OPAL: From Today to Tomorrow

Andreas Adelmann for the OPAL developer team

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- General Introduction
  - OPAL in a nutshell
  - Release roadmap
  - Flavours in OPAL
  - OPAL architecture
  - Future plans
- OPAL-X
  - Why are we interested in exascale

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 13 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

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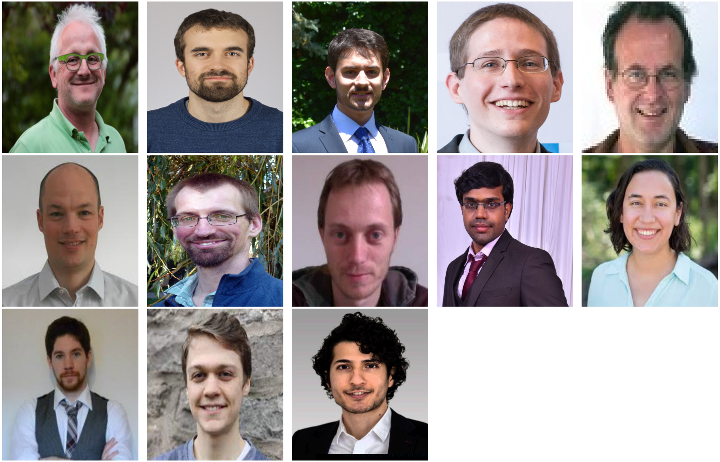
The Active OPAL Developer Team



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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

University of St Andrews

NIU Northern Illinois University

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Two OPAL flavours, OPAL-T & OPAL-CYCL

- Common features
  - 3D space charge: in unbounded, and bounded domains
  - particle Matter Interaction (protons)
  - parallel hdf5 & SDDS output
  - sampler & multi-objective optimisation
  - from e, p to Uranium (q/m is a parameter)
- OPAL-CYCL (+ FFAs + Synchrotrons)
  - neighbouring turns
  - time integration, 4th-order RK, LF, adaptive schemes
  - find matched distributions with linear space charge
  - spiral inflector modelling with space charge
- OPAL-T
  - rf-guns, injectors, beamlines [1]
  - auto-phasing (with veto)
  - full EM in `undulator` element since OPAL 2021.1
  - Particle-Particle-Particle-Mesh solver since OPAL 2022.1

[1] Proton therapy gantries & degrader

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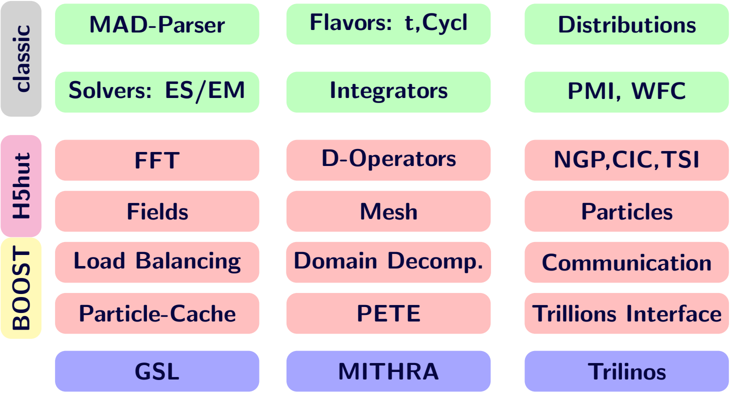
Software Architecture

MPI based

OPAL



Collision-less (non relativistic) Vlasov-Maxwell equation

$f_s \subset (\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R} :\rightarrow \mathbb{R}$ and s are the species.

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_x f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f_s = 0,$$

$$\left.\begin{array}{ll} \partial_t \mathbf{E} - c^2 \mathbf{curl}\,\mathbf{B} = \dfrac{\mathbf{J}}{\varepsilon_0}, & \nabla \cdot \mathbf{E} = \dfrac{\rho}{\varepsilon_0}, \\ \partial_t \mathbf{B} + \mathbf{curl}\,\mathbf{E} = 0, & \nabla \cdot \mathbf{B} = 0, \end{array}\right\} \quad \text{Maxwell's equations}$$

where the source terms are computed by

$$\rho = \sum_s q_s \int f_s \, d\mathbf{v}, \qquad \mathbf{J} = \sum_s q_s \int f_s \mathbf{v} \, d\mathbf{v}.$$

In some cases Maxwell's equations can be replaced by a reduced model like Poisson's equation. The electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ are superpositions of external fields and self-fields (space charge),

$$\mathbf{E} = \mathbf{E}_{\text{ext}} + \mathbf{E}_{\text{sc}}, \quad \mathbf{B} = \mathbf{B}_{\text{ext}} + \mathbf{B}_{\text{sc}}.$$

