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Update on OPAL

A. Adelmann (PSI-AMAS) on behalf of the OPAL team

FFAG 2014 - BNL

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Outline

1. OPAL in a Nutshell
2. New Features in OPAL
   - Fieldsolver (T. Kaman PSI/ETH)
   - Cyclotron Tracker (D. Winklehner MIT/PSI)
   - Time Dependent Fields (Ch. Rogers ASTeC)
   - Geometry (A. Gsell PSI)
   - Binary Distribution (A. Gsell PSI)
   - Even more but not FFAG related
3. Future plans

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Outline

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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 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 (and all other used frameworks) are written in C++ using OO-techniques, hence OPAL is easy to extend.
- Documentation is taken very seriously at both levels: source code and user manual
- Regression tests running every day on the head of the repository

OPAL in a Nutshell II

- At the moment we have an international team of 15 scientists
  - A. Gsell (PSI), T. Kaman (PSI/ETH), Ch. Kraus (PSI), Y.Ineichen (IBM), S. Russell X. Pang (LANL), Y. Bi, Ch. Wang, J. Yang (CIAE), H. Zha (Thinghua University) C. Mayes (Cornell), D. Winklehner (MIT/PSI) Ch. Rogers, S. Sheehy (Rutherford) & AA (PSI)
- webpage: `https://amas.psi.ch/OPAL`
- manual: `http://amas.web.psi.ch/docs/opal/opal_user_guide.pdf`
- problems, suggestion etc. mailing: opal AT lists.psi.ch
- the OPAL Discussion Forum: `https://lists.web.psi.ch/mailman/listinfo/opal`

OPAL Object Oriented Parallel Accelerator Library

Field Maps &
Analytic Models

$$\nabla \cdot \boldsymbol{E}_{sc} = -\rho/\varepsilon_0 = \nabla \cdot \nabla \phi_{sc}$$
$$\Delta \phi_{sc} = -\frac{\rho}{\varepsilon_0}$$
& BC's

Electro
Magneto
Optics

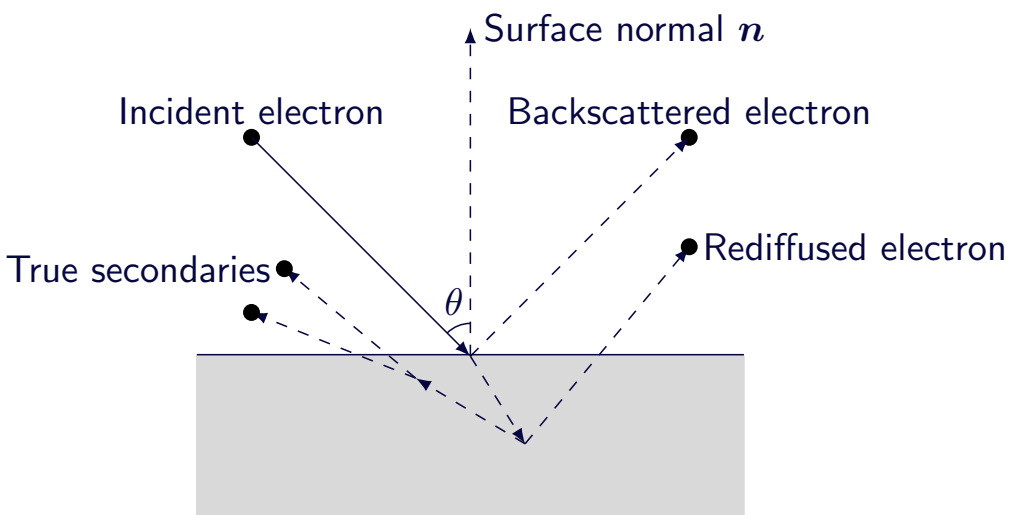
$$\boldsymbol{H} = \boldsymbol{H}_{\text{ext}} + \boldsymbol{H}_{\text{sc}}$$

N-Body
Dynamics

- OPAL-T
  - tracks particles which 3D space charge
- OPAL-ENVELOPE
  - is based on the 3D-envelope equation
- OPAL-CYCL
- OPAL-MAP (not yet released)
  - tracks particles with 3D space charge using split operator techniques.

