An Update on OPAL - the Open Source Charged Particle Accelerator Simulation Library

A. Adelmann for the OPAL developer team

Overview

Selection of Past Achievements

Code Benchmarking

Work in Progress
The OPAL Developer Team
Please join the OPAL Developer Team

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OPAL & Open Source Development

Frequency of master commits 2013-2019 (today):

- hosted on gitlab.psi.ch
- anonymous read-only access with https://gitlab.psi.ch/OPAL/src.git
- binaries (Linux, MAC OS-X soon again)
- reproducibility of results → more than 200 regression tests
- 4th developer week hosted by SLAC, March 28 to April 3 2020
OPAL in a Nutshell

OPAL is an open-source tool for charged-particle optics in large accelerator structures and beam lines including 3D space charge, particle matter interaction, partial GPU support and multi-objective optimisation.

- 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 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.
- Webpage: https://gitlab.psi.ch/OPAL/srcwikis/home
- the OPAL Discussion Forum: https://lists.web.psi.ch/mailman/listinfo/opal
- \( \mathcal{O}(40) \) users
2 OPAL flavours, OPAL-t & OPAL-cycl are released

- **Common features**
  - 3D space charge: in unbounded, and bounded domains
  - particle Matter Interaction (protons)
  - parallel hdf5 & SDDS output
  - 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
  - auto-phasing (with veto)

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1Proton therapy gantries & degrader
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Vlasov-Poisson Equation

When neglecting collisions, and taking advantage of the electrostatic approximation, the Vlasov-Poisson equation describes the (time) evolution of the phase space $f(x, v; t) > 0$ when considering electromagnetic interaction with charged particles.

$$ \frac{df}{dt} = \frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{q}{m} (E(x, t) + v \times B(x, t)) \cdot \nabla_v f = 0. \quad (1) $$

Solving with ES-PIC

- Hockney and Eastwood, $h_x(t), h_y(t), h_z(t)$, $M = M_x \times M_y \times M_z$
- SAAMG-PCG solver with geometry [AA et al., JCP, 229 12 (2010)]
- change $M$ during simulation (many different field solver instances)
- adaptive in $\Delta t$
- modern computational architectures
Software Architecture

MPI based + HW accelerators + Optimiser
**Example 1: FFT Poisson solver**

**Example:** simulation for the PSI Ring Cyclotron.

**Host code 8 cores:** 2x Intel Xeon Processor E5-2609 v2

**Accelerator:** Nvidia Tesla K20 or Nvidia Tesla K40

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Example 2: Degrader for proton therapy

[Rizzoglio et al. Phys. Rev. AB 20 (2017)]

PROSCAN facility
Beam line toward Gantry-3

COMET-cyclotron
(proton - 250 MeV)

Graphite degrader
(230 - 70 MeV)
Example 2: MC simulations for the degrader - results

Example: OPAL 1cm thick graphite degrader example.
Host code: 2x Intel Xeon Processor E5-2609 v2
Accelerator: Nvidia Tesla K20, K40 or Intel Xeon Phi 5110p

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Multi-Objective Optimisation with OPAL


- Access to **all** OPAL statistics data as QoIs.
- Access to **all** OPAL variables as design variables
- Specify the MOOP in the OPAL input file
- Runs smoothly with more than 10000 cores
- No tight coupling to parallelisation mechanism
- No tight coupling to optimisation algorithm
- Finds Pareto optimal solutions (NSGA-II)
Example High Charge Argonne Wakefield Accelerator
Assume particles incident on a homogeneous medium subjects to a process with a mean free path $\lambda$ between interactions

- Residual gas interaction

Mean free path $\rightarrow \frac{1}{\lambda} = N_{Total} \sigma_{Total}$

Ideal gas law $\rightarrow$ Gas density $\rightarrow N$

- Electromagnetic stripping

- model validated for a large drift for $H^-$ beam
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Precise high intensity cyclotron modelling
[Y. Bi, AA, et al., PR-STAB 14(5) (2011)]

Neighbouring bunch modelling
[J. Yang, AA, et al., PR-STAB 13(6) (2010)]

Realistic Injection Simulations of a Cyclotron Spiral Inflector
[Winklehner et al. PR-STAB 20 (2017)]

Intensity limits of the PSI Injector II cyclotron
[Kolano et al. NIM-A 885 (2018)]
Simulation of the DAEδALUS Cyclotron

[Winklehner et al. PR-STAB 20 (2017)]

- OPAL-\texttt{CYCL} flavour with SAAMG-PCG solver
- Geometry loaded as *.h5, OPAL performs initialization with voxelization for fast intersection tests at runtime
- Consider complicated spiral inflector- and grounded electrodes as boundary conditions for field solver (mirror charges) and particle termination
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Benchmarking - Single Particle Tracking

[S. L. Sheehy, et al.]
Space Charge Benchmarking
[N. Neveu. NAPAC 2016]

Transverse Beam Size

Normalized Emittance

Bunch Length

Energy
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New OPAL Element **Ring**
Mostly contributed by C. Rogers

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
- ramps for rf and magnets can be specified (via. polynomial)
- analytic field scaling for FFAs
- rf fringe-fields
High Power FFA Modeling
Ch. Rogers, S. Sheehy (RAL)

- ramps for rf and magnets can be specified (via. polynomial)
- analytic field scaling for FFAs
- rf fringe-fields
Vertical FFA Model
Ch. Rogers (RAL)

VFFA analytical field (magnet coordinates):

\[ B_x = \sum_n B_0 \exp(mz) \frac{1}{m} \partial_x f_n y^n \]
\[ B_y = \sum_n B_0 \exp(mz) \frac{n + 1}{m} f_{n+1} y^n \]
\[ B_z = \sum_n B_0 \exp(mz) f_n y^n \]

With end field \( f(x) \) and

\[ f_0 = f(x) \]
\[ f_1 = 0 \]
\[ f_{n+2} = \frac{-1}{(n+2)(n+1)} [\partial_x^2 f_n + m^2 f_n]. \]

- 15 cell FODO lattice
- Two rectangular magnets in each cell
- Many orbits are shown – trajectory in plan is the same
  - Fundamental property of vFFA
Vertical FFA Model

Ch. Rogers (RAL)

800 MeV

400 MeV
OPAL-MAP (work in progress)

PSI Gantry-2 optics (MSc. thesis P. Ganz)

- truncated power series and Lie-Methods
- maps up to arbitrary
- space charge maps
Adaptive Mesh Refinement (AMR) in OPAL
Ph.D. project M. Frey [M. Frey et al. accepted for publication in CPC]

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

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

- **Solution:**
  - Block-structured adaptive mesh-refinement (AMR)
Adaptive Mesh Refinement (AMR) in OPAL

- General interface to AMR libraries (in use: AMReX$^2$)
- Hardware independent implementation (CPU/GPU/XXX)

$^2$https://amrex-codes.github.io/amrex/
Miscellaneous

- pyOPAL (maybe after the retreat in 2020)
- OPAL and Exascale: hardware independent
- Opus magnum: OPAL paper [arXiv:1905.06654]

OPAL a Versatile Tool for Charged Particle Accelerator Simulations

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References I


[Rizzoglio et al. NIM-A 889 (2018)]  V. Rizzoglio, AA, et al. NIM-A Volume 898, 1 August 2018, Pages 1-10


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