial \boldsymbol{E}}{\partial t}}\,, \\ \mathbf{E} = \mathbf{E}_{\text{ext}} + \mathbf{E}_{\text{self}}, \quad \mathbf{B} = \mathbf{B}_{\text{ext}} + \mathbf{B}_{\text{self}}\,, \end{cases} \Rightarrow \begin{cases} \underbrace{\boldsymbol{\nabla}^2\Phi = \rho/\varepsilon_0\,,}_{\text{in co-moving frame}} \\ \text{with appropriate} \\ \text{boundary conditions.} \end{cases}$$

Modeling Electrons in Undulators and Wigglers

Solving full Maxwell equations is hard because:

- We have space charge **and** radiation that affects all particles,
- Hyperbolic PDE (stability issues, dispersion, huge computational demand...),
- Often simplifications are required (electrostatic, 1D wakefields, ...).

Table: Common approximations in modeling free electron laser radiation.

code name	approximation					
	steady state approximation	wiggler-average electron motion	slow wave approximation	forward wave	no space-charge	slice
GENESIS 1.3	optional	✓	✓	✓	—	optional
MEDUSA	optional	—	✓	✓	—	✓
TDA3D	✓	✓	✓	✓	—	no time-domain
GINGER	—	✓	✓	✓	—	—
PERSEO	—	—	—	✓	✓	—
CHIMERA	—	—	—	✓	—	—
EURA	—	✓	✓	✓	—	—
FAST	—	✓	✓	—	—	✓
PUFFIN	—	—	—	✓	✓	—

A. Fallahi et al. (2018), DOI:10.1016/j.cpc.2018.03.011

Mithra: Full EM Solver from First-Principles

Computer Physics Communications
Volume 228, July 2018, Pages 192-208

MITHRA 1.0: A full-wave simulation tool for free electron lasers ☆

Arya Fallahi [a], Alireza Yahaghi [a], Franz X. Kärtner [a, b]

Maxwell equations rearranged into wave equations:

$$\begin{cases} \nabla \cdot \boldsymbol{E} &= \dfrac{\rho}{\varepsilon_0}, \\ \nabla \wedge \boldsymbol{E} &= -\dfrac{\partial \boldsymbol{B}}{\partial t}, \\ \nabla \cdot \boldsymbol{B} &= 0, \\ \nabla \wedge \boldsymbol{B} &= \mu_0 \boldsymbol{j} + \dfrac{1}{c^2}\dfrac{\partial \boldsymbol{E}}{\partial t}, \end{cases} \Rightarrow \begin{cases} \nabla^2 \boldsymbol{A} - \dfrac{1}{c^2}\dfrac{\partial^2 \boldsymbol{A}}{\partial t^2} &= -\mu_0 \boldsymbol{j}, \\ \nabla^2 \phi - \dfrac{1}{c^2}\dfrac{\partial^2 \phi}{\partial t^2} &= -\dfrac{\rho}{\varepsilon_0}. \end{cases} \quad (1)$$

Integrate wave equations with non-standard FDTD, in co-moving frame.

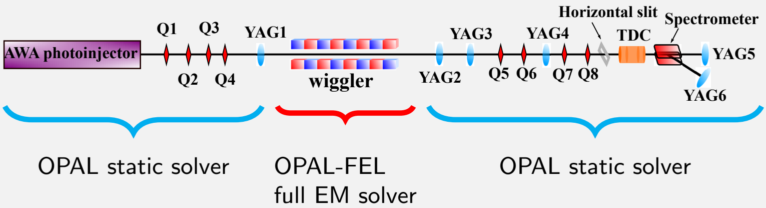
A. Fallahi et al. (2018), DOI:10.1016/j.cpc.2018.03.011
J.-L. Vay (2007), DOI: 10.1103/PhysRevLett.98.130405

