Key Figures 2010

PSI funds (global budget)		249	MCHF
External funding	~	60	MCHF
Staff	~	1400	PJ
Of which externally financed	~	370	PJ
Doctoral students	~	300	
Apprentices		80	
External users	~	2000	
Number of scientific publications	~	900	
PSI-employees with teaching duties at ETH and universities	~	80	

Precise Beam Dynamics Simulations: from High Power Cyclotron to (X)FEL Modeling

A. Adelmann (PSI-AMAS)
Acknowledgments: Y. Ineichen Ch. Kraus (PSI)
Y. Bi, J. Yang, Ch. Wang (CIAE) &
S. Russel (LANL)
SwissFEL Folks: B. Beutner, A. Falone, G L Orlandi and T. Schietinger

LBL - Wednesday, March 9 2011

Outline

Outline

Why Precise Beam Dynamics Simulations?

- consider a n MW (Cyclotron) proton driver - understanding halo
- H_2^+ versus a scheme with p (DAEδALUS)
- compact XFEL
  - providing 6D phase space at the undulator
  - bunch compression is a 3D process
  - transverse deflecting cavities
  - dark current & non uniform emission
  - many challenges of Bruce ......

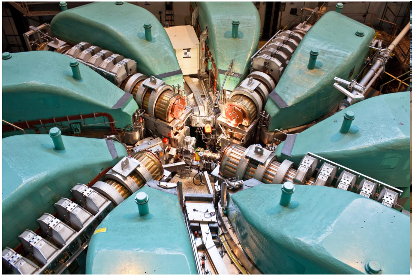
Dark Current Simulations

(Dark Current)

The High Intensity Challenge

Consider a 0.59 GeV, 2.3 mA (CW) Proton Cyclotron facility.

- uncontrolled & controlled beam loss $\mathcal{O}(2\mu A = const)$ in large and complex structures
- PSI Ring: 99.98% transmission $\rightarrow \mathcal{O}(10^{-4}) \rightarrow 4\sigma$
- small changes at injection affects extraction




The High Intensity Challenge

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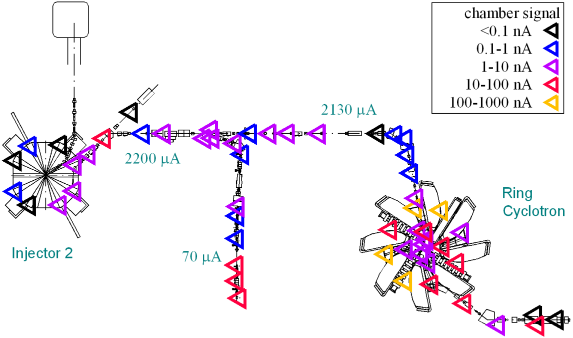


Consequences for a Beam Dynamics Model

- Multiscale / Multiresolution
  - Maxwell's equations or reduced set combined with particles
  - N-body problem $n \sim 10^9$ per bunch in case of PSI
  - Spatial scales: $10^{-4} \dots 10^4$ (m) $\rightarrow \mathcal{O}(1e5)$ integration steps
  - $v \ll c \dots v \sim c$
  - Large (complicated structures)
  - Neighboring bunches
- Multiphysics
  - Particle mater interaction: monte carlo
  - Secondary particles i.e. multi specis

Given an appropriate **physics model** it is necessary to combining state of the art **numerical methods** together with a **massively parallel implementation**.

Outline

Collision-less (non relativistic) Vlasov-Maxwell equation

$f_s \subset (\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^3 :\longrightarrow \mathbb{R}^3$ and s are the species.

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_x f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f_s = 0,$$

$$\left.\begin{aligned} \partial_t \mathbf{E} - c^2 \mathbf{curl}\, \mathbf{B} &= \frac{\mathbf{J}}{\varepsilon_0}, \qquad & \operatorname{div} \mathbf{E} &= \frac{\rho}{\varepsilon_0}, \\ \partial_t \mathbf{B} + \mathbf{curl}\, \mathbf{E} &= 0, \qquad & \operatorname{div} \mathbf{B} &= 0, \end{aligned}\right\} \quad \text{Maxwell's equations}$$

where the source terms are computed by

$$\rho = \sum_s q_s \int f_s \, d\mathbf{v}, \qquad \mathbf{J} = \sum_s q_s \int f_s \mathbf{v} \, d\mathbf{v}.$$

The electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ are superpositions of external fields and self-fields (space charge),

$$\mathbf{E} = \mathbf{E}_{\text{ext}} + \mathbf{E}_{\text{sc}}, \quad \mathbf{B} = \mathbf{B}_{\text{ext}} + \mathbf{B}_{\text{sc}}.$$

If $\mathbf{E}$ and $\mathbf{B}$ are known, then each particle can be propagated according to the equation of motion for charged particles in an electromagnetic field,

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}(t)}{dt} = \frac{q}{m_0}\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right).$$

Maxwell's Equation in the Electrostatic approximation

Field Maps &
Analytic Models

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

Electro
Magneto
Optics

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

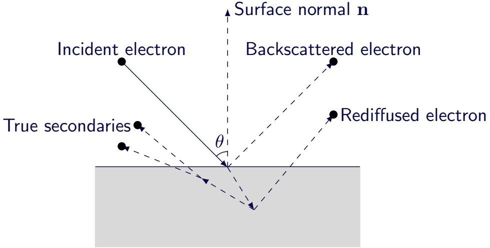
N-Body
Dynamics

With G the 3D open space Green's function $G(\mathbf{x},\mathbf{x}') = \frac{1}{\sqrt{(\mathbf{x}-\mathbf{x}')^2}}$ the solution of the Poisson equation at point $\mathbf{x}$ can be expressed by

$$\phi_{sc}(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0}\int G(\mathbf{x},\mathbf{x}')\rho(\mathbf{x},\mathbf{x}')d\mathbf{x}'.$$

