Development of the simulation code OPAL

Pedro Calvo Portela

on belhalf of the OPAL developer team

Snowmass'21 Workshop on High Power Cyclotrons

September 9, 2021

Contents

OPAL [1]

Open-source tool for charged-particle optics in large accelerator structures and beam lines including 3D space charge, particle matter interaction and multi-objective optimization

- OPAL is built from the ground up as a parallel application exemplifying the fact that HPC (High Performance Computing) is the third leg of science, complementing theory and the experiment
- OPAL provides parallel calculations on your laptop as well as on the largest HPC clusters
- OPAL uses the MAD language with extensions.

[1] A. Adelmann *et al.*, arXiv:1905.06654 (2019)

Open Source Development

- OPAL is hosted on gitlab ⟶ https://gitlab.psi.ch/OPAL/src
- Stable release versions available via binaries on Linux and macOS
- Continuous bugfixes and enhancements following the issue tracker and the OPAL discussion forum
- The OPAL framework ⟶ Manual
- Quality assurance and reproducibility of results through more than 200 regression tests
- International developer team


PAUL SCHERRER INSTITUT

Open Source Development

The *OPAL* Framework: Version 2.5

Andreas Adelmann (PSI) · Pedro Calvo (CIEMAT) · Matthias Frey (PSI) · Achim Gsell (PSI) · Uldis Locans (PSI) · Christof Metzger-Kraus · Nicole Neveu (SLAC) · Chris Rogers (RAL) · Steve Russell (LANL) · Suzanne Sheehy (Oxford) · Jochem Snuverink (PSI) · Daniel Winklehner (MIT) – 2021-07-02

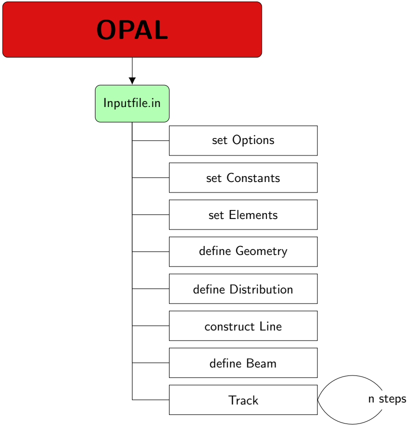
Users (~70)

The OPAL framework in the latest release version 2021.1 comes in two flavours:

- **OPAL-CYCL**
  - Track particles in cyclotrons and FFAs with time as the independent variable.
  - Time integration ⟶ 4th-order RK, LF, adaptive schemes
  - Neighbouring turns
  - Matched distribution generator
  - Geometry modelling
- **OPAL-T**
  - Beam lines, linacs, RF-photo injectors and complete X-ray Free-Electron Laser
  - Auto-phasing

Common features:

- 3D space charge
- Particle-Matter Interactions
- Parallel hdf5 & SDDS output
- Multi-objective optimization
- OPAL Sampler
- Post Processing ⟶ pyOPALTools



The phase space evolution in OPAL is based on the collisionless Vlasov-Poisson equation considering electromagnetic interaction with charged particles and taking advantage of the electrostatic approximation:

$$\frac{df(\boldsymbol{x},\boldsymbol{p},t)}{dt} = \gamma m_0\, \partial_t f + \boldsymbol{p}\cdot\nabla_x f + q\left(\boldsymbol{E}(\boldsymbol{x},t) + \frac{1}{\gamma m_0}\,\boldsymbol{p}\times\boldsymbol{B}(\boldsymbol{x},t)\right)\cdot\nabla_{\boldsymbol{p}} f = 0$$

$$\boldsymbol{E} = \boldsymbol{E}_{ext} + \boldsymbol{E}_{sc}$$

$$\boldsymbol{B} = \boldsymbol{B}_{ext} + \boldsymbol{B}_{sc}$$

- Accelerator description $\longrightarrow$ Elements $\longrightarrow$ External fields $\equiv$ $\boldsymbol{E}_{ext}$, $\boldsymbol{B}_{ext}$
- Self-fields $\equiv$ $\boldsymbol{E}_{sc}$, $\boldsymbol{B}_{sc}$ $\longrightarrow$ Poisson's equation $\longrightarrow$ `FIELDSOLVER` command
- Initial beam $\longrightarrow$ `DISTRIBUTION` command
- Particle definition $\longrightarrow$ `BEAM` command

Multi-Objective Optimization [2][3]

