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

A. Adelmann (PSI), A. Albà (PSI) & A. Fallahi (ETH Zurich)

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ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

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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 12 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 developer team

A. Adelmann (PSI), A. Albà (PSI), P. Calvo (CIEMAT), M. Frey (U. St Andrews), A. Gsell (PSI), Ch. Kraus, S. Muralikrishnan (JSC), N. Neveu (SLAC), P. Piot (NIU), Ch. Rogers (RAL), J. Snuverink (PSI), D. Winklehner (MIT)

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Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

SLAC NATIONAL ACCELERATOR LABORATORY

UKRI Science and Technology Facilities Council

MIT Massachusetts Institute of Technology

JÜLICH Forschungszentrum

University of St Andrews

NIU Northern Illinois University

The Need for a Full EM Solver

Sven Reiche (PSI) c.f. 2021 UC-XFEL workshop:

- **Goodby ~~SVEA~~** $\Rightarrow$ **Hello PIC**

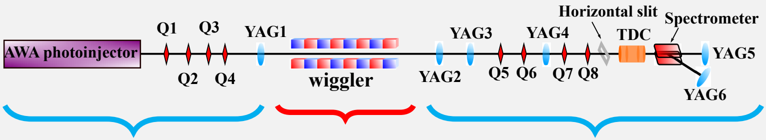
Alexander Zholents (ANL):

- when $K^2 \gg 1$, the wiggler strongly influence the longitudinal SCF
- now the frequency of plasma oscillations inside the electron bunch propagating through the wiggler become larger than the frequency of the plasma oscillations in a drift section
- the wiggler can be conveniently used to control the plasma oscillation frequency

- this feature can be useful for microbunched electron cooling
- an LDRD enabled a super cool POP experiment at AWA

The Need for a Full EM Solver

AWA Wiggler Experiment



Only space charge

(electrostatic approximation okay)

Space charge and radiation

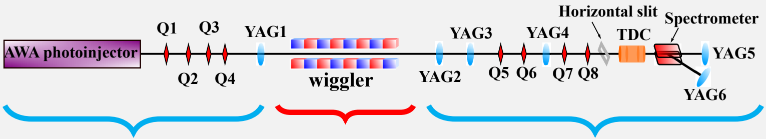
(requires full EM)

Only space charge

(electrostatic approximation okay)

The Need for a Full EM Solver

AWA Wiggler Experiment



Only space charge	Space charge and radiation	Only space charge
(electrostatic approximation okay)	(requires full EM)	(electrostatic approximation okay)

OPAL electrostatic solver:

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

Adelmann et al. (2019), DOI:10.48550/ARXIV.1905.06654

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

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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]

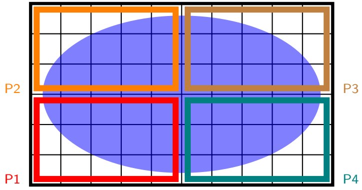
Maxwell equations rearranged into wave equations:

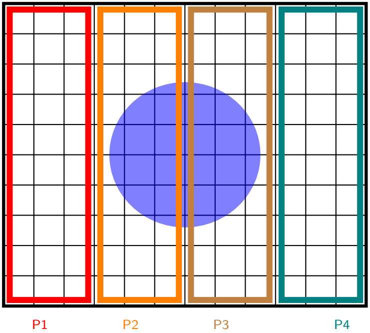
$$
\begin{cases}
\boldsymbol{\nabla} \cdot \boldsymbol{E} &= \dfrac{\rho}{\varepsilon_0}, \\
\boldsymbol{\nabla} \wedge \boldsymbol{E} &= -\dfrac{\partial \boldsymbol{B}}{\partial t}, \\
\boldsymbol{\nabla} \cdot \boldsymbol{B} &= 0, \\
\boldsymbol{\nabla} \wedge \boldsymbol{B} &= \mu_0 \boldsymbol{j}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

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

Space Decomposition and Load Balancing

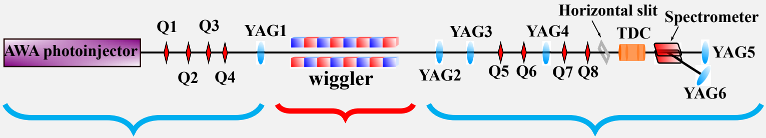




- The static solver (left) adapts the grid to tightly surround the bunch
- The full-wave solver (right) cannot resize the grid, and equally shares the number of cells among processors

