OPAL a versatile Parallel Tool for Precise 3D Beam Dynamics Studies including Collective Effects

A. Adelmann (PSI-AMAS)

Acknowledgments: A. Gsell, Y. Ineichen Ch. Kraus (PSI)
Y. Bi, J. Yang, Ch. Wang (CIAE)
Hao Zha (Tsinghua Univ. Beijing) & S. Russel (LANL)

ERL-2011 - October 20. 2011

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Outline

1. Motivation for OPAL & Problem Setup
2. OPAL in a Nutshell
   - Space Charge
   - Particle Matter Interaction & Multipacting
   - 3D Geometry Handling Capability of OPAL
3. Examples of OPAL Simulations
   - Precise Simulations of the PSI Ring Cyclotron
   - CTF3 gun, with thermal emittance
   - Dark Current Simulations of the CTF3 RF-Photo Gun
4. Conclusion and Outlook

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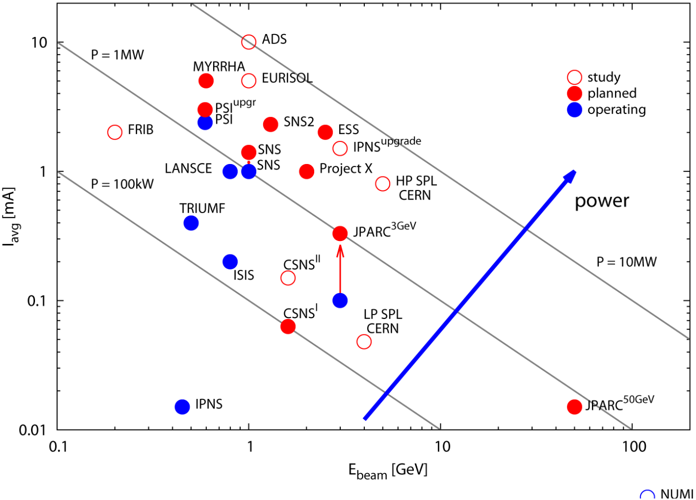
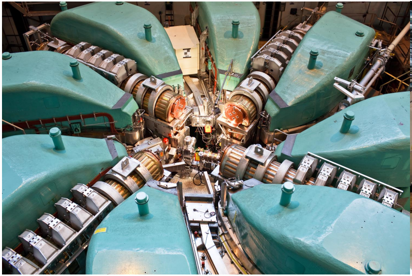


ADS
P = 1MW
MYRRHA
EURISOL
study
planned
operating
PSI^upgr
PSI
FRIB
SNS2
ESS
IPNS^upgrade
SNS
SNS
LANSCE
Project X
HP SPL
CERN
P = 100kW
power
TRIUMF
JPARC^3GeV
CSNS^II
ISIS
P = 10MW
CSNS^I
LP SPL
CERN
IPNS
JPARC^50GeV
10
1
0.1
0.01
0.1
1
10
100
I_avg [mA]
E_beam [GeV]
NUMI

The High Intensity Challenge

Consider the PSI 0.59 GeV, 2.4 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

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 (Cyclotrons & FFAG)
- Multiphysics
  - Particle mater interaction: monte carlo
  - Field Emission
  - 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**.

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OPAL in a Nutshell (amas.web.psi.ch)

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
- Towards an international/community code
- Mailing List `lists.web.psi.ch/mailman/listinfo/opal`

OPAL and its Flavours

3 OPAL flavors are released:

- OPAL-T
  - OPAL-T tracks particles which 3D space charge uses time as the independent variable, and can be used to model beamlines, guns, linac's (SW,TW), hence complete FEL's but without the undulator.
  - 1D CSR (soon 2&3D)
  - short range wakefields ($\perp, ||$)
  - autophasing
  - field emission (dark current studies) & particle matter interaction
  - arbitrary overlapping fields
  - code comparison: IMPACT-T, Astra & GPT
- OPAL-ENVELOPE
  - OPAL-ENVELOPE is based on the 3D-envelope equation (à la HOMDYN) and can be used to design FEL's.
  - is the forward solver for an ongoing Ph.D project on Multi-objective Optimization