A Direct Fast FFT-Based Poisson Solver

Assume you know G the Green's function

The solution of the Poisson's equation

$$\nabla^2 \phi = -\rho/\varepsilon_0,$$

for the scalar potential, ϕ can be expressed as:

$$\phi(x,y,z) = \int\int\int dx'dy'dz'\rho(x',y',z')G(x-x',y-y',z-z'), \quad (1)$$

where G is the Green function and ρ is the charge density.
Discretisation of Eq. (1) on a grid with cell sizes h_x, h_y and h_z leads to:

$$\phi_{i,j,k} = h_x h_y h_z \sum_{i'=1}^{M_x} \sum_{j'=1}^{M_y} \sum_{k'=1}^{M_z} \rho_{i',j',k'} G_{i-i',j-j',k-k'}, \quad (2)$$

The solution of Eq. (2) can be obtained using FFT based convolution:

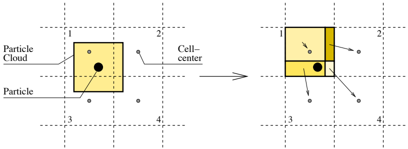
$$\phi_{i,j,k} = h_x h_y h_z \; \mathsf{FFT}^{-1}\{(\mathsf{FFT}\{\rho_{i,j,k}\}) \otimes (\mathsf{FFT}\{G_{i,j,k}\})\}$$

A fast Direct FFT-Based PIC Poisson Solver

Assume you know G the Green's function

Solving for ϕ using $\phi(\mathbf{x}) = \dfrac{1}{4\pi\varepsilon_0}\displaystyle\int G(\mathbf{x},\mathbf{x}')\rho(\mathbf{x})d\mathbf{x}'$ is expensive $\mathcal{O}(N^2)$ with N number of particles/grid-points.

1. Let Ω be spanned by a Cartesian structured mesh of $l \times n \times m$ with $l = 1 \dots M_x$, $n = 1 \dots M_y$ and $m = 1 \dots M_z$. The mesh size is a function of time: $h_x(t), h_y(t)$ and $h_z(t)$
2. Discretize $\rho \to \rho_h$ and $G \to G_h$ on a regular grid (PIC)



3. Go to Fourier space $\rho_h \to \widehat{\rho}_h$, $G_h \to \widehat{G}_h$ and convert the convolution into a multiplication $\widehat{\phi}_h = \widehat{\rho}_h * \widehat{G}_h$ in $\mathcal{O}(N \log N)$
4. Use a parallel FFT, particle and field load balancing

OPAL Releases I

- Consolidation has begun with V 2.0
  - ✓ major rewrite of OPAL-T, Distribution class
  - major rewrite of OPAL-CYCL, (ongoing)
  - ✓ strong typing, versioning of input files
  - ✓ no multipacting
  - ✓ no envelope model
  - ✓ Manual is converted to Wiki
  - ✓ `gitlab` and issue tracker
- new features (V. 2.1)
  - ✓ **Sampler - create random samples easily**
  - ✓ GA based MOOP fully integrated
- new features (V. 2.2)
  - ✓ curved multipoles (FFAG and Proton Therapy Modelling)
  - map tracking (experimental)

OPAL Releases II

- ✓ $\mathcal{M}_{sc}$ based on moments of the distribution
  - AMR-Fieldsolver
- new features (V. 2.4)
  - MultiGauss distribution for microbunched beams
  - `SOURCE` element can be made `TRANPARENT` for backtracking particles
  - many more plus all bug fixes can be found here

New Release Numbering since 2021

- OPAL 2021.1
  - New Undulator element with its own FDTD electromagnetic solver
  - Energy loss calculation and beam scattering for all light ions
  - ALPHA particles are supported in BEAM command
  - Gas stripping for DEUTERON beams and H2P beams in AIR
- OPAL 2022.1
  - Python interface for OPAL

OPAL Releases III

- P3M solver (Particle-Particle-Particle-Mesh)

Papers and Presentations: https://gitlab.psi.ch/OPAL/src/-/wikis/OPALPresentations

Future Plans for OPAL

$\Longrightarrow$ we will release one more “old“ OPAL i.e. OPAL 2023.1
$\Longrightarrow$ after that only bugfixes

Expecting for OPAL 2023.1:

- several documented issues are fixed
- pyOPAL is ready for FFA modelling
- more on FFA modelling

OPAL-X

Massive Parallelism, Performance, and Portability

- New hardware capabilities: **Exascale** (10^{18} FLOPS)

  $\Longrightarrow$ **Massive parallelism.**

- Must **efficiently** use these high operations per second

  $\Longrightarrow$ **Performance.**

- Architectures are **heterogeneous** i.e. CPUs & GPUs

  $\Longrightarrow$ **Portability.**

- Algorithm considered: **Particle-In-Cell** codes.

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OPAL-X

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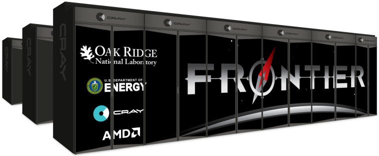
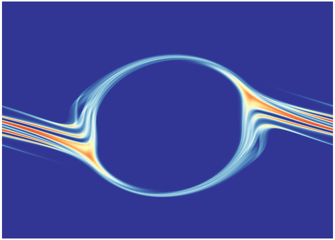


Why Exascale Particle-in-Cell?