Large-scale multi-objective design optimization enables the automated identification of working points in high dimensional search and decision spaces. Multi-object optimization algorithms tackle the non-trivial task of beam dynamics studies for particle accelerators

- Multi-Objective Genetic Algorithm NSGA-II
- Optimizer is fully integrated in the OPAL framework
- Access to all OPAL statistics data
- Access to all OPAL variables as design variables
- Specify the MOOP in the OPAL input file
- Runs smoothly with more than 10000 cores
- Finds Pareto optimal solutions

[2] Y. Ineichen *et al.*, Comput. Sci. Res. Dev. 28, 185 (2013)

[3] N. Neveau *et al.*, Phys. Rev, Accel. Beams 22, 054602 (2019)

Particle-matter interactions

OPAL combines the particle tracking through an accelerator or beamline with a Monte Carlo simulation of the beam interaction with matter [4][5]

- Energy loss

  Stopping power of light ions ⟶
  - Semi-empirical formulas of Andersen and Ziegler
  - Bethe-Bloch equation
  - Energy straggling

- Scattering physics
  - Multiple Coulomb Scattering
  - Large Angle Rutherford Scattering

[4] V. Rizzoglio *et al.*, Phys. Rev, Accel. Beams 20, 124702 (2017)

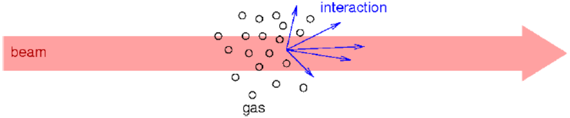
[5] V. Rizzoglio *et al.*, Nucl. Instrum. Methods A. 898, 1 (2018)

Beam stripping

Assume particles incident on a homogeneous medium subjects to a process with a mean free path λ between interactions:

$$\text{Interaction probability} \longrightarrow P(x) = 1 - e^{-x/\lambda}$$

- Residual gas interaction



- Mean free path $\rightarrow \dfrac{1}{\lambda} = N_{Total}\,\sigma_{Total}$
- Analytic expressions for cross section as a function of particle energy [6][7][8]

[6] C. F. Barnett, Tech. Rep. ORNL-6068/V1, Oak Ridge National Laboratory (1990)

[7] Y. Nakai *et al.*, At. Data Nucl. Data Tables 37, 69 (1987)

[8] T. Tabata and T. Shirai, At. Data Nucl. Data Tables 76, 1 (2000)

Electromagnetic stripping

Ions + Magnetic field $\longrightarrow$ Electrons and nucleus are bent in opposite direction

$$\text{Mean free path} \longrightarrow \frac{1}{\lambda} = \frac{1}{\beta c \gamma \tau}$$

$\tau \longrightarrow$ Lifetime from formal theory of decay [9]

Beam stripping in OPAL[10]

- New physics model implemented in OPAL-CYCL
- Beam species: p, d, H^-, H_2^+
- Residual gas composition $\rightarrow$ air, H_2
- Secondary ions could be traced
- Beam fraction lost is evaluated individually for each particle in each step through a random number generator

[9] L. R. Scherk, Can. J. Phys. 57, 558 (1979)

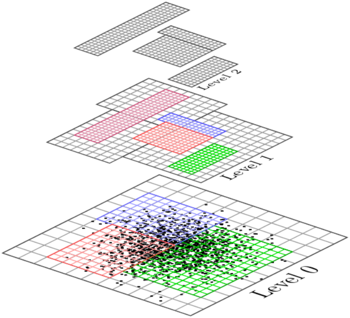
[10] P. Calvo *et al.*, *Beam stripping interactions in compact cyclotrons*, ZC10188, paper accepted to be published in Phys. Rev, Accel. Beams

Adaptive Mesh Refinement [11]

- Requirements on Particle-in-Cell (PIC) Model:
  - Solving large-scale N-body problems of $\mathcal{O}(10^9 \ldots\ 10^{10})$ particles coupled with Maxwell's equations in the electrostatic approximation
  - High resolution to cover tiny halo effects = Extremely fine mesh of $\mathcal{O}(10^8 \ldots\ 10^9)$ grid points