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)
  - striper foil
  - single particle tracking mode & tune calculation
  - particle matter interaction
  - multipacting capabilities
- OPAL-MAP (not yet released)
  - OPAL-MAP tracks particles with 3D space charge using split operator techniques.
  - $\mathcal{M}(s) = \mathcal{M}_{\mathsf{ext}}(s/2) \otimes \mathcal{M}_{\mathsf{sc}}(s) \otimes \mathcal{M}_{\mathsf{ext}}(s/2) + \mathcal{O}(s^3)$

Maxwell's Equation in the Electrostatic approximation

1,2 or 3D Field Maps $\&$
Analytic Models $(\boldsymbol{E},\boldsymbol{B})_{\boldsymbol{ext}}$

$$\mathrm{div}\, \boldsymbol{E'}_{sc} = \rho'/\varepsilon_0 = \mathrm{div}\, \nabla\phi'_{sc}$$
$$\Delta\phi'_{sc} \;=\; -\frac{\rho'}{\varepsilon_0}$$
& BC's
$$\boldsymbol{\mathcal{L}^b(E')} \rightarrow \boldsymbol{(E,B)_{SC}}$$

Electro
Magneto
Optics

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

N-Body
Dynamics

If $\mathbf{E}(\mathbf{x},t)$ and $\mathbf{B}(\mathbf{x})$ are known:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}(t)}{dt} = k_s\left[\mathbf{E}(\mathbf{v},t) + \mathbf{v}\times\mathbf{B}(\mathbf{x})\right]$$

- Boris-pusher (adaptive version soon!)
- Leap-Frog
- RK-4.

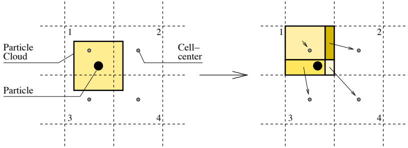
A fast Direct FFT-Based Poisson Solver

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

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

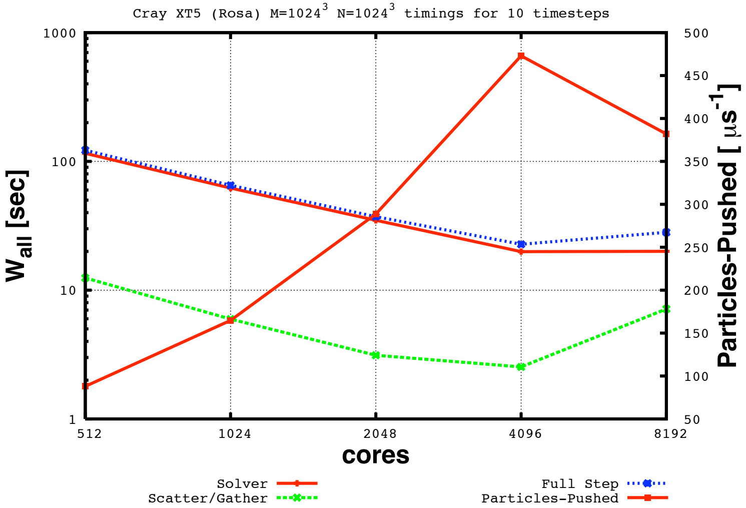
but this is very expensive $\mathcal{O}(N^2)$ with N number of particles.

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.

A fast Direct FFT-Based Poisson Solver cont.



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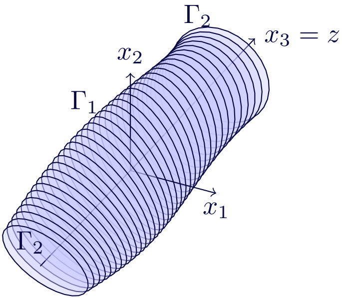
Iterative Poisson Solver SAAMG-PCG

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

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

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

- $\Omega \subset \mathbb{R}^3$: 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

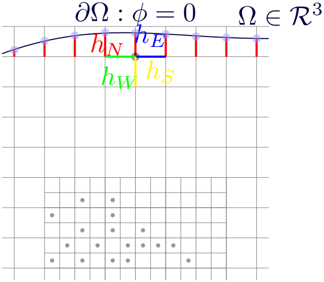
1. elliptic beam-pipe
2. arbitrary beam-pipe element

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.