Particle Matter Interaction

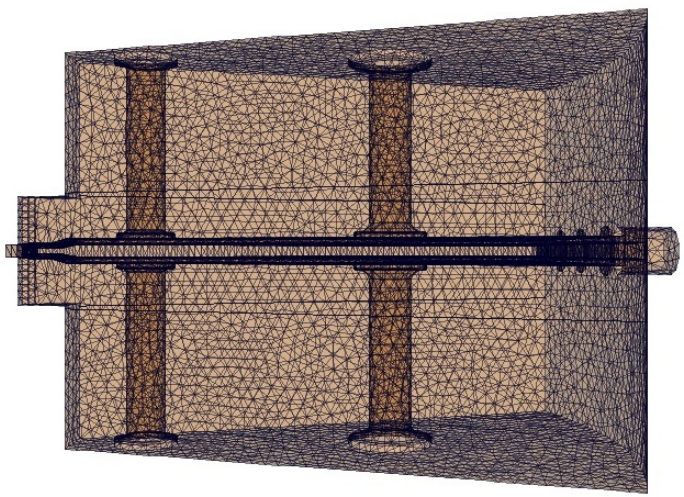
- Energy loss $-dE/dx$ (Bethe-Bloch)
- Coulomb scattering is treated as two independent events:
  - multiple Coulomb scattering
  - large angle Rutherford scattering
- Field Emission Model (Fowler-Nordheim)
- Secondary Emission Model

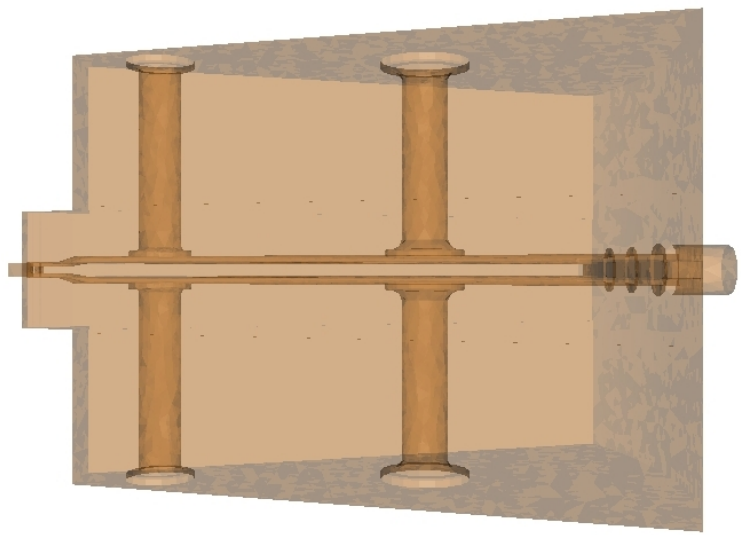


- Phenomenological- don't involve secondary physics but fit the data.
- Model 1 developed by M. Furmann and M. Pivi
- Model 2 (Vaughan) is easier to adapt to SEY curves

3D Geometry Handling Capability of OPAL

- obtain geometry in `STEP` format
- mesh geometry with `GMSH` and export to native `VTK`
- convert to `h5` with `vtk2h5grid`





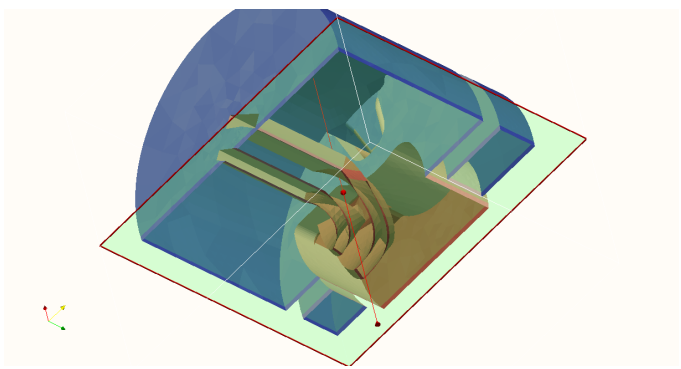
Outline

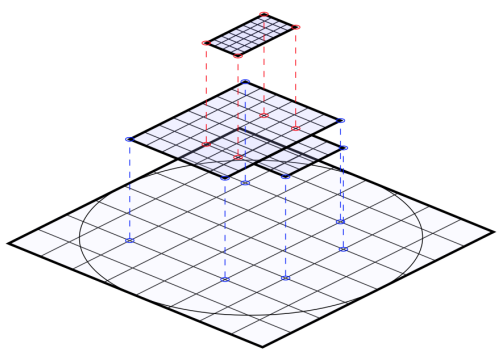
3D space-charge calculation in OPAL

T. Kaman (PSI/ETH)

The space-charge forces are calculated by solving the 3D Poisson equation. Types of the FieldSolver:

1. FFT (default): with open boundary conditions using a standard or integrated Green function method
2. SAAMG_SOLVER: iterative solvers that takes into account
   - simple domains such a cylinder with an elliptic area
   - complicated, irregular domains NEW
3. AMR_SOLVER: efficient and precise iterative solver with multi-scale capabilities NEW





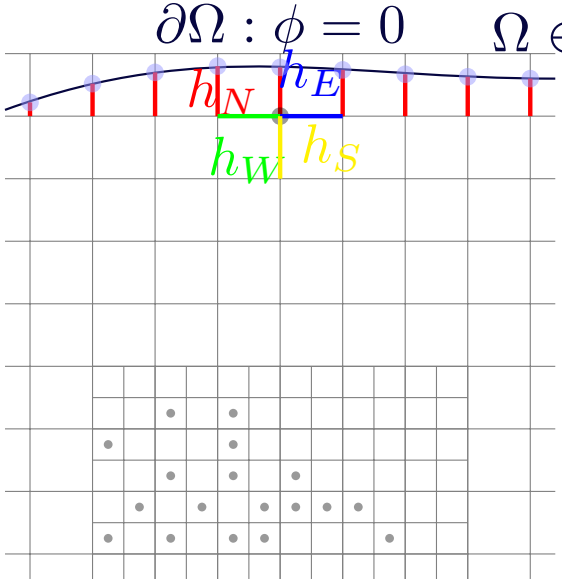
SAAMG_SOLVER FieldSolver [*]

T. Kaman (PSI/ETH)

We apply a second order finite difference scheme which leads to a set of linear equations

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

where $\mathbf{b}$ denotes the charge densities on the mesh.



- solve anisotropic electrostatic Poisson PDE with an iterative solver
- reuse information available from previous time steps
- tierative solver on irregular geometry for space charge calculations is new in OPAL
- The solver is enabled with `-DENABLE_SAAMG_SOLVER=TRUE` on `cmake`.

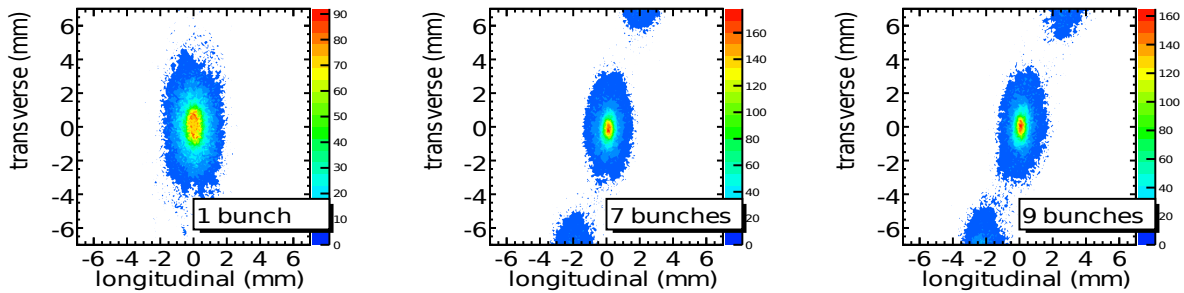
[*] D. Winklehner et.al. "Realistic Spiral Inflector Simulations with OPAL ", in Preparation

AMR_SOLVER FieldSolver [*]

T. Kaman (PSI/ETH)

Iterative solver with multi scale capability is new in OPAL

- BoxLib an AMR software framework (LBNL) is used in OPAL to add the adaptive mesh refinement (AMR) technique
- More efficient and accurate space-charge calculation
- Heterogeneous problem with respect to the spatial discretization : only small areas of interest require a fine resolution



- AMR_Solver is enabled with `-DENABLE_AMR_SOLVER=TRUE` on cmake.