Particle Matter Interaction & Space Charge

- 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 ([Furman & Pivi] & [Vaughan])



- 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

Outline

OPAL in a Nutshell

OPAL is a tool for charged-particle optics in large accelerator structures and beam lines including 3D space charge and particle matter interaction

- 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 very easy to extend.
- Documentation is taken very seriously at both levels: source code and user manual (`http://amas.web.psi.ch/docs/index.html`)
- Regression tests running evert day on the head of the repository

`www.amas.psi.ch`

OPAL and its Flavours

4 OPAL flavours exist:

- OPAL-T
  - OPAL-T tracks particles which 3D space charge uses time as the independent variable, and can be used to model beamlines, guns, injectors and complete FEL's but without the undulator.
  - Field emission (dark current studies)
  - many more linac features ...
- OPAL-ENVELOPE
  - OPAL-ENVELOPE is based on the 3D-envelope equation (à la HOMDYN) and can be used to design FEL's.
  - OPAL-ENVELOPE could also be used for an on-line model (incl. space charge)
  - same lattice than OPAL-T
- OPAL-MAP (not yet released)
  - OPAL-MAP tracks particles with 3D space charge using split operator techniques.
  - $\mathcal{M}(s) = \mathcal{M}_{\text{ext}}(s/2) \otimes \mathcal{M}_{\text{sc}}(s) \otimes \mathcal{M}_{\text{ext}}(s/2) + \mathcal{O}(s^3)$

OPAL and its Flavours cont.

- OPAL-CYCL
  - 3D space charge
  - neighboring turns
  - time is the independent variable.
  - from p to Uranium (q/m is a parameter)
  - Solve Poisson equation with spectral methods
  - Use 4th-order RK and Leap Frog
  - Single particle tracking mode & tune calculation
  - Particle Matter Interaction
  - Multipacting capabilities

OPAL is developed by an international collaboration including Los Alamos (LANL), China Institute of Atomic Energy (CIAE) and Tsinghua University, Beijing.
Parallel I/O (H5hut) PSI-LBL collaboration.

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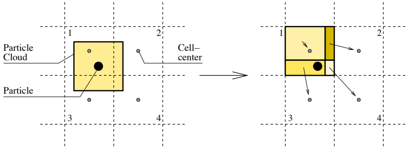
A fast Direct FFT-Based Poisson Solver

Solving for ϕ using $\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0}\int G(\mathbf{x},\mathbf{x}')\rho(\mathbf{x},\mathbf{x}')d\mathbf{x}'$ is expensive $\mathcal{O}(N^2)$ with N number of particles.

1. Discretize $\rho \rightarrow \rho_h$ and $G \rightarrow G_h$ on a regular grid (PIC).



2. Go to Fourier space $\rho_h \rightarrow \widehat{\rho}_h$, $G_h \rightarrow \widehat{G}_h$ and convert the convolution into a multiplication $\mathcal{O}(\log N)$.
3. Use a parallel FFT, particle and field load balancing.

Iterative Poisson Solver SAAMG-PCG

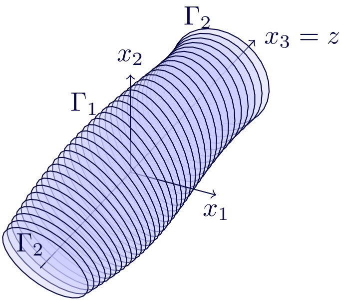
Boundary Problem

$$\Delta\phi = -\frac{\rho}{\varepsilon_0}, \text{ in } \Omega \subset \mathbb{R}^3,$$

$$\phi = 0, \text{ on } \Gamma_1$$

$$\frac{\partial\phi}{\partial\mathbf{n}} + \frac{1}{d}\phi = 0, \text{ on } \Gamma_2$$

- $\Omega \subset \mathbb{R}^3$: simply connected computational domain
- ε_0: the dielectric constant
- $\Gamma = \Gamma_1 \cup \Gamma_2$: boundary of Ω
- d: distance of bunch centroid to the boundary



Γ_1 is the surface of an

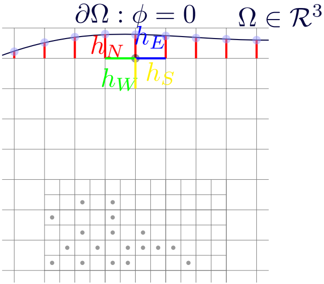
1. elliptic beam-pipe
2. arbitrary beam-pipe element

Iterative Poisson Solver $\mathrm{SAAMG\text{-}PCG}$ cont.

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

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

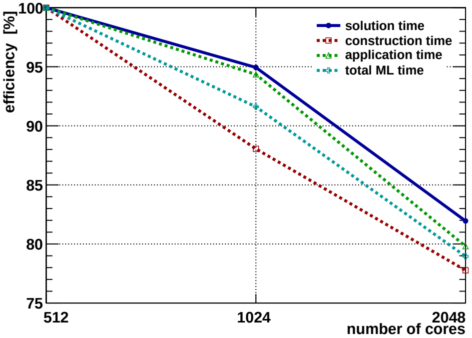
where **b** denotes the charge densities on the mesh.