OPAL-FEL: start-to-end simulation of undulator-based facilities

OPAL-FEL $=$ OPAL static solver $+$ additional full EM solver based on MITHRA

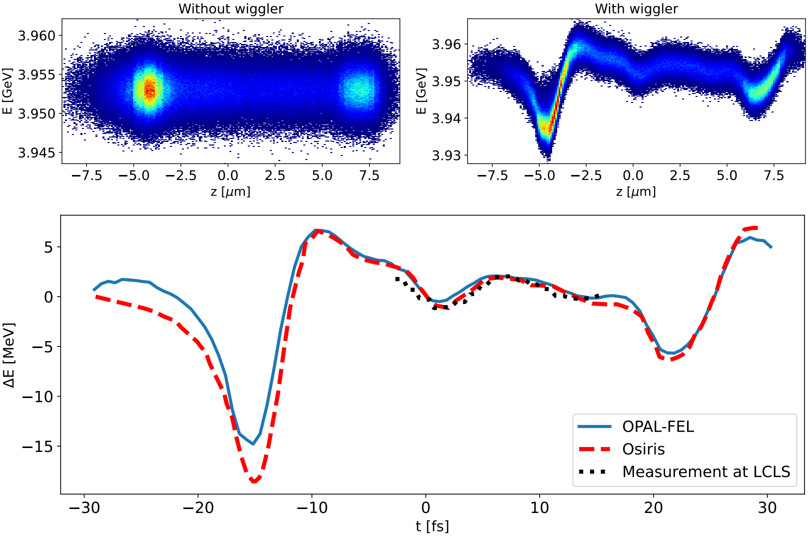
To the best of our knowledge, there are no single particle-tracking codes that can do start-to-end tracking of accelerators including wigglers/undulators.

AWA Wiggler Experiment



Benchmarking OPAL-FEL: LCLS Experiment

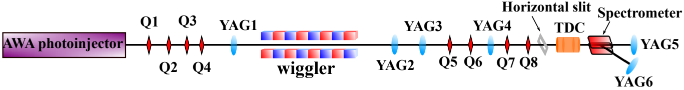
Experiment at LCLS tested wiggler effects in **radiation dominated regime**.

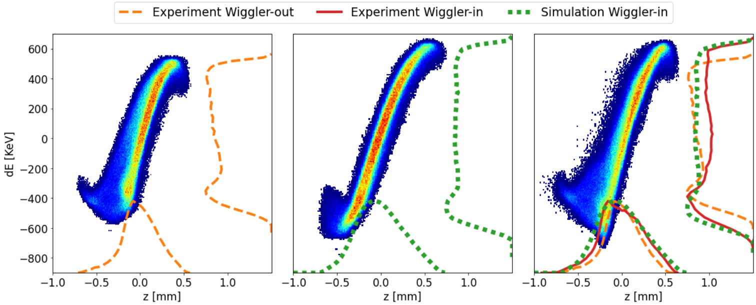


J. P. MacArthur et al. (2019), DOI:10.1103/PhysRevLett.123.214801
A. Albà et al. (2022), DOI:10.1016/j.cpc.2022.108475

The AWA POP Experiment

Testing wiggler effects in **space charge dominated regime**.





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Computer Physics Communications

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Benchmarking collective effects of electron interactions in a wiggler with OPAL-FEL ☆

Arnau Albà [a], Jimin Seok [b, c], Andreas Adelmann [a], Scott Doran [b], Gwanghui Ha [b], Soonhong Lee [b], Yinghu Piao [b], John Power [b], Maofei Qian [b], Eric Wisniewski [b], Joseph Xu [b], Alexander Zholents [b]

Summary and Outlook

- OPAL can simulate start-to-end beamlines with undulators,
- Benchmarked in radiation dominated regime (LCLS 3.95 GeV) and space charge dominated regime (AWA 45 MeV),
- Optimal use of computational resources combining electrostatic with full EM solver in different parts of beamline.

What's next (potentially):

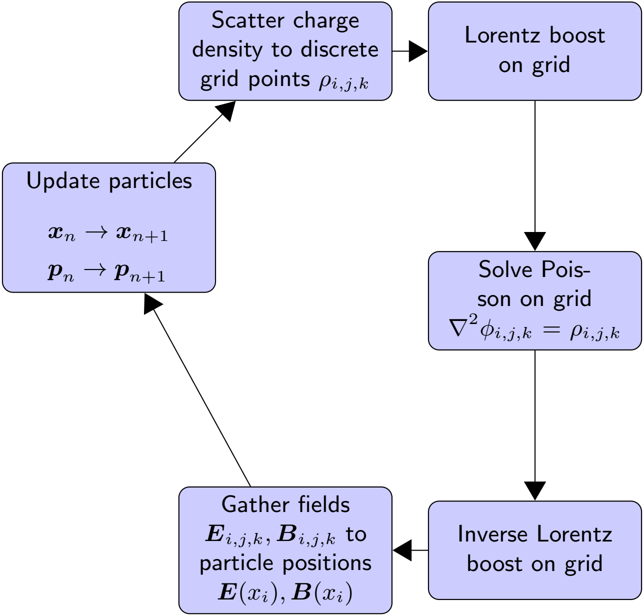
- Modeling full FELs,
- First-principle simulation of cooling schemes that use wigglers.

