

### Update on OPAL V.1.4.0

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### Outline

1 OPAL in a Nutshell

2 New Features in OPAL

#### 3 Future plans



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

- OPAL is built from the ground up as a parallel 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
- Regression tests are running on every git change
- Webpage: https://amas.psi.ch/OPAL
- Manual: http://amas.web.psi.ch/docs/opal/opal\_user\_guide.pdf
- OPAL Discussion Forum: https://lists.web.psi.ch/mailman/listinfo/opal
- $\bullet$  International team of 13 developers &  $\mathcal{O}(40)$  users



- OPAL is designed for 4 flavours:
  - OPAL-т
    - time as the independent variable
    - capable to build S2E models (beamlines, rf-guns, linac)
    - auto-phasing, wake fields, 1D CSR
    - 3D space charge & particle matter interaction
    - field emission (dark current studies), multipacting capabilities
    - from e, p to Uranium (q/m is a parameter)
  - OPAL-CYCL [Y. Bi, et al., PR-STAB 14(5) (2011)],
    - J. Yang, et al., NIM-A **704**(11) (2013)]
      - neighbouring turns [J. Yang, et al., PR-STAB 13(6) (2010)]
      - time integration, 4th-order RK, LF, adaptive schemes
        - [M. Toggweiler, AA, et al. (2014)]
      - single particle tracking mode & tune calculation
      - find matched distributions with linear space charge
  - OPAL-ENVELOPE (not yet released)
    OPAL-MAP (not yet released)



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### Outline



#### New Features in OPAL

- Fieldsolver (AA PSI)
- Cyclotron Tracker (D. Winklehner MIT & A. Gsell PSI)
- Time Dependent Fields (Ch. Rogers ASTeC)
- Binary Distribution (A. Gsell PSI)
- GPU Support (PhD. project U. Locans PSI/Univ. Latvia)
- Matched Distribution (Ch. Baumgarten, M. Frey & AA PSI)

#### 3 Future plans



# 3D space-charge calculation in $\operatorname{OPAL}_{\text{AA (PSI)}}$

The space-charge forces are calculated by solving the electrostatic 3D Poisson equation.

- FFT (default): with open boundary conditions using a standard or integrated Green function method
- FFT is GPU accelerated NEW
- SAAMG-PCG: iterative solvers that takes into account [AA et al., JCP, **229** 12 (2010)]
  - simple domains such a cylinder with an elliptic area
  - complicated, irregular domains NEW
  - default since version 1.4.0



# Complex Geometry in Action

#### D. Winklehner MIT & A. Gsell PSI





### Changes to OPAL-CYCL |

D. Winklehner MIT & A. Gsell PSI

- Capability to include the central region of a compact cyclotron.
  - Generalization of reference coordinate system from 2D to 3D.
  - Loading of a mesh containing the geometry data. This is important for:
    - particle termination
    - 2 boundary conditions within the iterative field solver
  - Support for geometries with several disconnected surfaces





# Time Dependent RF-Fields

Ch. Rogers (ASTeC)

This is all within the Ring definition:

- A field map routine to calculate the RF field at x, y, z, t
- The ability to enable overlapping field maps
- A user interface to enable displacement and rotation of field maps
  - enable drift (field free) regions

```
rf_f0 = 0.0028583; // GHz
rf_f1 = 9.80429e-09;
rf_f2 =-3.204e-14;
rf_f3 =-4.69392e-21;
phi = 2.*PI*0.365;
rf_frequency: POLYNOMIAL_TIME_DEPENDENCE, PO=rf_f0, P1=...;
rf_amplitude: POLYNOMIAL_TIME_DEPENDENCE, P0=1.;
rf_phase: POLYNOMIAL_TIME_DEPENDENCE, P0=phi;
```



#### Time Dependent RF-Fields cont. Ch. Rogers (ASTeC)

```
rf_cavity: VARIABLE_RF_CAVITY,
PHASE_MODEL="rf_phase",
AMPLITUDE_MODEL="rf_amplitude",
FREQUENCY_MODEL="rf_frequency", ...;
triplet: SBEND3D, FMAPFN="fdf-tosca-field-map.table", ... ;
ringdef: RINGDEFINITION, HARMONIC_NUMBER=1,
         LATTICE_RINIT=2350.0, LATTICE_PHIINIT=0.0, ...
         BEAM RINIT=x closed orbit. SYMMETRY=1.0:
11: Line = (ring, probe1, triplet, triplet, triplet,
triplet, triplet, triplet, triplet, triplet,
cavity_offset, rf_cavity);
. . .
```



# Time Dependent RF-Fields cont.

Ch. Rogers (ASTeC)

- Run with fixed frequency
  - rf\_frequency: POLYNOMIAL\_TIME\_DEPENDENCE, PO=rf\_f0;
- Particles track through stationary bucket for 1000 turns (ERIT)



Update on OPAL V.1.4.0



# Time Dependent RF-Fields cont.

Ch. Rogers (ASTeC)

- Now vary the rf frequency
  - rf\_frequency: POLYNOMIAL\_TIME\_DEPENDENCE, PO=rf\_f0, P1=rf\_f1, P2=rf\_f2, P3=rf\_f3;
- See particles accelerating
  - Small distortions due to variation in frequency



Precise FFAG simulations with 3D space charge possible



# Time Dependent RF-Fields cont.

Ch. Rogers (ASTeC)