- solve anisotropic electrostatic Poisson PDE with an iterative solver
- reuse information available from previous time steps
- achieving good parallel efficiency
- irregular domain with "exact" boundary conditions
- easy to specify boundary surface

[A. Adelmann, P. Arbenz and Y. Ineichen]

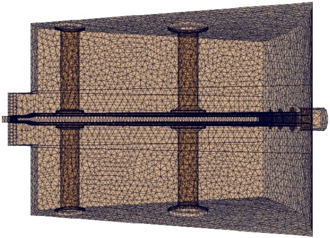
SAAMG-PCG Parallel Efficiency

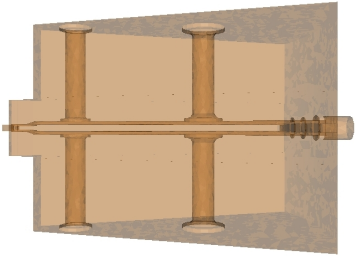


- obtained for a tube embedded in a $1024 \times 1024 \times 1024$ grid
- construction phase is performing the worst with an efficiency of 73%
- influence of problem size on the low performance of the aggregation in ML

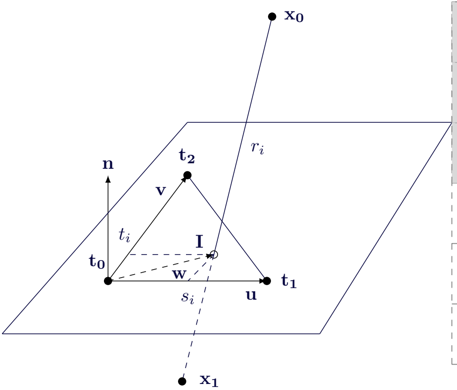
3D Geometry Handling Capability of OPAL

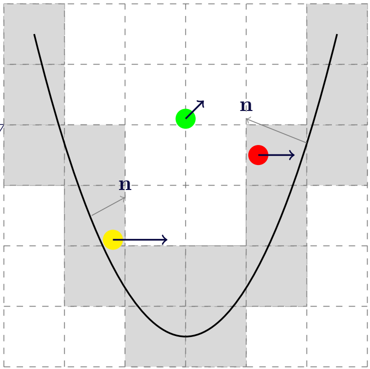
- Read in surface mesh generated by Heronion or GMSH
- Triangulated surface representation of geometry



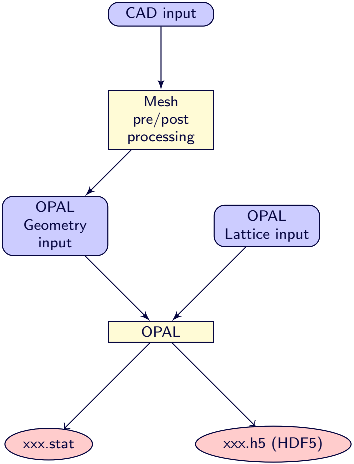


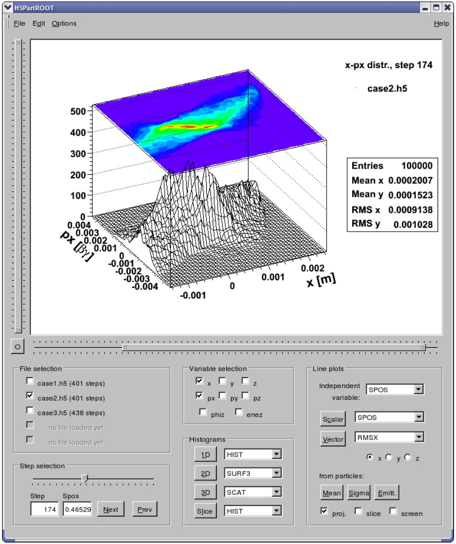
- Triangle-line segment intersection
- Boundary bounding box to speedup the collision tests
- We can handle arbitrary structure as long as it is closed





Parallel I/O (H5hut) & Postprocessing (H5Root)