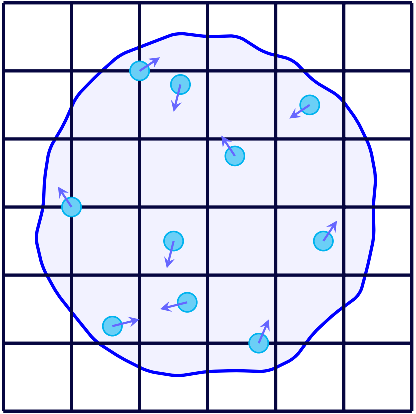
Two-stream instability.

$\implies$ Compute-intensive

$\implies$ High resolution

- Method used in **plasma physics**, **astrophysics**, and **accelerator physics**.
- Lends itself well to parallelization.
- Massive parallelism $\implies$ higher resolution simulations.

The Particle-in-Cell (PIC) method



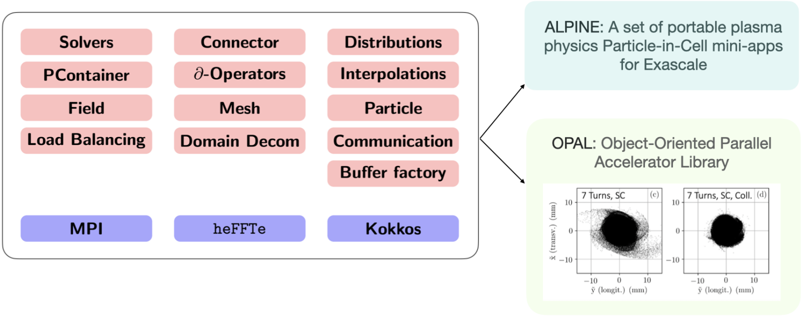
- macro ... real particles.
- Track evolution in phase space, but compute fields on the grid.
- Avoid pairwise computation $\mathcal{O}(N^2)$, $N =$ no. particles.
- Equations of motion:

$$\frac{d\boldsymbol{r}}{dt} = \frac{\boldsymbol{p}}{m\gamma}$$

$$\frac{d\boldsymbol{p}}{dt} = q\left(\boldsymbol{E} + \frac{\boldsymbol{p}}{m\gamma} \times \boldsymbol{B}\right)$$

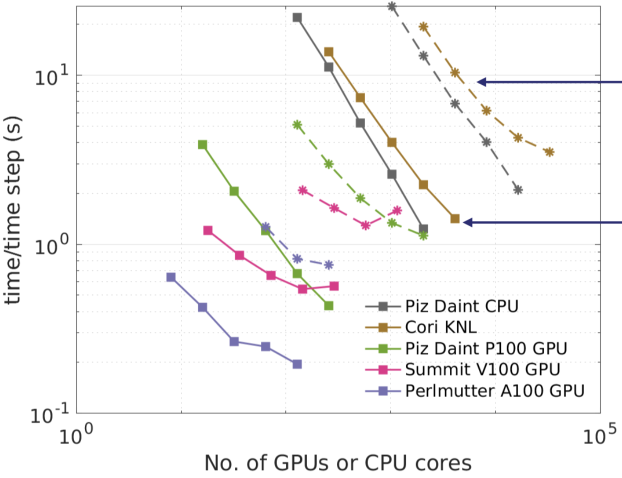
IPPL the base of OPAL

IPPL V2.0 Open source C++ library for Particle-in-Cell



For ALPINE see preprint

IPPL: Scaling across architectures



Dashed: 1024^3 grid, 8B particles

Solid: 512^3 grid, 1B particles

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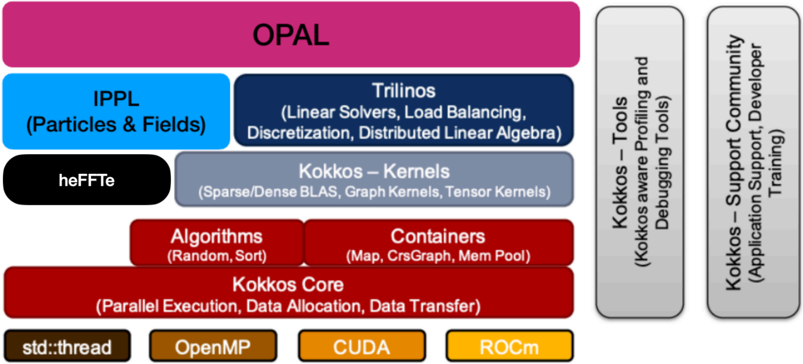
OPAL-X I

getting getting ready for Exascale



Biggest changes are:

- C++20 (massive reduction of lines of code)

OPAL-X II

getting getting ready for Exascale

- no more OPAL flavours
- full FEM electromagnetic solver (PhD project)
- new $2\frac{1}{2}$ dimensional solver for long bunches
- add collisions beyond P3M
- OPAL can be controlled from Python (pyOPAL-X)