- Now vary the rf frequency
  - rf\_frequency: POLYNOMIAL\_TIME\_DEPENDENCE, PO=rf\_f0, P1=rf\_f1, P2=rf\_f2, P3=rf\_f3;
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#### Binary Distribution A. Gsell (PSI)

Building OPAL in non trivial, hence we provide pre-build binaries

- for Linux and Mac OS X
- the distribution includes everything to run OPAL and tools ...
- Easy installation procedure
  - download from the OPAL webpage
  - Ochoose an installation directory \$DIR and change to this directory
  - Inpack with tar xvf OPAL-VERSION-XXX.tar.bz2
  - setup your environment source \$DIR/OPAL-VERSION/etc/profile.d/opal.sh



# GPU Support I

GPU Support (PhD. project U. Locans PSI/Univ. Latvia)

Dynamic Kernel Scheduler (DKS) [AA, U. Locans, A. Suter (2016)] is a slim software layer between host application and hardware accelerator





# GPU Support II

GPU Support (PhD. project U. Locans PSI/Univ. Latvia)

#### **DKS** concept

- **Communication:** common interface to communicate with different types of devices hiding all the details of different frameworks used for each device
- Function library: library of predefined algorithms written using CUDA, OpenCL, OpenMP
- Auto-tuning: based on the system setup and executable tasks select appropriate implementation and configuration to execute the code (not yet available)





### Monte Carlo Computation on HW Accelerators

- A degrader is a slab of matter (incl. gas) with a thickness adjusted to the amount of energy to be lost
- Energy loss: using Bethe-Bloch
- Scattering: including Multiple Coulomb Scattering and large angle Rutherford Scattering





### Monte Carlo Computation on HW Accelerators

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

#### Matched Distribution with Linear Space Charge Ch. Baumgarten, M. Frey & AA (PSI)

• **Goal:** Find a stationary distribution  $\sigma$ , i.e.

$$\sigma(s+L) = M\sigma(s)M^T$$
$$\sigma = \sigma(s+L) \stackrel{!}{=} \sigma(s)$$

with linear transfer map M.

- Assumptions:
  - azimuthal symmetry
  - coasting beam
  - isochronicity
- Input: energy, emittances, intensity, field map
- Additional Output ClosedOrbitFinder:
  - radial and vertical tune
  - field index
  - orbit radius
  - radial momenta

THC02 - Matched Distributions with Linear and Non-Linear Space Charge, M. Frey



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- Adaptive Mesh Refinement (AMR) Solver
- OPAL-т-**3d**
- Multiobjective Optimiser



# Adaptive Mesh Refinement (AMR) Solver

PhD. Project M. Frey (PSI), T. Kaman (UZH), A. Almgreen (LBNL) & AA

• efficient and precise iterative solver with multi-scale capabilities



- BoxLib an AMR software framework (LBNL)
- More efficient and accurate space-charge calculation
- Heterogeneous problem with respect to the spatial discretization : only small areas of interest require a fine resolution







### ОРАL-т-**Зd**

Towards fully 3D, work in progress, lead by Ch. Metzger (HZB)

- Elements in input file placed along design path (ELEMEDGE)
- Is simple for user and works fine for straight machines

#### Major drawbacks for dipoles:

- no overlap between dipole field and field of any other element
- misalignment is problematic
- Solution: place elements in 3D space.



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### OPAL-T-3d |

Towards fully 3D, work in progress, lead by Ch. Metzger (HZB)

#### For ERL bERLinPro

- include all elements only once although traversed twice  $(n \times)$
- add apertures to all elements
- add origin and initial orientation of beamline (elements)
- IPAC 16 paper : WEPOY034 Latest Improvements of OPAL







## Multiobjective Optimiser

[Y. Ineichen, AA, et al. (2012), Y. Ineichen, AA, et al. (2014)]

#### **Dynamic Kernel Scheduler**





#### References I

[AA et al., JCP, 229 12 (2010)] A. Adelmann, P. Arbenz, et al., J. Comp. Phys, 229 (12): 4554 (2010)

[Y. Bi, et al., PR-STAB 14(5) (2011)] Y. Bi, A. Adelmann et al., Phys. Rev. STAB 14(5) 054402 (2011)

[J. Yang, et al., PR-STAB 13(6) (2010)] J. Yang, Adelmann et al., Phys. Rev. STAB 13(6) 064201 (2010)

[J. Yang, et al., NIM-A 704(11) (2013)] J. Yang, Adelmann et al., NIM-A 704(11) 84-91 (2013)

[C. Wang, AA, et al. arXiv:1208.6577] C. Wang, A. Adelmann, et al., arXiv:1208.6577

[Y. Ineichen, AA, et al. (2014)] A Parallel General Purpose Multi-Objective Optimization Framework, with Application to Beam Dynamics Y. Ineichen, A. Adelmann, A. Kolano, C. Bekas, A. Curioni, P. Arbenz, arXiv:1302.2889, 2013

[Y. Ineichen, ETH Ph.D Thesis (2013)] Y. Ineichen ETH-Diss 21114, 2013

[Y. Ineichen, AA, et al. (2012)] Y. Ineichen, A. Adelmann et al., Computer Science - Research and Development, pp. 1-8. Springer, Heidelberg, 2012.

[AA, U. Locans, A. Suter (2016)] A. Adelmann, U. Locans A. Suter, Computer Physics Communication (CPC) (207): 83-90, (2016)

<sup>[</sup>M. Toggweiler, AA, et al. (2014)] M. Toggweiler, A. Adelmann, P. Arbenz, J.J. Yang, J. Comp. Phys. 273 : 255-267 (2014)