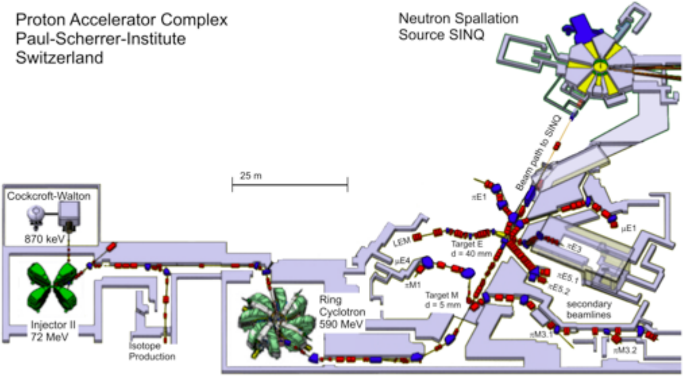




Outline

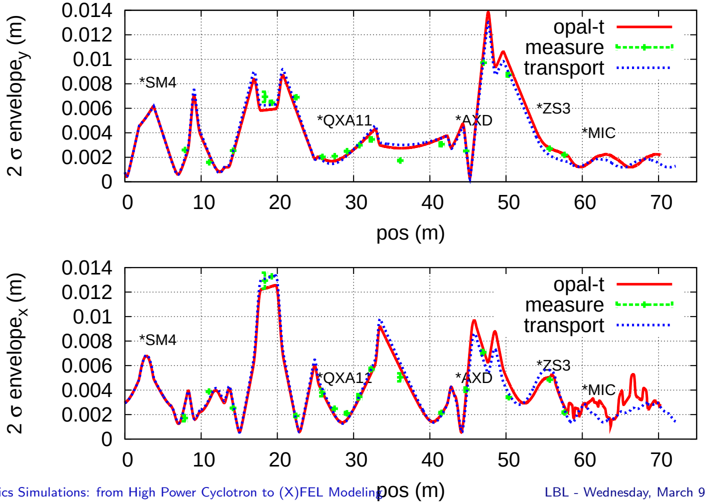
Outline

PSI HIPA Overview

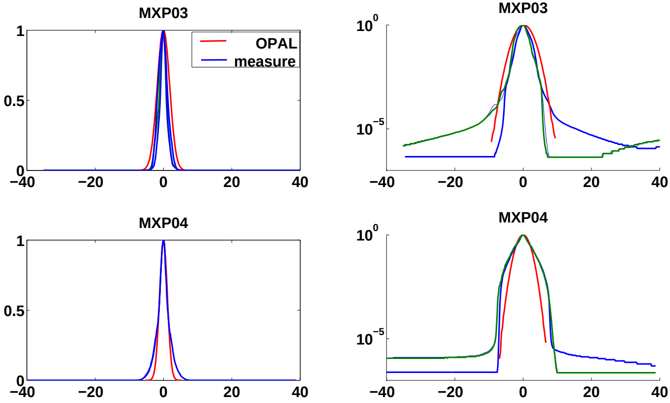


OPAL-T Simulations of the PSI IW2 Line (72 MeV p)

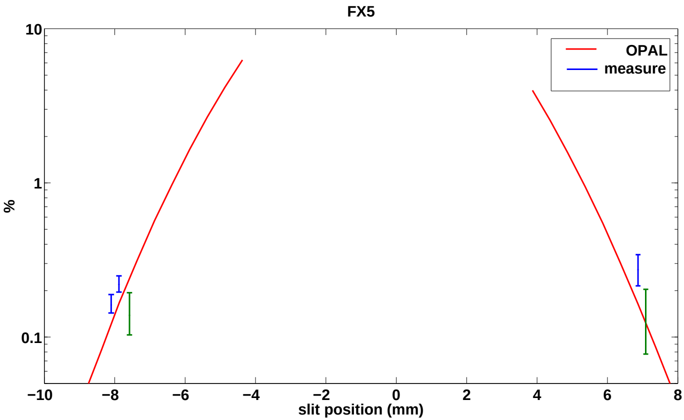
Production run setup (2.2 mA)



Comparison of beam profile monitors in the PSI-IW2 Line

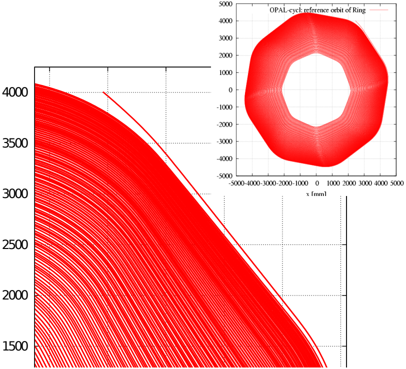


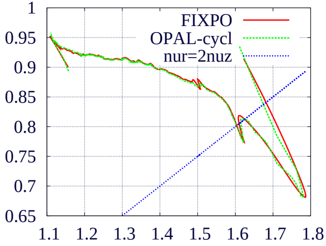
Comparison of beam losses on the slits with measurements



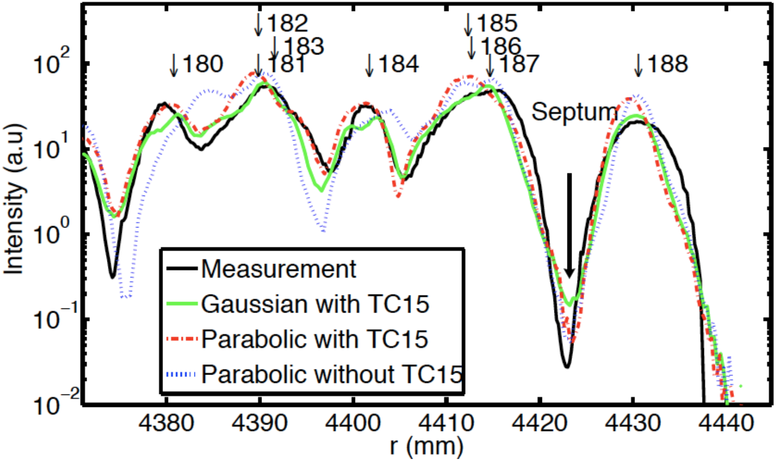
PSI 590 MeV Ring - last 8 turns

- initial conditions from 72 MeV transfer line simulation (OPAL-T)
- rf parameters from control room
- using measured mid-plane field and analytic trim-coil (tc15)
- single particle run to verify tun numbers and tunes





PSI 590 MeV Ring - last 8 turns @ 2.2 mA



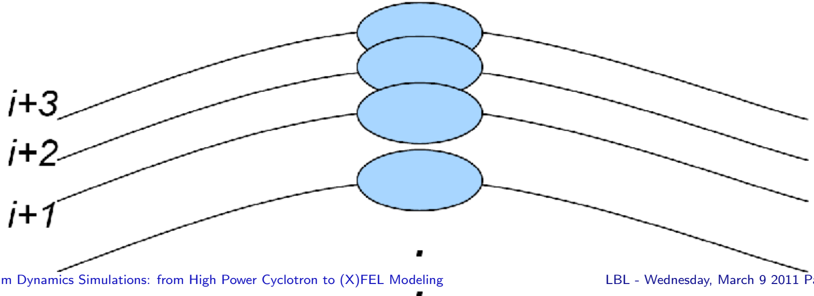
[Y. Bi, A. Adelmann]