[*] T. Kaman et.al., "High Resolution Beam Dynamics Simulations using Adaptive Mesh Refinement", in Preparation

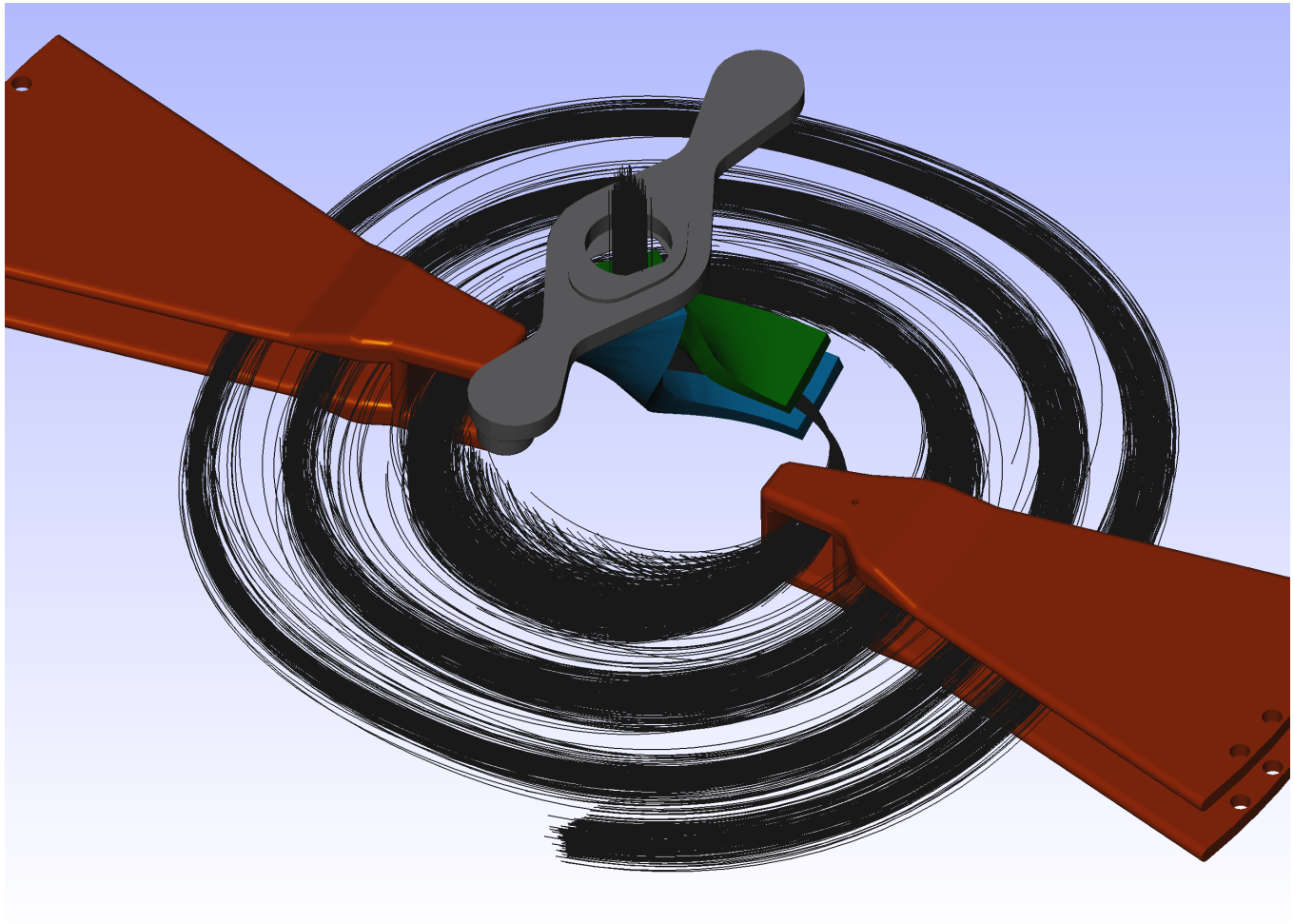
Changes to OPAL-cycl

D. Winklehner (MIT/PSI)

1. Capability to include the central region of a compact cyclotron. This includes complex objects like spiral inflectors and mirror inflectors in which particles enter the cyclotron along the z-axis.
   - Generalization of reference coordinate system in cyclotron tracker from 2D to 3D.
   - Loading of a mesh containing the geometry data..
     This is important for (1) particle termination, and (2) boundary conditions in the field solver.
2. Particle distributions is not saved in local frame anymore (for simplification and to avoid issues during restarts). Statistics information (e.g. emittance) are still be calculated in a local frame