- Bottlenecks
  - Waste of memory and resolution in regions of void

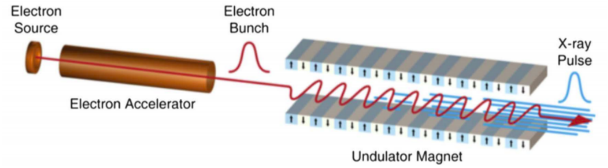
- Solution:
  - Block-structured adaptive mesh-refinement (AMR)
  - General interface to AMR libraries (in use: AMReX 2)
  - Hardware independent implementation (CPU/GPU/XXX) $\longrightarrow$ Trilinos



[11] M. Frey *et al.*, Comput. Phys. Commun. 247, 106912 (2020)

OPAL and Radiation [12]

- New OPAL Element ⟶ `UNDULATOR`
- Full-wave solver (3D) attached to the undulator element
- External C++ library ⟶ MITHRA [13] ⟶ Full-Wave Simulation Tool for Free Electron Lasers maintained and improved externally
- MITHRA + OPAL ⟹ OPAL-FEL

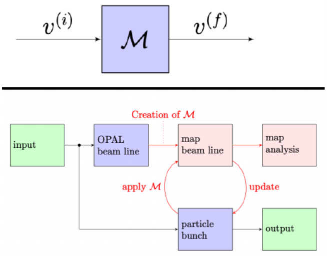


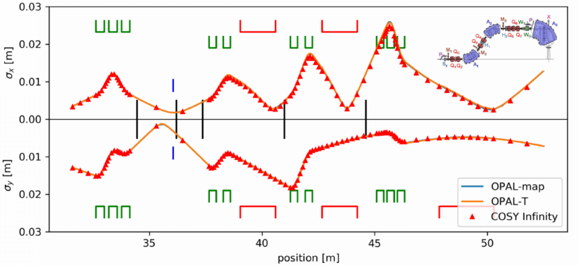
[12] A. Alba, MSc. thesis, ETH Zurich (2020)

[13] A. Fallahi *et al.*, Comput. Phys. Commun. 228, 192 (2018)

OPAL-MAP

- Map tracking beam optics code that computes maps for each beam line element to describe the action of the system
- The map creation is done by applying the Lie Operator on the element Hamiltonian and calculated in the Truncated Power Series
- OPAL elements available $\longrightarrow$ DRIFT, DIPOLE and QUADRUPOLE





OPAL Ring Element

OPAL requires modification to adequately track FFA field maps

- OPAL-T allows tracking through a set of beam elements in linac-type geometry
- OPAL-CYCL previously hard coded to use 2D mid-plane field map + single RF cavity
- Aim to introduce the capability to track through a set of arbitrary beam elements in ring-type geometry
- Additionally introduce specific capability to track through a 3D field map in a sector-type geometry
- Analytic field scaling for FFAs

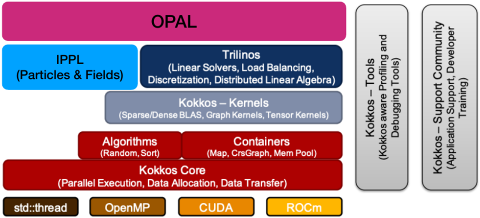
Miscellaneous

- ▷ Computing Hardware Independence and scalability ⟶ Kokkos integration
- ▷ Respond to user needs ⟶ pyOPAL
- ▷ Improving computational time ⟶ Continue consolidation & code cleanup
- ▷ Enhance physics models

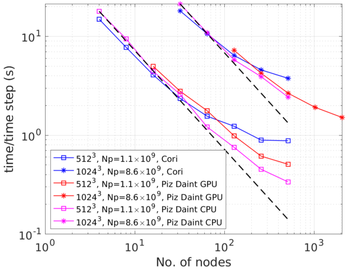
Two problems for the future we need to address now!

- ▷ Computing HW topologies are changing toward ML & data science (portability)
- ▷ Need to perform well on large heterogeneous HPC systems (scalability)

Future OPAL architecture ⟶ Exascale Machines



Preliminary scaling of relevant OPAL Kernels



curtesy of Dr. Muralikrishnan Sriramkrishnan

Thank You!

To the OPAL developer collaboration

- Andreas Adelmann
- Achim Gsell
- Chris Rogers
- Arnau Albà
- Christof Metzger-Kraus
- Jochem Snuverink
- Matthias Frey
- Nicole Neveu
- Daniel Winklehner

PAUL SCHERRER INSTITUT PSI

Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

UKRI Science and Technology Facilities Council

SLAC NATIONAL ACCELERATOR LABORATORY

MIT Massachusetts Institute of Technology

And to all of you for your attention!