Arnau Albà, PhD student

Start-to-end Modelling of FELs with OPAL-FEL Full Maxwell Solver

OPAL Retreat, June 10th 2021

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Electrostatic Approximation Downfalls

$$\begin{cases} \vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}, \\ \vec{\nabla} \wedge \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \\ \vec{\nabla} \cdot \vec{B} = 0, \\ \vec{\nabla} \wedge \vec{B} = \mu_0 \vec{j} + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t}, \end{cases} \Rightarrow \begin{cases} \nabla^2 \phi - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \phi = -\frac{\rho}{\epsilon_0}, \\ \nabla^2 \vec{A} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \vec{A} = -\mu_0 \vec{j}. \end{cases}$$

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Wave equations for fields

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Wave equations for fields

However, OPAL's FFT solver uses the **electrostatic approximation**:

$$\frac{\partial}{\partial t} \to 0 \Rightarrow \begin{cases} \nabla^2 \phi = -\frac{\rho}{\epsilon_0}, \\ \nabla^2 \vec{A} = -\mu_0 \vec{j}. \end{cases}$$

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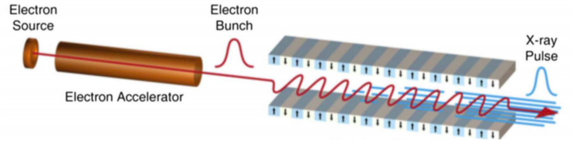
$$\frac{\partial}{\partial t} \to 0 \Rightarrow \boxed{\begin{cases} \nabla^2 \phi = -\frac{\rho}{\epsilon_0}, \\ \nabla^2 \vec{A} = -\mu_0 \vec{j}. \end{cases}}$$

Fields are **not** time dependent.

Undulators and FELs

Electrostatic approximation breaks down in wigglers and undulators because:

- Particles emit radiation
- Wiggly motion means particles in bunch move in different directions
- Wave-particle interaction effects cannot be neglected



Credit: A. Marinelli [1]

Wigglers are used to produce radiation and to shape phase-space in:

- Synchrotrons
- Free Electron Lasers
- Experimental beamlines [2], [3], [4]

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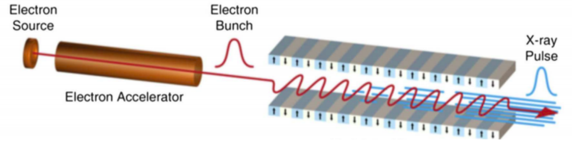

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So how do we model undulators?

Modelling Wigglers

MITHRA [5], [6] is an open source “Full-Wave Simulation Tool for Free Electron Lasers” developed by Arya Fallahi. It solves the full Maxwell equations in 3D space with an FDTD-PIC scheme, separately **integrating particles and fields**:

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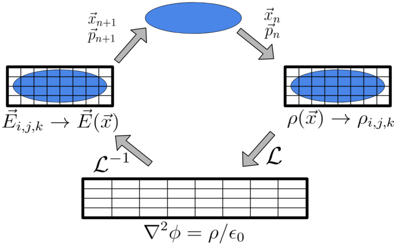
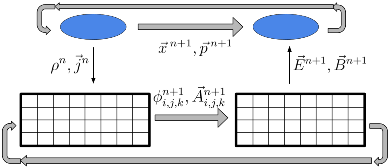


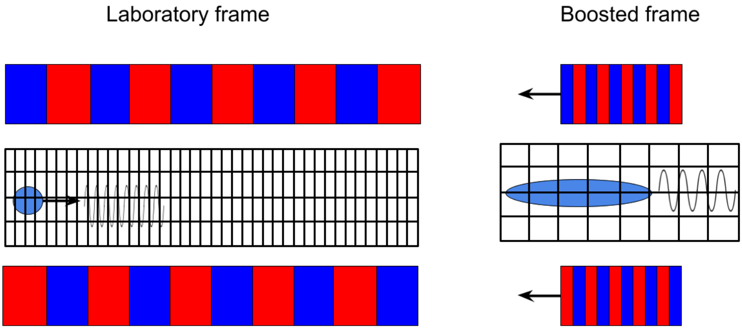
OPAL FFT solver



MITHRA (and OPAL-FEL) full-wave solver

Modelling Wigglers

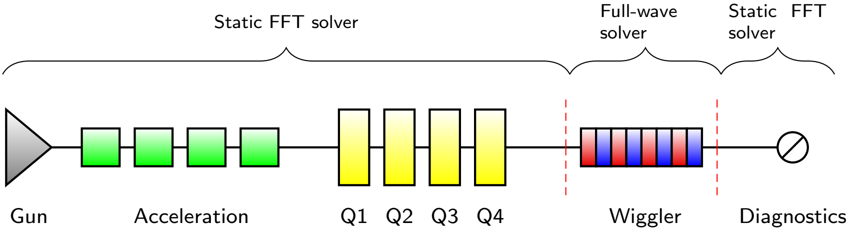
In MITHRA the mesh and fields need to be in a **inertial frame of reference**, so **an adaptive grid is not possible**.



