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

A. Adelmann for the OPAL developer team

FFA 2019 - Villigen - 21. November 2019

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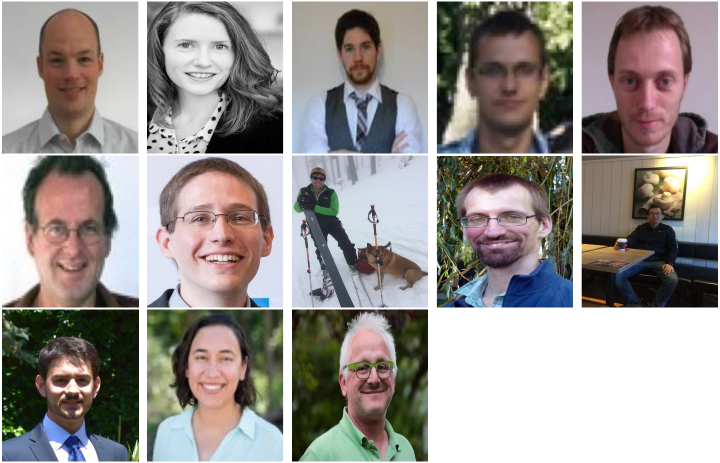
The OPAL Developer Team



Please join the OPAL Developer Team

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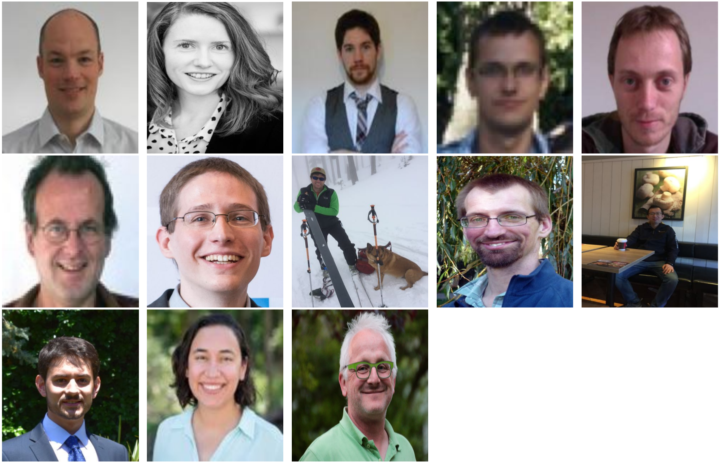

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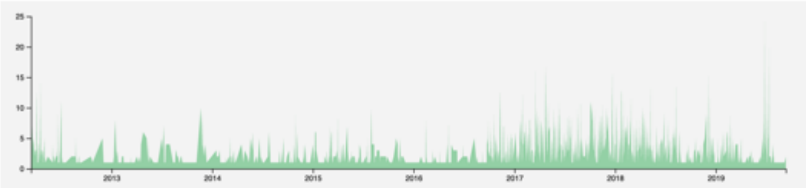
OPAL & Open Source Development

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 I

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/src/wikis/home
- the OPAL Discussion Forum: https://lists.web.psi.ch/mailman/listinfo/opal
- $\mathcal{O}(40)$ users

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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[1]
  - auto-phasing (with veto)

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[1] Proton therapy gantries & degrader
[Rizzoglio et al. Phys. Rev. AB 20 (2017) , Rizzoglio et al. NIM-A 889 (2018)]

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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 $f(\mathbf{x}, \mathbf{v}; t) > 0$ when considering electromagnetic interaction with charged particles.

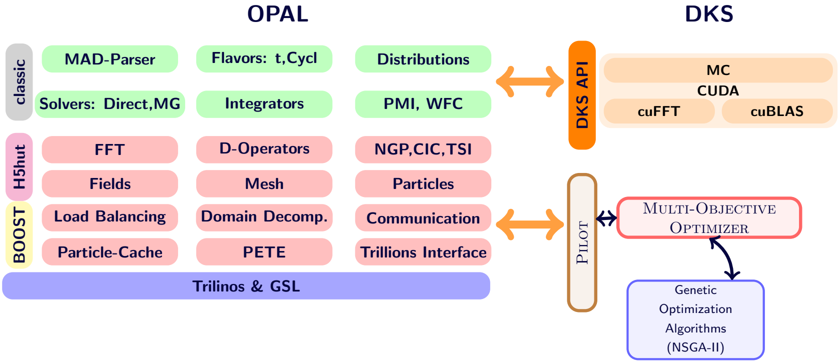
$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \frac{q}{m}(\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t)) \cdot \nabla_v f = 0. \qquad (1)$$

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 Δt
  [M. Toggweiler, AA, et al. J. Comp. Phys. **273** (2014)]
- modern computational architectures