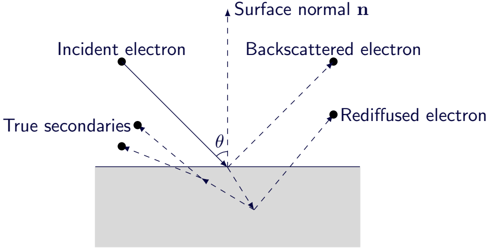


- solve anisotropic ($\mathcal{L}$) electrostatic Poisson PDE with an iterative solver (PCG)
- reuse information available from previous time steps
- achieving good parallel efficiency
- irregular domain with “exact” boundary conditions
- easy to specify boundary surface

[A. Adelmann, P. Arbenz and Y. Ineichen, J. Comp. Phys, 229 (12) (2010)]

Particle Matter Interaction & Multipacting

- 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])

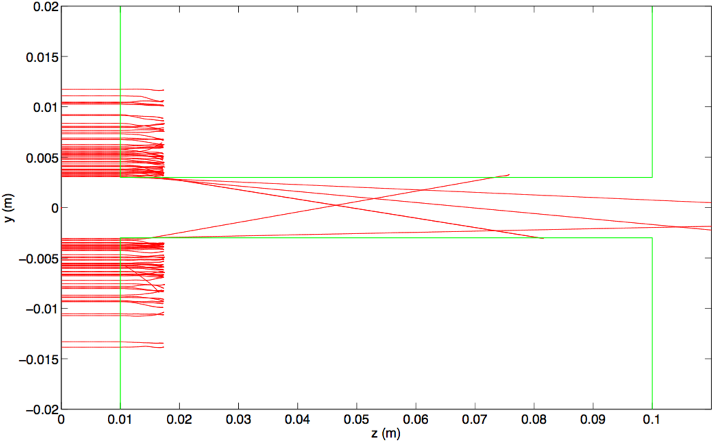


Phenomenological- don't involve secondary physics but fit the data.

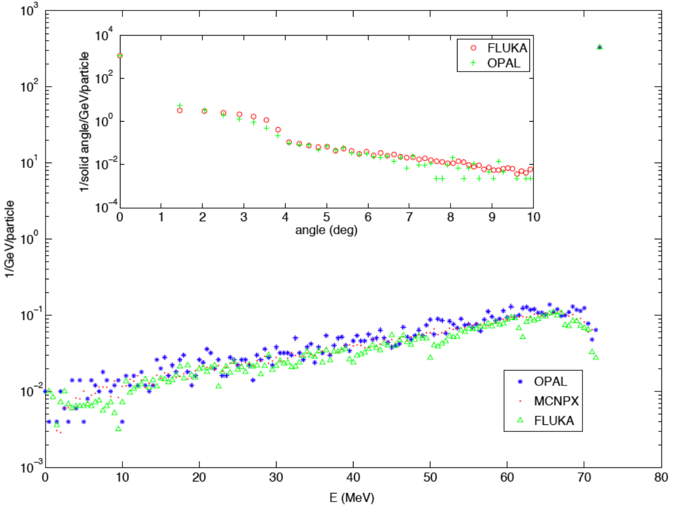
- Model 1 developed by M. Furmann and M. Pivi
- Model 2 (Vaughan) is easier to adapt to SEY curves

Particle Matter Interaction & Multipacting cont.

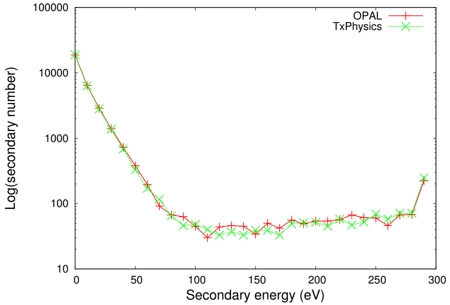
A 72 MeV cold Gaussian beam with $\sigma_x = \sigma_y = 5$ mm passing a copper slit with the half aperture of 3 mm from 0.01 m to 0.1 m.