Central Region Example

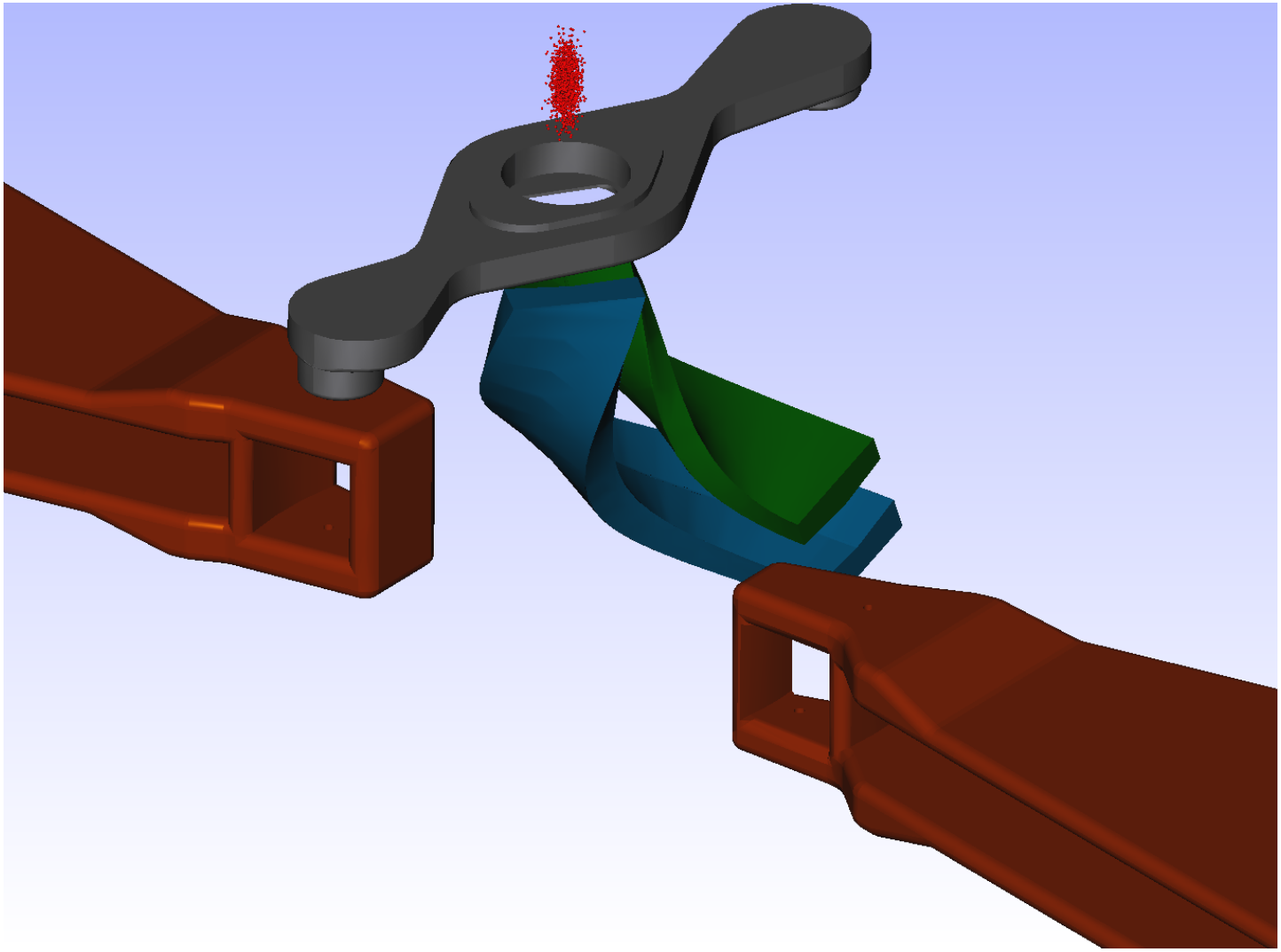
D. Winklehner (MIT/PSI)