Software Architecture

MPI based + HW accelerators + Optimiser



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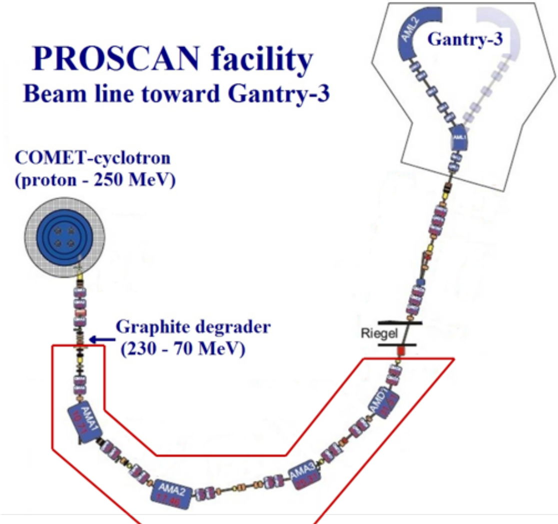
Example 1: FFT Poisson solver

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

FFT size	DKS	Total time (s)	OPAL speedup	Solver t (s)	Solver speedup
64x64x32	no	324.98		22.53	
	K20	**311.17**	$\times$**1.04**	**7.42**	$\times$**3**
	K40	**293.7**	$\times$**1.10**	**7.32**	$\times$**3**
128x128x64	no	434.22		206.73	
	K20	**262.74**	$\times$**1.6**	**32.15**	$\times$**6.5**
	K40	**245.08**	$\times$**1.8**	**25.87**	$\times$**8**
256x256x128	no	2308.05		1879.84	
	K20	**625.37**	$\times$**3.6**	**202.63**	$\times$**9.3**
	K40	**542.73**	$\times$**4.2**	**160.87**	$\times$**11.7**
512x512x256	no	3760.46		3327.14	
	K40	**716.86**	$\times$**5.2**	**302.49**	$\times$**11**

Example 2: Degrader for proton therapy

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



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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

Particles	DKS	t_{degr} (s)	Degrader speedup	t_{integ} (s)	Integration speedup
10^5	no	20.30		3.46	
	MIC	**2.29**	×**8**	**0.89**	×**4**
	K20	**0.28**	×**72**	**0.15**	×**23**
	K40	**0.19**	×**107**	**0.14**	×**24**
10^6	no	206.77		34.93	
	MIC	**5.38**	×**38**	**4.62**	×**7.5**
	K20	**1.41**	×**146**	**1.83**	×**19**
	K40	**1.18**	×**175**	**1.21**	×**29**
10^7	no	2048.25		351.64	
	K20	**14.4**	×**142**	**17.21**	×**20**
	K40	**12.79**	×**160**	**11.43**	×**30**

Multi-Objective Optimisation with OPAL

[Y. Ineichen, AA, et al. (2012), N. Neveu, AA, et al. (2019)]

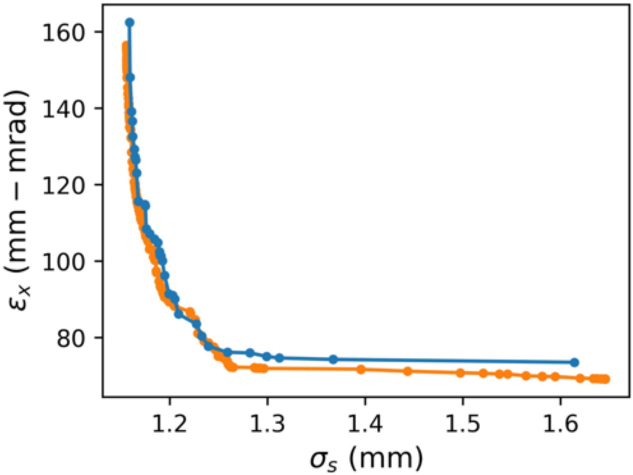
- Access to **all** OPAL statistics data as QoIs.
- Access to **all** OPAL variables as design variables
- Specify the MOOP in the OPAL input file
- Runs smoothly with more than 10000 cores

➡ No tight coupling to parallelisation mechanism

➡ No tight coupling to optimisation algorithm

➡ Finds Pareto optimal solutions (NSGA-II)

Example High Charge Argonne Wakefield Accelerator

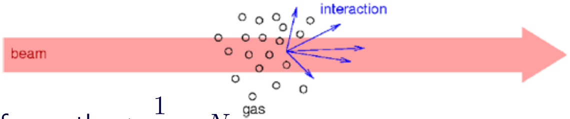


Beam stripping in OPAL-CYCL

Pedro Calvo (Ciemat) Poster & Paper: **MOP034**

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

- Residual gas interaction



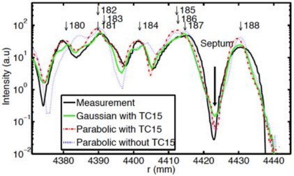
Mean free path $\rightarrow \dfrac{1}{\lambda} = N_{Total}\,\sigma_{Total}$