Particle Matter Interaction & Multipacting cont.

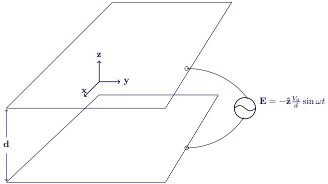


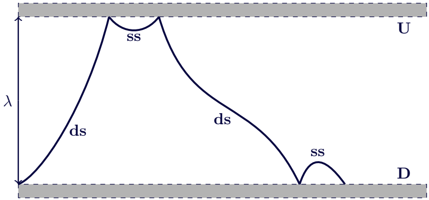
Particle Matter Interaction & Multipacting cont.



- 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

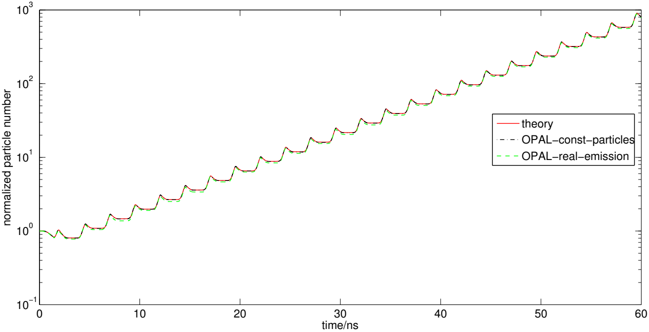
Particle Matter Interaction & Multipacting cont.





- 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]!

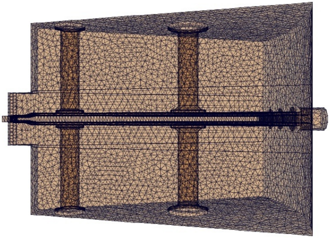
Particle Matter Interaction & Multipacting cont.

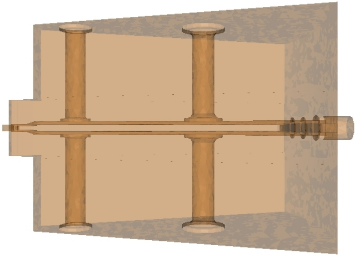


$f = 200MHz$, $V_0 = 120V$, $d = 5mm$, Furman-Pivi's model, copper and re-normalize to a const number of simulation particles

3D Geometry Handling Capability of OPAL

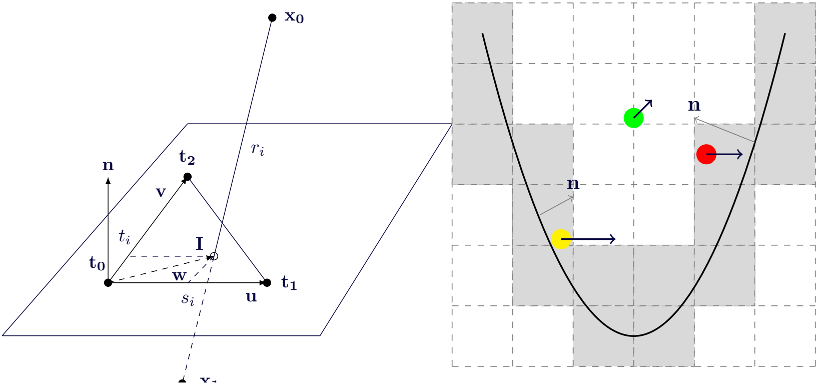
- Read CAD data and generate the surface mesh (Heronion or GMSH)
- Triangulated surface representation of geometry





3D Geometry Handling Capability of OPAL cont.