Thus MITHRA can only work as long as the bunch has a constant mean velocity, i.e. it can only simulate the bunch inside the undulator!

Modelling Wigglers

By including MITHRA as a solver in OPAL we obtain OPAL-FEL [7], capable of **automatically switching between solvers**, and simulating full beamlines including an undulator!

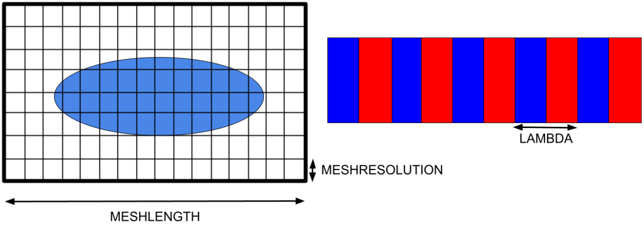


Using OPAL-FEL

Install with `cmake -DENABLE_OPAL_FEL=yes ...` (see manual for details).

The parameters of the `UNDULATOR` element also define the full-wave solver, because the full-wave solver is attached to the element:

```
UND: UNDULATOR, ELEMEDGE = 44.0e-2, K = 10.81, LAMBDA = 8.5e-2,
NUMPERIODS = 5,
MESHLENGTH = { 12e-3, 12e-3, 4e-3 }, MESHRESOLUTION = { 1e-5, 1e-5, 8e-6},
FNAME = "output.job";
```



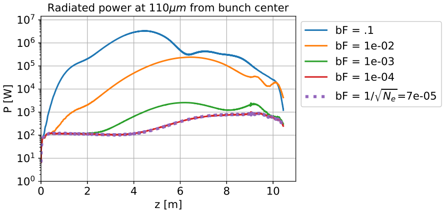
Using OPAL-FEL

Output from the full-wave solver depends on `output.job`:

```
BUNCH
{
  bunch-sampling
  {
    sample    = true
    directory = ./
    base-name = bunch-sampling/bunch
    rhythm    = 100e-12
  }
}

FIELD
{
  field-sampling
  {
    sample    = false
    type      = at-point
    field     = Ex
    field     = Ey
    field     = Ez
    directory = ./
    base-name = field-sampling/field
    rhythm    = 3.2e-12
    position  = (0.0, 0.0, 110.0e-6)
  }
}

FEL-OUTPUT
{
  radiation-power
  {
    sample          = true
    type           = at-point
    directory      = ./
    base-name      = power-sampling/power
    plane-position = 1.1e-4
  }
}
```



OPAL-FEL implementation

The `UNDULATOR` element is a drift with a wrapper function

```
void Undulator::apply(
    PartBunchBase<double, 3>* itsBunch,
    CoordinateSystemTrafo const& refToLocalCSTrafo)
```

which

- is called when bunch enters undulator fringe field (in `computeExternalFields(oth);` for OPAL-t)
- does coordinate transformation on particles before undulator
- initialises fields and mesh
- initialises and runs MITHRA full-wave solver

```
MITHRA::FdTdSC solver(mesh, bunch, seed,
    undulators, externalFields, FELs);
solver.solve();
```

- coordinate transformation back to lab frame when bunch exits undulator
- reference particle placed in bunch centroid after full-wave simulation

OPAL-FEL implementation

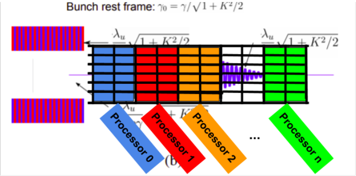
Some characteristics of the MITHRA full-wave solver:

- Uses openMPI
- Undulator field is

$$B_x = B_0 \cosh(kx)\sin(kz),$$
$$B_z = B_0 \sinh(kx)\cos(kz),$$

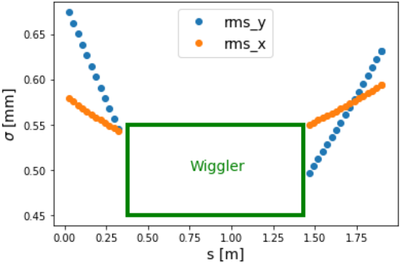
plus fringe fields with $\vec{\nabla} \cdot \vec{B} \neq 0$

- Domain decomposition uniformly divides grid, no load balancing



OPAL-FEL implementation

Full-wave solver **does not write in the OPAL stat file**:



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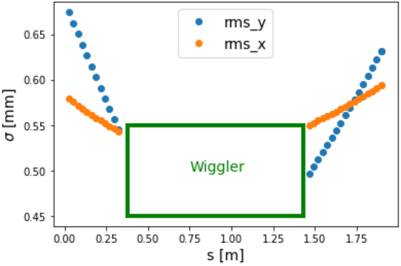
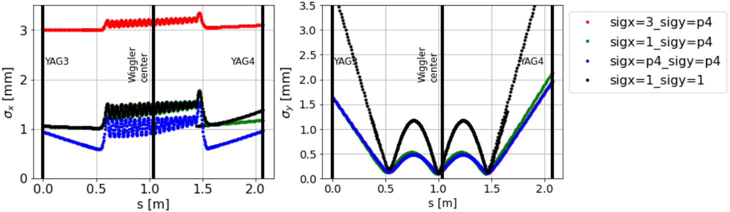
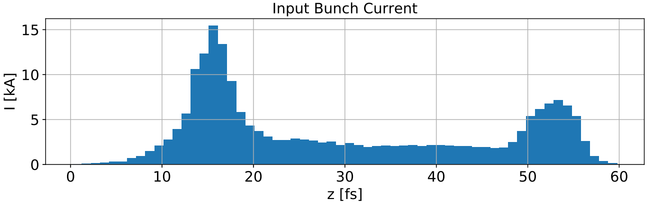


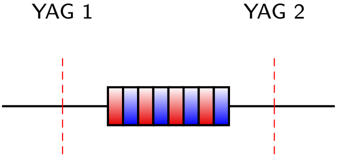
Can be fixed with Lorentz transformation of output from full-wave solver (approximation):



OPAL-FEL benchmark

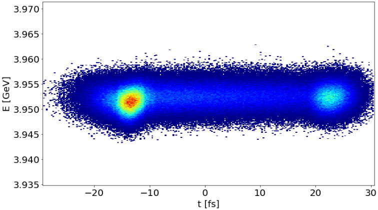
- Reproduce findings and LCLS experiment from paper by MacArthur et al. [3].
- Radiation from high current tail expected to create energy modulation in beam core.

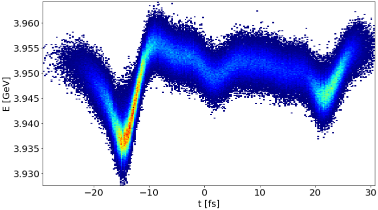


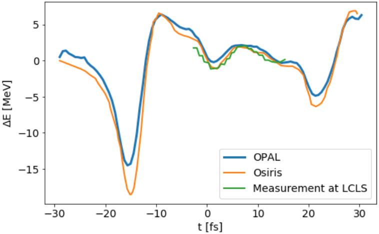



```
D1: DRIFT, ...
YAG1: MONITOR, ...
D2: DRIFT, ...
UND: UNDULATOR, ...
D3: DRIFT, ...
YAG2: MONITOR, ...
D4: DRIFT, ...
```

OPAL-FEL benchmark

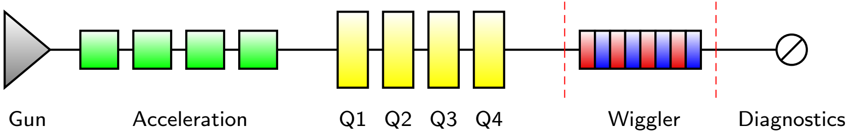






OPAL-FEL for AWA experiment

Whole beamline was modelled to prepare AWA experiment for micro-bunched electron cooling [4], [8], [9].



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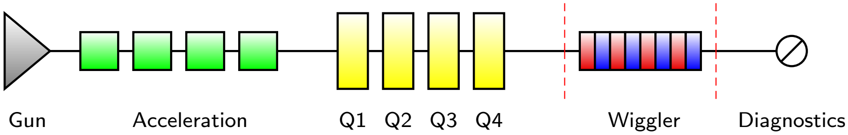

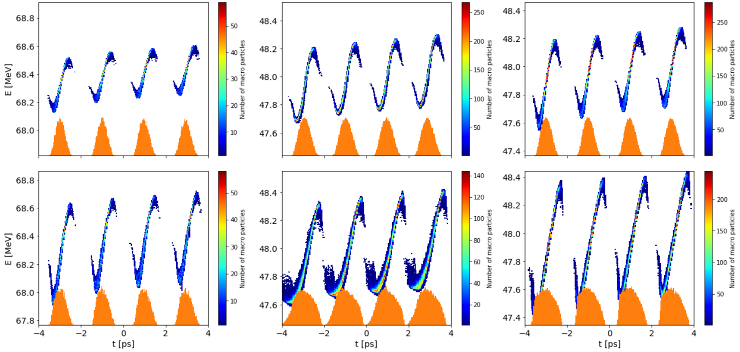

63 MeV | 44 MeV case 1 | 44 MeV case 2

Summary and Possible Improvements

- OPAL can now successfully model undulators and wigglers
- Can automatically switch between solvers
- Benchmarked and used in experiments
- Uses external MITHRA library $\Rightarrow$ full-wave solver maintained and improved externally

Drawbacks and room for improvement:

- Hacky implementation
  - Full-wave solver cannot write to stat file
  - Solver attached to undulator element only, rather than being a solver class
  - Reference particle does not see undulator
- Only available in OPAL-t
- Can only model standard flat-pole undulators, rather than arbitrary fieldmaps
- No load balancing
- Many more particles required for full-wave solver than for FFT solver

Thank you to Andreas, Arya, and all OPAL developers for the help in developing this tool.

Thank you for your attention. Questions?

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