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

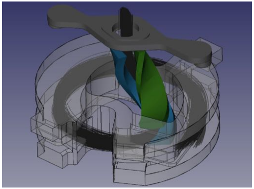
- Electromagnetic stripping
- model validated for a large drift for H^- beam

Selection of Past Achievements

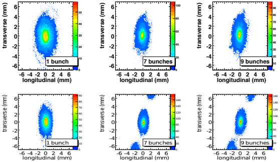
Precise high intensity cyclotron modelling
[Y. Bi, AA, et al., PR-STAB **14**(5) (2011)]



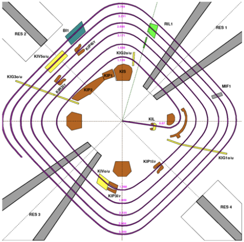
Realistic Injection Simulations of a Cyclotron Spiral Inflector
[Winklehner et al. PR-STAB **20** (2017)]



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



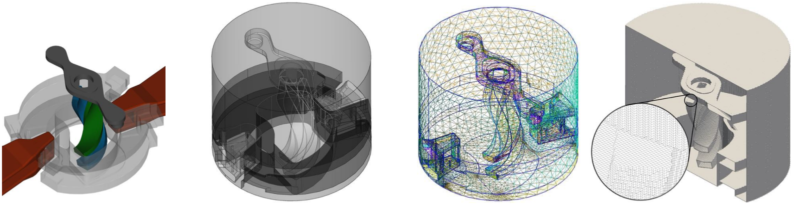
Intensity limits of the PSI Injector II cyclotron [Kolano et al. NIM-A **885** (2018)]



Simulation of the DAEδALUS Cyclotron

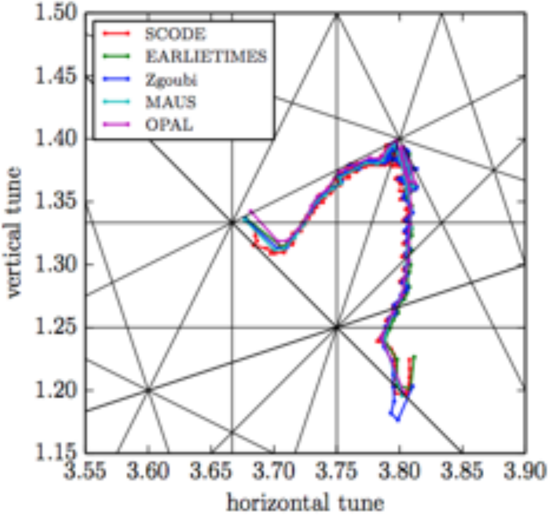
[Winklehner et al. PR-STAB **20** (2017)]

- OPAL-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**



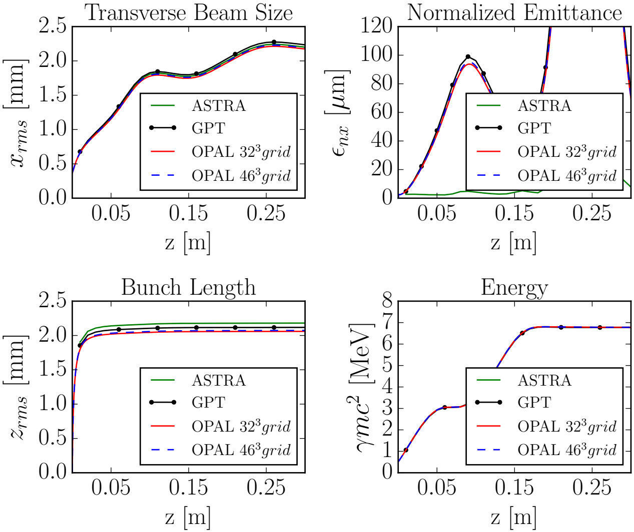
Benchmarking - Single Particle Tracking

[S. L. Sheehy, et al.]



Space Charge Benchmarking

[N. Neveu, NAPAC 2016]



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New OPAL Element **Ring**

Mostly contributed by C. Rogers

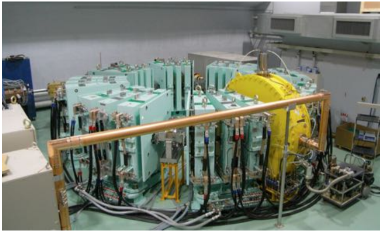
OPAL requires modification to adequately track FFA field maps