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



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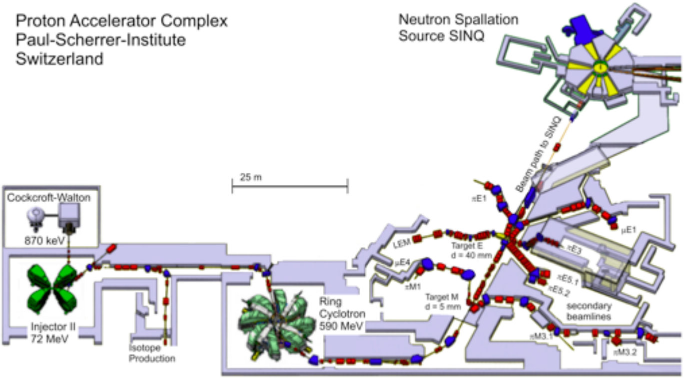
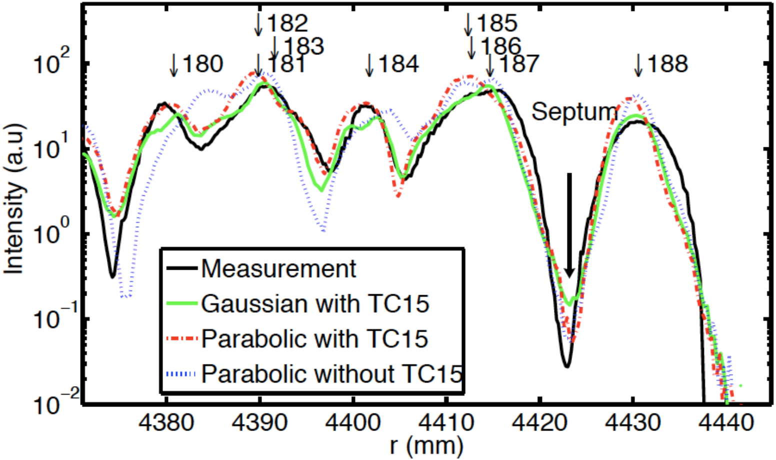
Precise Simulations of the PSI Ring Cyclotron

The PSI High Power Proton Facility



Precise Simulations of the PSI Ring Cyclotron cont.

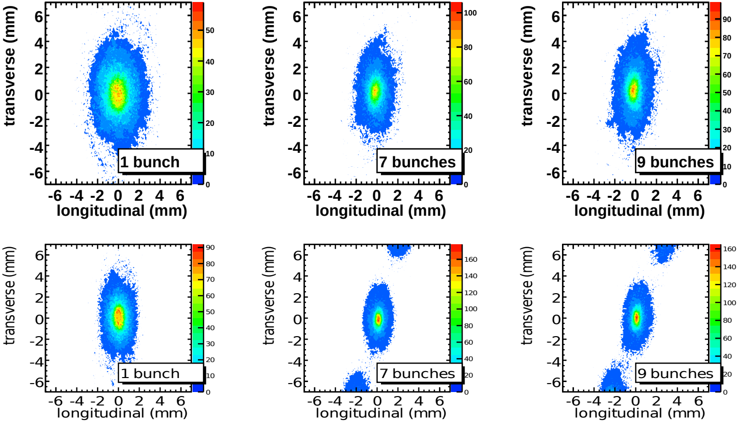
PSI 590 MeV Ring - last 8 turns @ 2.2 mA



[Y. Bi, A. Adelmann, et.al Phys. Rev. STAB Volume 14 Issue 5 (2011)]

Precise Simulations of the PSI Ring Cyclotron cont.

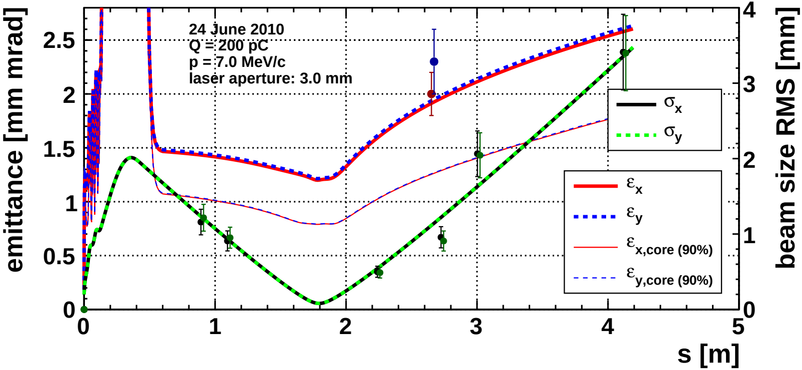
Single bunch and multiple bunches at turn 80 and 130



[J. Yang, Adelmann, et.al Phys. Rev. STAB Volume 13 Issue 6 (2010)]

CTF3 gun, with thermal emittance

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).