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

AWA Wiggler Experiment



OPAL static solver | OPAL-FEL full EM solver | OPAL static solver

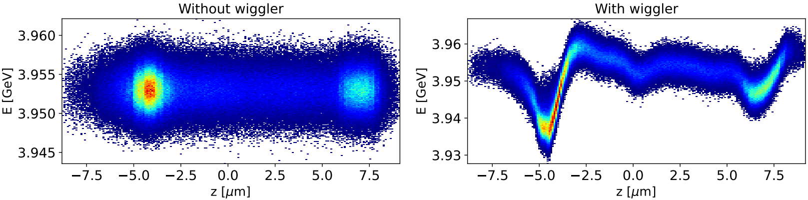
To the best of our knowledge, there are no single particle-tracking codes that can do start-to-end tracking of accelerators including wigglers/undulators.

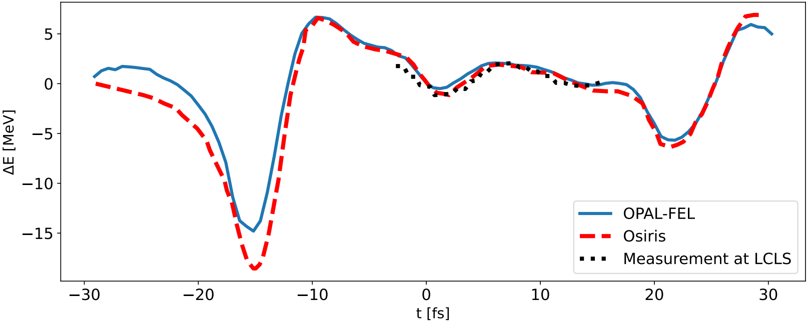
Experiment Parameters for the Benchmarks

	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 µm	250 µm
$\sigma_{x,y}$	74 µm	400 µm

Benchmarking OPAL-FEL: LCLS Experiment

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

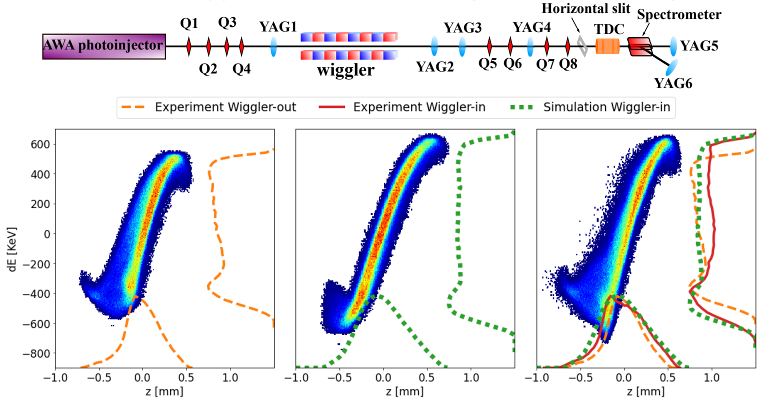




J. P. MacArthur et al. (2019), DOI:10.1103/PhysRevLett.123.214801
A. Albà et al. (2022), DOI:10.1016/j.cpc.2022.108475

The AWA POP Experiment

Effect of the wiggler in eth **space charge dominated regime**.



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Computer Physics Communications

Volume 280, November 2022, 108475

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]

Conclusions and Future work

Summary

- OPAL can simulate start-to-end accelerators 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.

Where is the gap regarding space charge computations?

1. even for compact FEL's the computational needs are substantial
2. such things like collisions are not included

What is needed to bridge this gap?

1. we need to make efficient use of field computational methods & computing hardware
2. research on what is the most efficient EM method