Neighboring Bunch Effects- Multi Bunch Model

In the model, the injection-to-extraction simulation is divided into two stages:

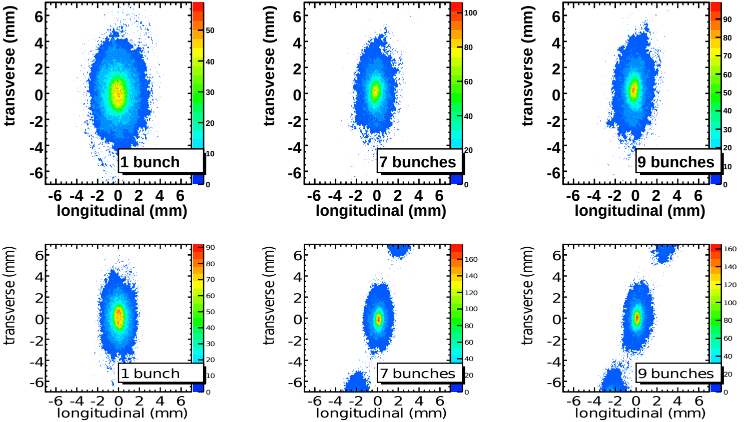
1. First stage, big $\Delta r \Rightarrow$ single bunch tracking
2. Second stage, small $\Delta r \Rightarrow$ multiple bunches tracking

- Full 3D
- Energy bins & re-binning
- Large grids needed



PSI 590MeV Ring

Single bunch and multiple bunches at turn 80 and 130



[J. Yang, Adelmann]

Outline

1. Motivation & Problem Setup
2. The Models upon OPAL is based
3. OPAL and its Flavours
4. Simulation Results
   - Precise Simulations of the PSI Ring Cyclotron
   - Particle Matter Interaction
   - Multipacting & Dark Current Modeling
5. The SwissFEL & the 250 MeV Accelerator Test Facility

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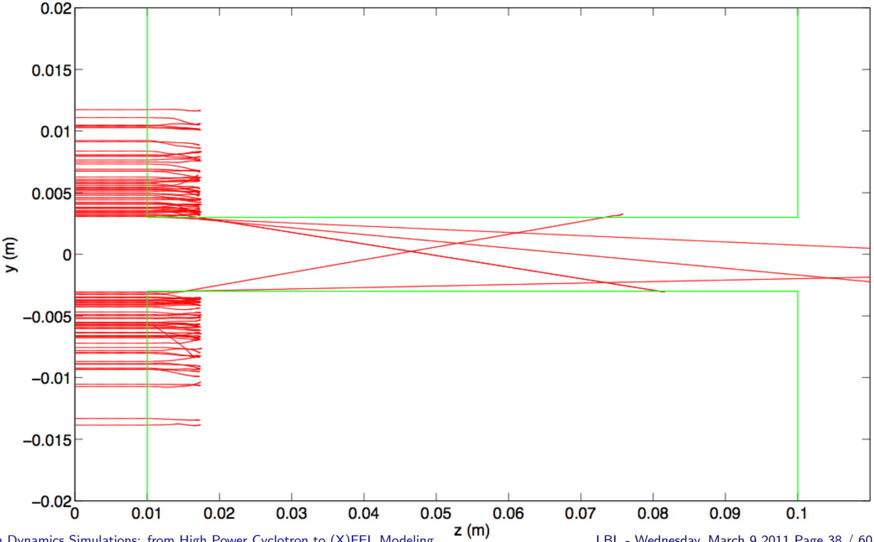
Particle Matter Interaction

- Energy loss $-dE/dx$ (Bethe-Bloch)
- Coulomb scattering is treated as two independent events: the multiple Coulomb scattering and the large angle Rutherford scattering
- Space charge & halo generated by the obstacle

A 72 MeV cold Gaussian beam with $\sigma_x = \sigma_y = 5$ mm passing a copper slit with the half aperture of 3 mm from 0.01 m to 0.1 m.

Particle Matter Interaction cont.



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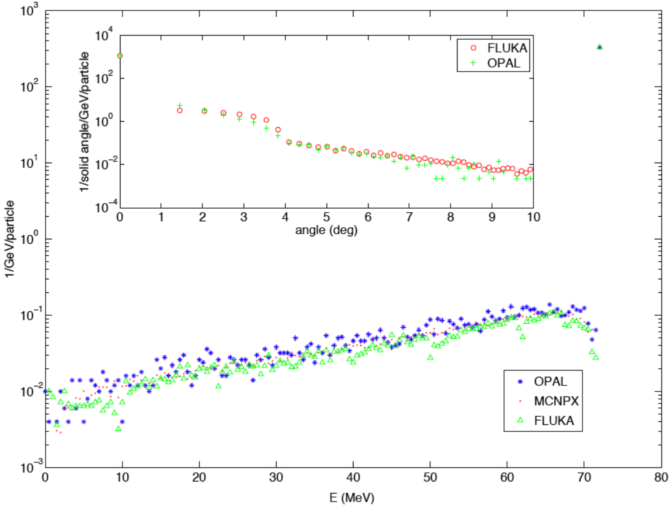
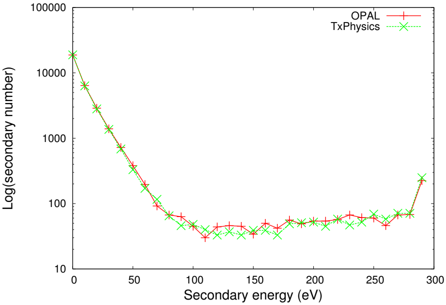
Particle Matter Interaction cont.