Best Cyclotron Systems, Inc. 1 MeV/amu Teststand, H_2^+

Coming back to IsoDAR

D. Winklehner (MIT/PSI)



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, P0=rf_f0, P1=...;
rf_amplitude: POLYNOMIAL_TIME_DEPENDENCE, P0=1.;
rf_phase:     POLYNOMIAL_TIME_DEPENDENCE, P0=phi;
```

Time Dependent RF-Fields cont.

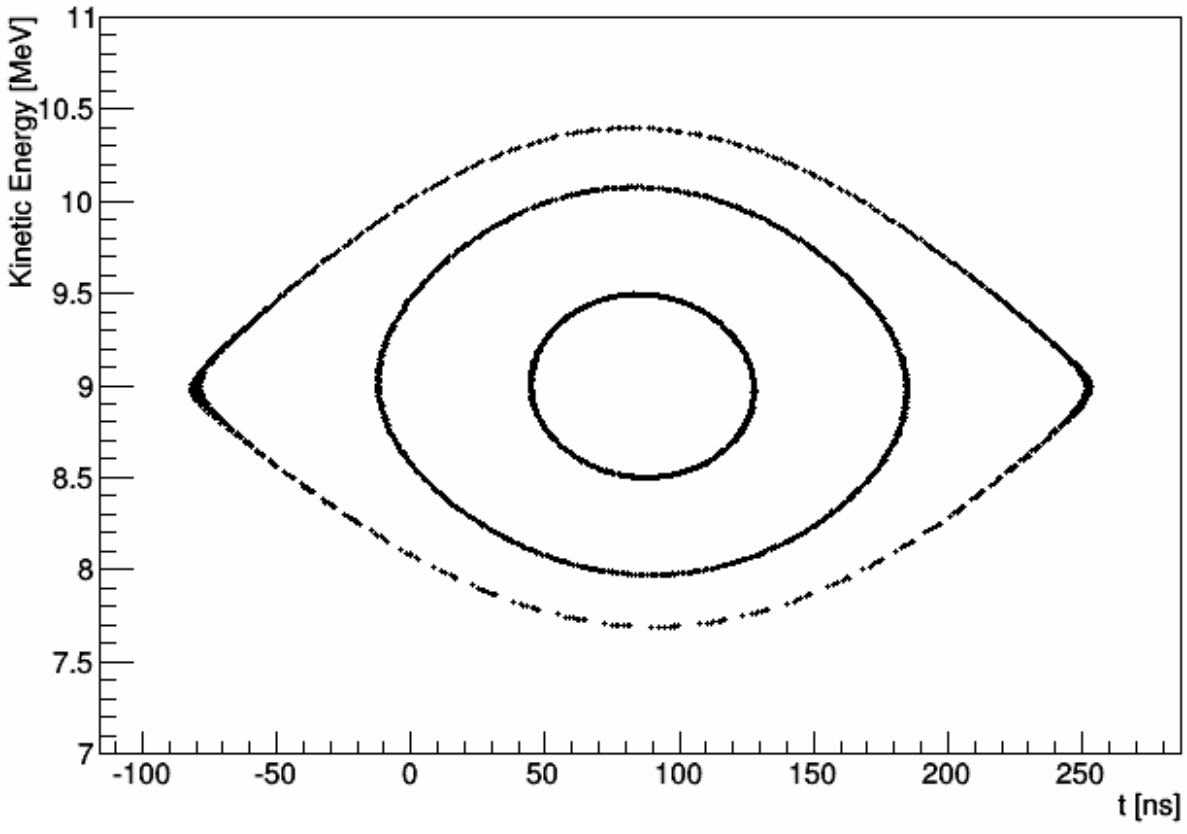
Ch. Rogers (ASTeC)

```
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;