Backup Slides: Experiment Parameters

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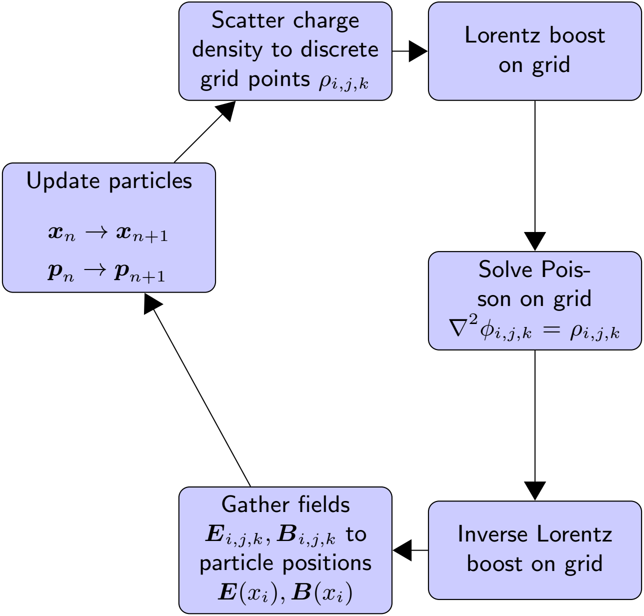
λ_w	35 cm	8.5 cm
Q	200 pC	300 pC
mean E	3.95 GeV	45.5 MeV
σ_z	4.75 μm	250 μm
$\sigma_{x,y}$	74 μm	400 μm

Backup Slides: OPAL Electrostatic Solver



Backup Slides: OPAL-FEL Full EM Solver

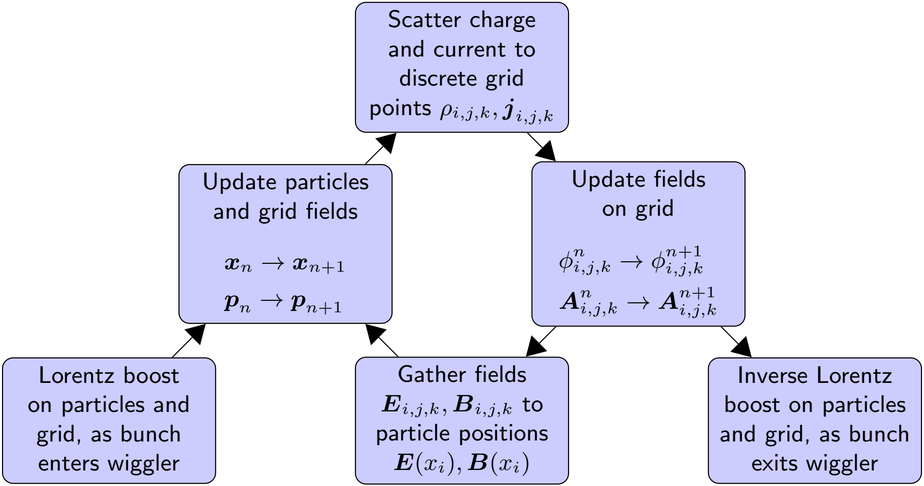
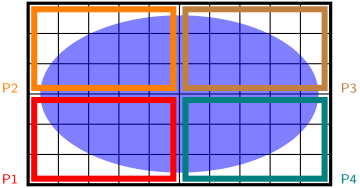


Figure: Schematic of OPAL-FEL's full-wave solver.

Backup Slides: Space Decomposition and Load Balancing



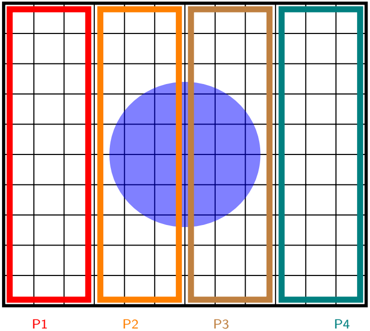


Figure: Parallelization schemes used by OPAL's solvers. The blue ellipse is the bunch, and in this example four processors share the computational load. The static solver (left) adapts the grid to tightly surround the bunch, and equally shares the number of particles among processors. The full-wave solver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

Backup Slides: Undulator in Co-moving Frame

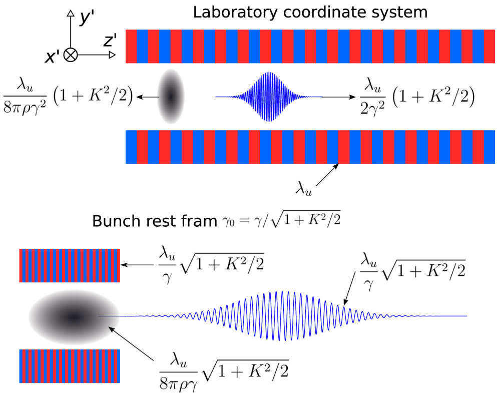


Figure: By doing the entire simulation in the co-moving frame, the bunch length, undulator period, and radiation wavelength become of comparable size. Then the computational grid can be smaller and coarser, than when solving in the lab frame.

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