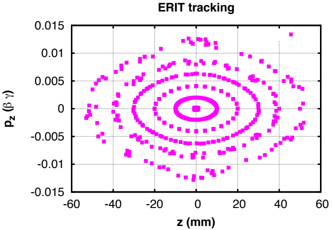
- OPAL-t allows tracking through a set of beam elements in linac-type geometry
- OPAL-cycl previously hard coded to use 2D mid plane field map + single RF cavity
- Aim to introduce the capability to track through a set of **arbitrary** beam elements in ring-type geometry
- Additionally introduce specific 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):

$$B_x = \sum_n B_0 \exp(mz) \frac{1}{m} \partial_x f_n y^n$$

$$B_y = \sum_n B_0 \exp(mz) \frac{n+1}{m} f_{n+1} y^n$$

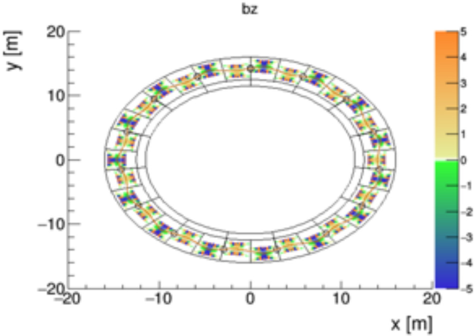
$$B_z = \sum_n B_0 \exp(mz) f_n y^n$$

With end field *f(x)* and

$$f_0 = f(x)$$

$$f_1 = 0$$

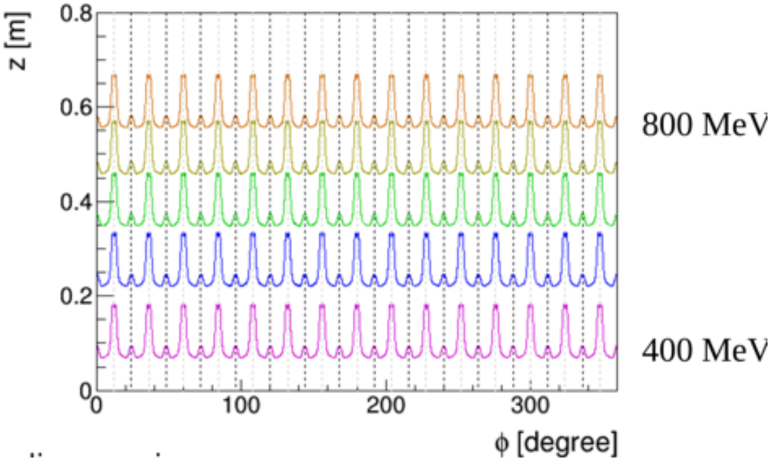
$$f_{n+2} = \frac{-1}{(n+2)(n+1)} [\partial_x^2 f_n + m^2 f_n].$$



- 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

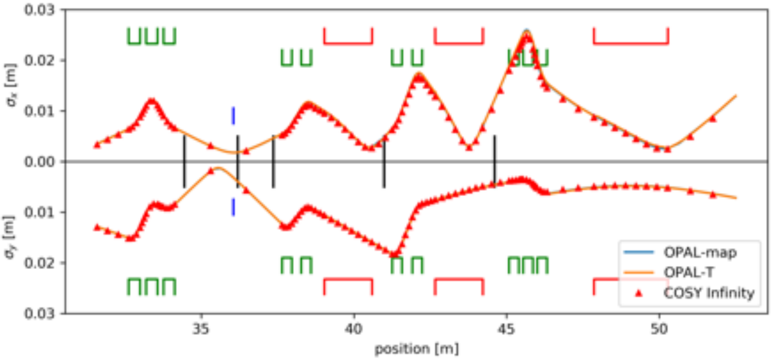
Ch. Rogers (RAL)



OPAL-MAP (work in progress)

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

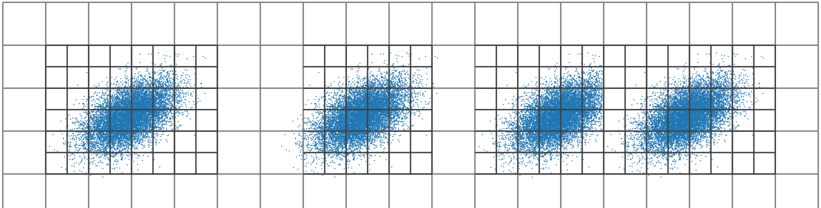
- truncated power series and Lie-Methods
- maps up to arbitrary
- space charge maps



Adaptive Mesh Refinement (AMR) in OPAL

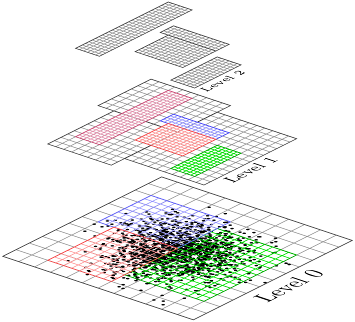
Ph.D. project M. Frey [M. Frey et al. accepted for publication in CPC]

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

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