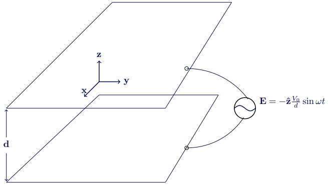
Outline

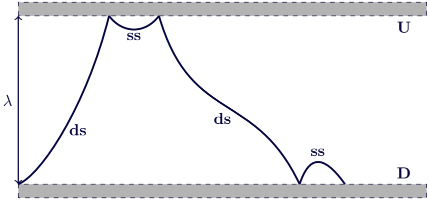
Multipacting & Dark Current Modeling



- Benchmark Against the TxPhysics Library
- Validate the implementation of Furman-Pivi's model
- Logarithm of total secondary emission number (backscattered + re-diffused + true secondaries) vs. energy of emitted particles

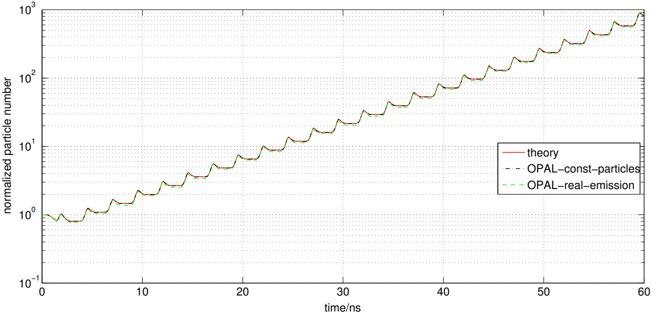
Multipacting & Dark Current Modeling cont.





- Benchmarking the secondary emission model is not sufficient!
    - There double-side(ds) and single-side(ss) impacting exist
    - This is the most complete description of multipacting [S. Anza et al]!

Multipacting & Dark Current Modeling cont.



$f = 200MHz$, $V_0 = 120V$, $d = 5mm$, Furman-Pivi's model, copper and re-normalize to a const number of simulation particle

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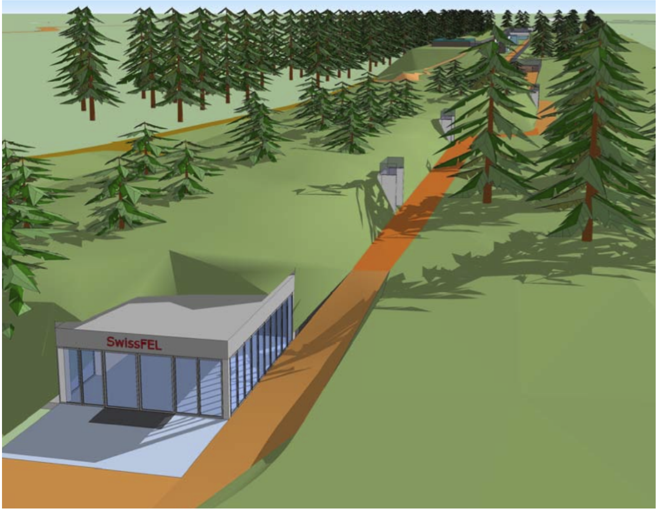
Outline

The SwissFEL http://www.psi.ch/swissfel/



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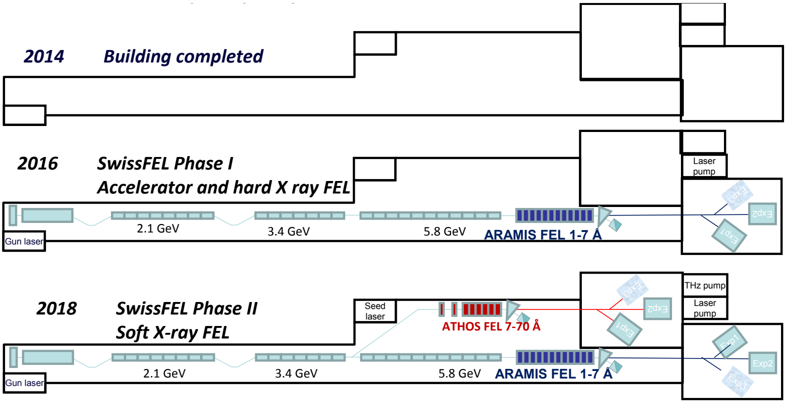
The SwissFEL http://www.psi.ch/swissfel/



The SwissFEL cont.

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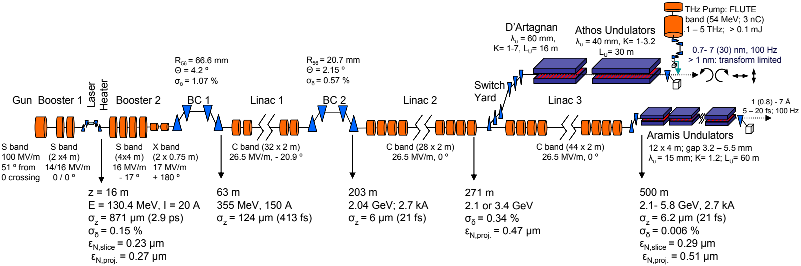
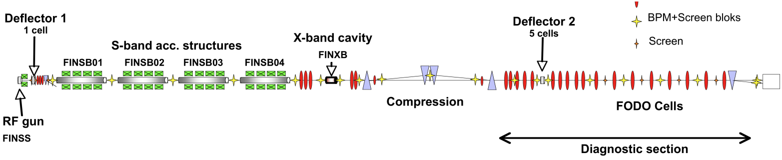
The SwissFEL cont.