l1: Line = (ring, probe1, triplet, triplet, triplet,
triplet, triplet, triplet, triplet, triplet,
cavity_offset, rf_cavity);
...
```

Time Dependent RF-Fields cont.

Ch. Rogers (ASTeC)

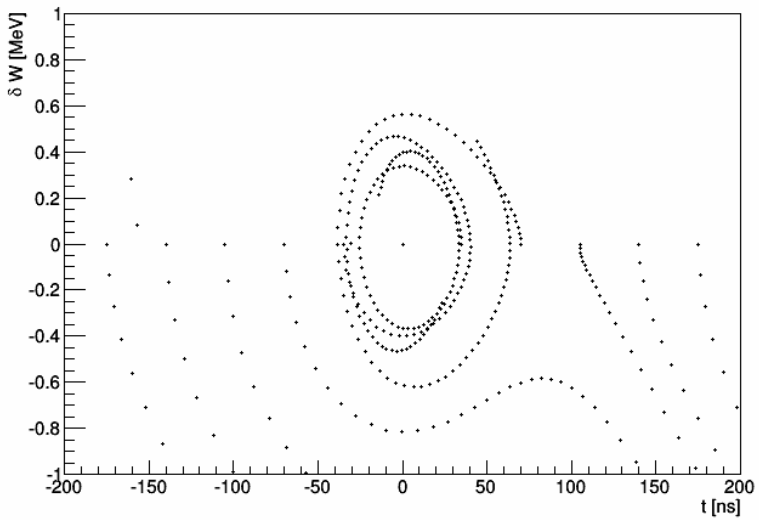
- Run with fixed frequency
  - `rf_frequency: POLYNOMIAL_TIME_DEPENDENCE, P0=rf_f0;`
- Particles track through stationary bucket for 1000 turns (ERIT)

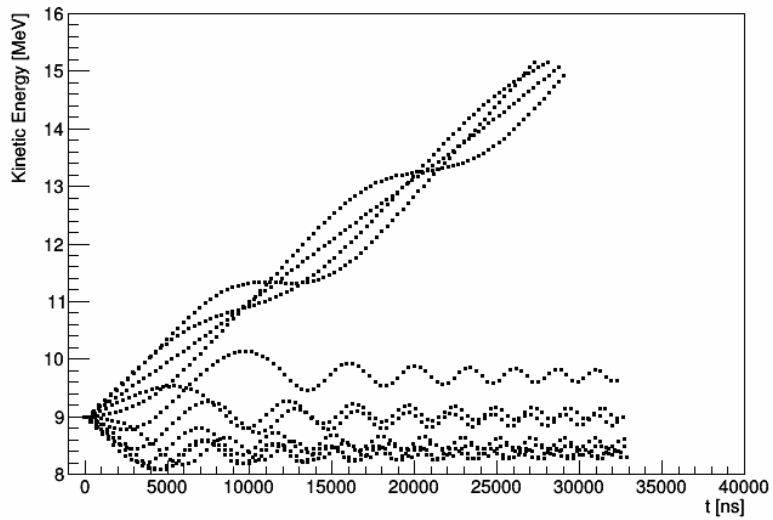


Time Dependent RF-Fields cont.

Ch. Rogers (ASTeC)

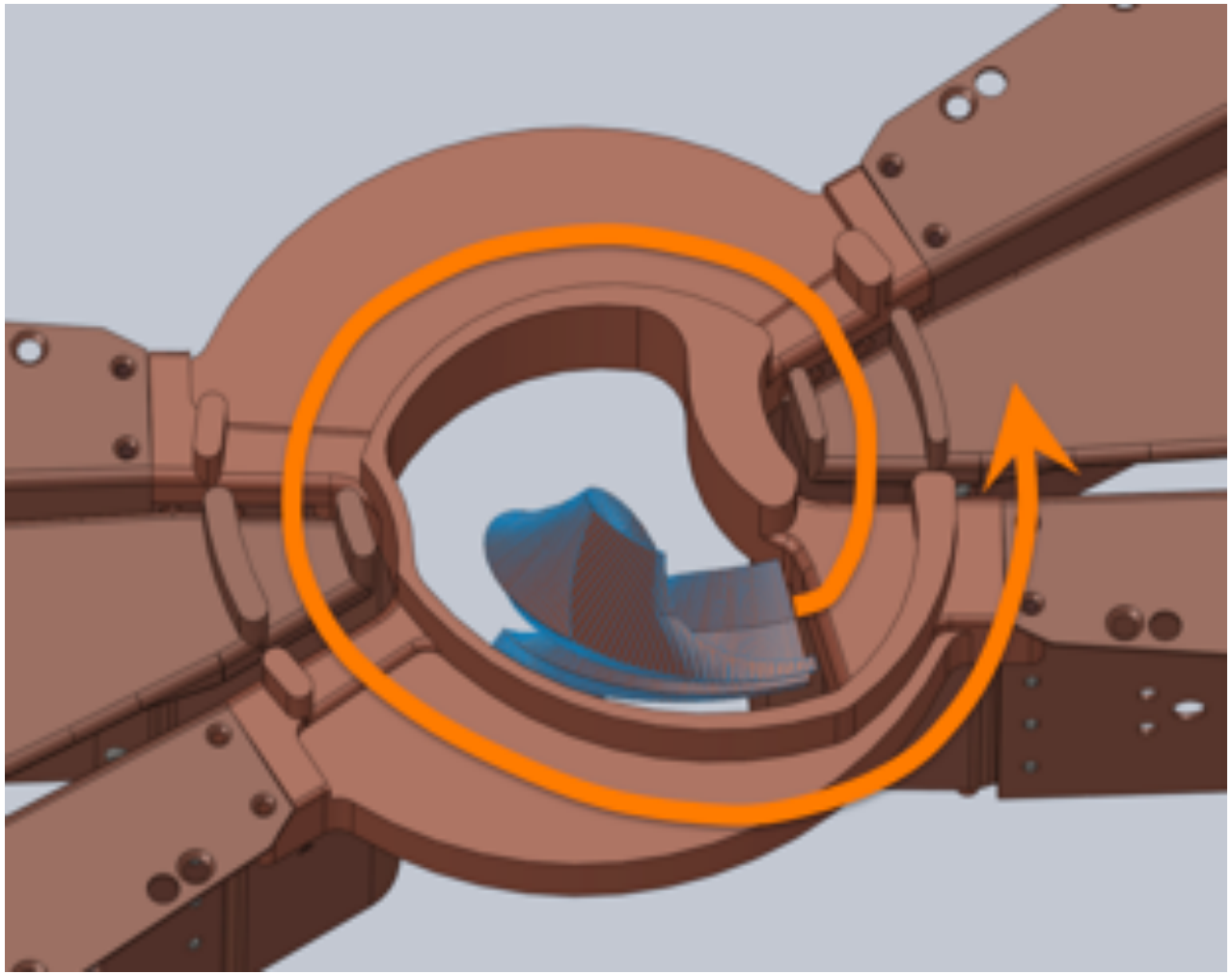
- Now vary the rf frequency
  - `rf_frequency: POLYNOMIAL_TIME_DEPENDENCE, P0=rf_f0, P1=rf_f1, P2=rf_f2, P3=rf_f3;`
- See particles accelerating
  - Small distortions due to variation in frequency
  - much more to come





Geometry: towards getting mature

A. Gsell (PSI)



Geometry: towards getting mature

A. Gsell (PSI)

- Some particles hitting the boundary were not absorbed
  - Problems with voxelisation of the geometry
  - The algorithm to orient the triangle was broken (required for the inside/outside test)
  - Almost complete rewrite of the geometry part
- Support for geometries with several disconnected surfaces

- Voxelization is now based on the voxels enclosing the bounding box of each triangle and fast box-triangle intersection tests
- This gives us a minimal set of voxels enclosing the geometry. This speed up the inside/outside tests
- Reliable and fast line-segment triangle intersection test, used by the inside/outside test

Binary Distribution

A. Gsell (PSI)

- Building OPAL and the related tools require:
  - up-to-date versions of: GLIBC, cmake, autotools Open-MPI, IPPL, Trilinos, VTK, root, gsl
  - a compiler supporting C++11
  - steps described in the OPAL manual

Because of all the non trivial involved steps we provide pre-build binaries

- We provide binary distributions for Linux and Mac OS X
- The binary distribution includes everything to run OPAL and tools ...
- On Mac's Mac OS X 10.9 plus Xquarz is required

Easy installation procedure

1. download from the OPAL webpage
2. choose an installation directory `$DIR` and change to this directory
3. unpack with `tar xvf OPAL-VERSION-XXX.tar.bz2`
4. setup your environment `source $DIR/OPAL-VERSION/etc/profile.d/opal.sh`

Even more but not FFAG related

- new 1D CSR model with examples/benchmarks (X. Pang LANL)
- Trace3D/Transport benchmarking (V. Rizzoglio PSI)
- Unit tests for any new code, using the google test framework (Ch. Rogers ASTeC)

Checkout the manual!

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Outline

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Future plans

- Version 1.3.0 to be released very soon (AA)
- change from `svn` to `git` (A. Gsell)
- `AMR` solver fully ready in 1.3.x (T. Kaman)
- Method to find matched distribution σ with linear space charge (AA & student)
  - coasting beam
  - accelerated beam
- H5root update to `root` 6.x (AA & ???)
- Overlapping 1D fringe fields (S. Russel LANL)
- Generalise OPAL for multiple ion species (D. Winklehner & AA)
- Update OPAL-T to include arbitrary geometries. (D. Winklehner & AA)