Questions?

Backup Slides: Experiment Parameters

	LCLS	**AWA**
L_w	2.10 m	1.1 m
K_w	51.5	10.81
N_w	6	10
λ_w	35 cm	8.5 cm
Q	200 pC	300 pC
mean E	3.95 GeV	45.5 MeV
σ_z	4.75 $\mu\mathrm{m}$	250 $\mu\mathrm{m}$
$\sigma_{x,y}$	74 $\mu\mathrm{m}$	400 $\mu\mathrm{m}$

Backup Slides: OPAL Electrostatic Solver



Backup Slides: OPAL-FEL Full EM Solver

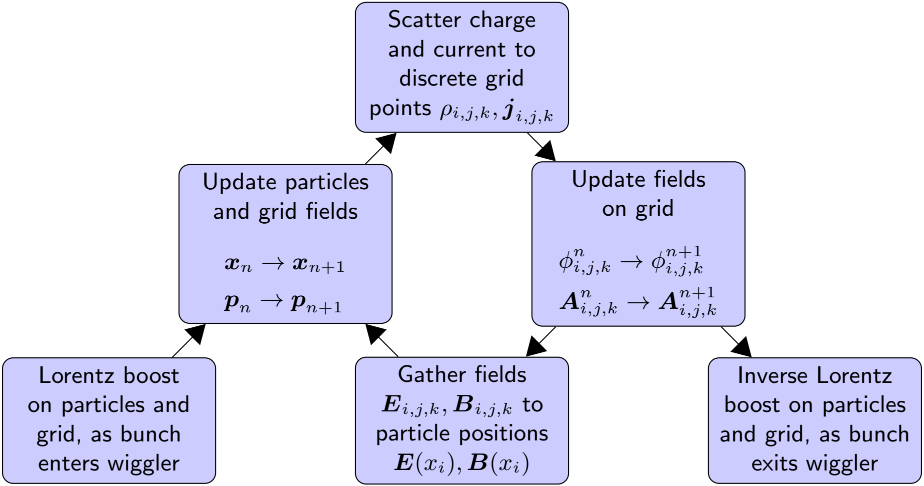
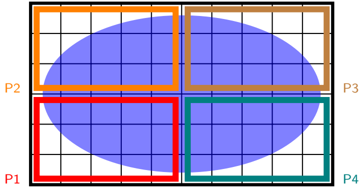


Figure: Schematic of OPAL-FEL's full-wave solver.

Backup Slides: Space Decomposition and Load Balancing



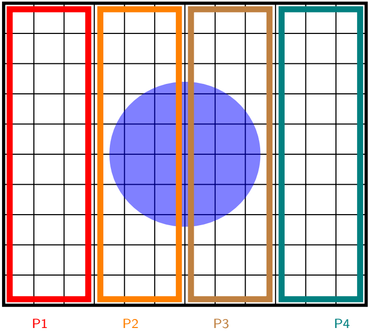


Figure: Parallelization schemes used by OPAL's solvers. The blue ellipse is the bunch, and in this example four processors share the computational load. The static solver (left) adapts the grid to tightly surround the bunch, and equally shares the number of particles among processors. The full-wave solver MITHRA (right) cannot resize the grid, and equally shares the number of cells among processors.

Backup Slides: Undulator in Co-moving Frame

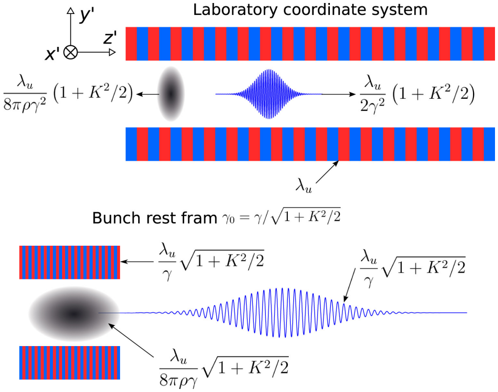


Figure: By doing the entire simulation in the co-moving frame, the bunch length, undulator period, and radiation wavelength become of comparable size. Then the computational grid can be smaller and coarser, than when solving in the lab frame.

A. Fallahi et al. (2018), DOI:10.1016/j.cpc.2018.03.011
J.-L. Vay (2007), DOI: 10.1103/PhysRevLett.98.130405