E	5.8	(GeV)
P	5	(MW)
f_{rep}	100	(Hz)
λ	$1 \ldots 70$	(Å)
L	713	(m)

- RF-Photo Gun (PSI development)
- frequency tripl. TiSa Laser
- S,C and X-Band RF structures
- norm. conducting



The 250 MeV Test Injector



What is primarily indispensable to get SwissFEL lasing?

Table: Critical Parameter to reach @ 250 MeV

Charge	20 pC	200 pC	
E	250	250	(MeV)
ΔE uncorr.	< 50	< 50	(keV)
ε_x rms proj	0.15	0.5	(mm-mr)
ε_x slice	0.11	< 0.4	(mm-mr)
I peak	100	350	(A)

Benchmarking OPAL-T & Astra

OPAL-T simulation of the CTF3 gun and 2 S-band TW structures and solenoids.

Table: Initial conditions

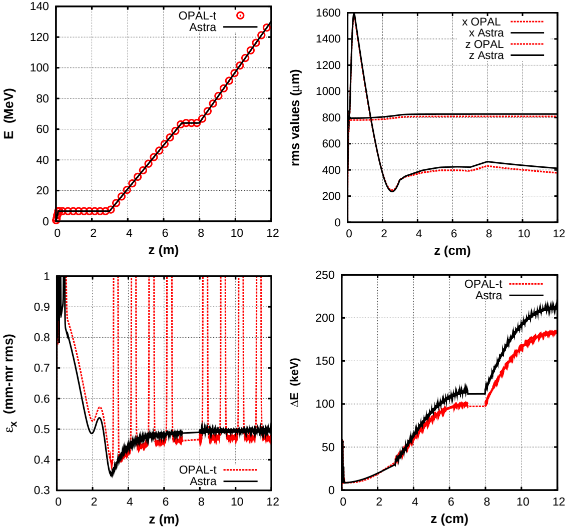
σ_x	249	μm
σ_y	249	μm
Q	200	pC
t_{fwhm}	9.9	ps
$t_{\text{rise}} = t_{\text{fall}}$	0.782	ps
E_{th}	0.65	eV
ϕ_{gun}	-3.5	deg
ϕ_{tw1}	0.0	deg
ϕ_{tw2}	0.0	deg

Table: $Q = 200$ pC at 12m

	OPAL	Astra	
E_{final}	130.249	130.290	(MeV)
ΔE_{final}	184.79	213.22	(keV)
ε_x rms	0.46990	0.49075	(mm-mr)
x rms	377.648	412.510	(μm)
z rms	809.092	826.860	(μm)

Both codes run autophase

Benchmarking OPAL-T & Astra cont.



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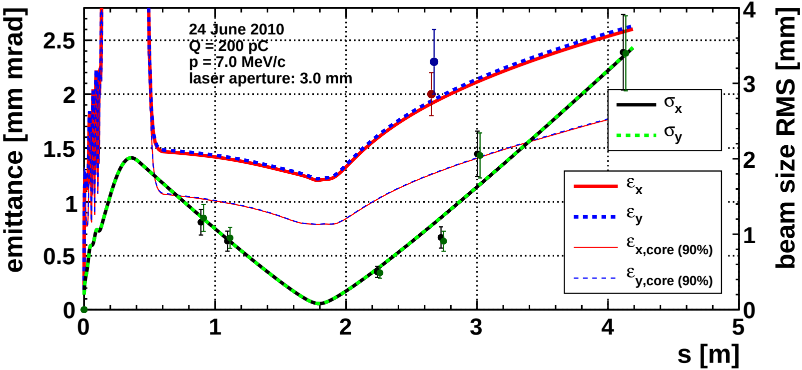
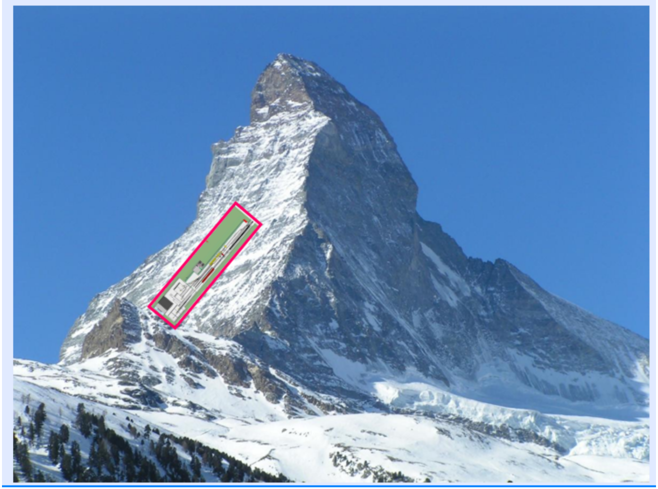
Comparing Simulations with Reality

OPAL-T simulation of the CTF3 gun, including thermal emittance (0.65 eV) and laser profile (0.7 ps rise time 9.8 ps flat-top).



The SwissFEL is a very compact machine



J. Rossbach / Univ. HH&DESY - Inauguration SwissFEL Injektor 24.8.2010

References

- A. Adelmann, P. Arbenz and Y. Ineichen, J. Comp. Phys, 229 (12): 4554-4566 (2010)
- M. A. Furman and M. Pivi, Phys. Rev. ST Accel. Beams 5, 124404 (2002)
- S. Anza, C. Vicente, J. Gil, V. E. Boria, B. Gimeno, and D. Raboso, Phys. Plasmas 17, 062110 2010
- Y. Bi, A. Adelmann et.al submitted Phys. Rev. STAB and `http://arxiv.org/abs/1012.0718`
- J. Yang, Adelmann et.al, Phys. Rev. STAB Volume 13 Issue 6 064201 (2010)
- J. R. M. Vaughan, IEEE Transactions on Electron Devices 40, 830 (Apr 1993)

Backup

```
GME:GEOMETRY, LENGTH=1, S=0.0, A=0.00085, B=0.00085;

Fs1:FIELDSOLVER, FSTYPE=MG, MX=32, MY=32, MT=64,
        PARFFTX=false, PARFFTY=false, PARFFTT=true,
        BCFFTX=dirichlet, BCFFTY=dirichlet, BCFFTT=open,
        GEOMETRY="GME", ITSOLVER="CG", INTERPL="linear",
        TOL=1e-6, MAXITERS=100, PRECMODE="reuse";

Fs2:FIELDSOLVER, FSTYPE=FFT, MX=32, MY=32, MT=64,
        PARFFTX=false, PARFFTY=false, PARFFTT=true,
        BCFFTX=open, BCFFTY=open, BCFFTT=open,
        BOXINCR=1.0, GREENSF=INTEGRATED;

beam1: BEAM, PARTICLE=ELECTRON, PC=P0, NPART=1e5,
      BFREQ=1498.953425154e6, BCURRENT=0.299598, CHARGE=-1;

SELECT, LINE=FIND1;
```

```
TRACK,LINE=FIND1, BEAM=beam1, MAXSTEPS=10000, DT=1.0e-12;
 RUN, METHOD = "PARALLEL-T", BEAM=beam1,
 FIELDSOLVER=Fs2, DISTRIBUTIONS={Dist1,Dist2};
endtrack;

f1: Filter, TYPE="FixedFFTLowPass", NFREQ=9;
f2: Filter, TYPE="Savitzky-Golay", NLEFT=64,
NRIGHT=64,POLYORDER=1;
CSRWAKE: Wake, TYPE="1D-CSR", FILTERS={f2, f1};

F10BC_MB01: RBend, L=0.282000, K0=0.1585,
FMAPFN="F10BC-MB01.T7", ELEMEDGE=29.964,
ALPHA=3.035,  DESIGNENERGY=247.6, WAKEF=CSRWAKE;
```

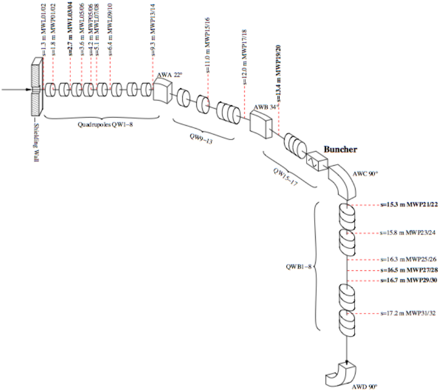
```
KX1I_PHYS: SurfacePhysics, TYPE="Collimator",MATERIAL="Cu";

KX0I: ECollimator, L=0.09, ELEMEDGE=0.01,
XSIZE=0.003, YSIZE=0.003,
APERTURE={0.003,0.003},SURFACEPHYSICS='KX1I_PHYS';

DR1:DRIFT, L=0.09, ELEMEDGE=0.01,
APERTURE={0.003,0.003}, SURFACEPHYSICS='KX1I_PHYS';

QXA1:QUADRUPOLE,L=0.19,ELEMEDGE=0.11,K1=1.0,
APERTURE={0.003,0.003}, SURFACEPHYSICS='KX1I_PHYS';

MXP00: Monitor, L=0.002, ELEMEDGE=0.1, OUTFN="MXP00.h5";

IW2Line: Line=(MXP00,KX0I);
```

870 keV Injection Line

Simulation and measurement DC beam 870 keV

Find $\mathcal{D}_{start}$ and ν_e by $min(F)$:

$$F = \sum_{n=1}^{\#monitors} (\widetilde{\mathcal{X}}_{mea}(s_n) - \widetilde{\mathcal{X}}_{sim}(s_n))^2.$$



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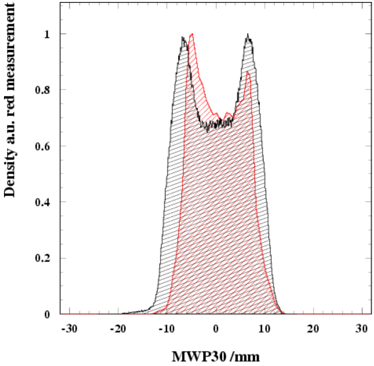
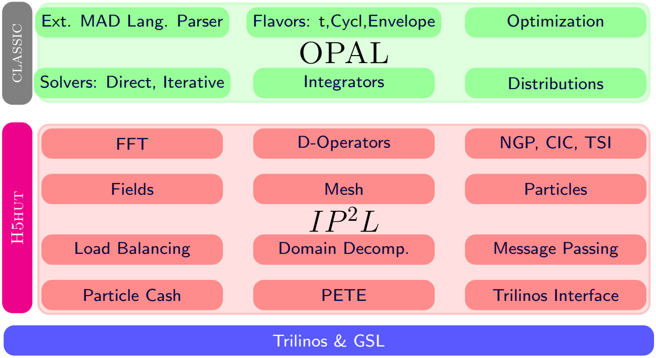


OPAL Architecture



- **OPAL Object Oriented Parallel Accelerator Library**
- IP^2L **Independent Parallel Particle Layer**
- **Class Library for Accelerator Simulation System and Control**
- **H5hut for parallel particle and field I/O (HDF5)**
- **Trilinos http://trilinos.sandia.gov/**

OPAL Parallel Scaling on Cray XT5 (FFT Solver)

- Tracking 10^8 Gaussian distributed particles
- 3D FFT on a 1024^3 grid