[T. Schietinger et.al., LINAC2010]

Dark Current Simulations of the CTF3 RF-Photo Gun

(Dark Current)

Dark Current Simulations with Secondary Emission

(Dark Current)

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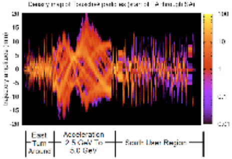
Charges from the Organizers

ERL 2011

Beam Loss

- Beam loss can be a huge operational problem for ERLs.
- Many potential sources:
  1) Touschek/IBS scattering
  2) Residual gas scattering
  3) Space charge and CSR effects
  4) Strayed light from a drive laser
  5) Bunch tail at photocathode
  6) RF fields and field emission of cavities



Trajectories of Touschek-scattered electrons at Cornell ERL

- Simulation codes are being implemented for some sources such as Tousch ek/IBS scattering.
- Further studies of beam halo formation and beam loss are needed.

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Other Issues

- Error tolerances
- Orbit stability
- Simulation codes (elegant, BMAD, GPT, IMPACT-T, ···.)
- Start-to-End(S2E) simulation
- Energy spread due to wakes
- Longitudinal space charge effects
- Light source performance
- Roles of test facilities and collaboration work

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Conclusions

- Some of the ongoing efforts towards precise beam dynamics simulations where sketched and results are presented
- Using the High Performance Computing (HPC) technology enable us to speedup computations while increasing the accuracy of the used models (statistics w.r.t losses)
- HPC is an enabler of new modeling capabilities: 3D space charge & secondary effects in large structures
- State-of-the-art numerical methods and adequate software technology are mandatory
- Active collaborations, today with CIAE, LANL, Cornell and LBL

Outlook & Plans for new Capabilities includes:

- 3D FEM Maxwell solver (Ph.D ETH/PSI to be completed in 1Q 2012)
- 3D CSR Model (Ph.D ETH/PSI to be completed in 1Q 2012)
- Multiobjective Optimization (Ph.D ETH/PSI/IBM started 2010)
- Adaptive Time Stepping (ETH-MS student project, available in version 2.x)
- P^3M solver for resolving scales smaller the h , available in version 2.x
- Adaptive Mesh Refinement (re-submit proposal)
- Multi Species

The OPAL framework combines essential factors

- physics modeling
- numerics
- high performance computing

which enables us to enter into new regimes of precise accelerator modeling and control.

References

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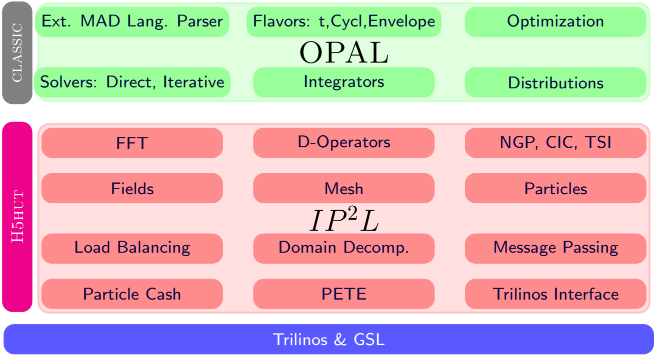
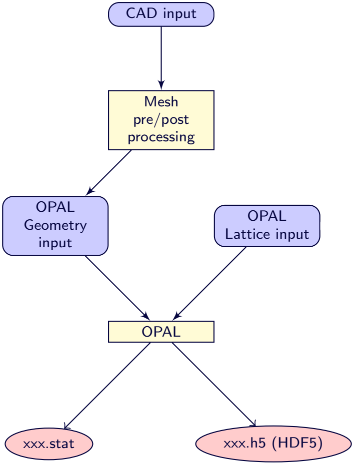
Backup Slides

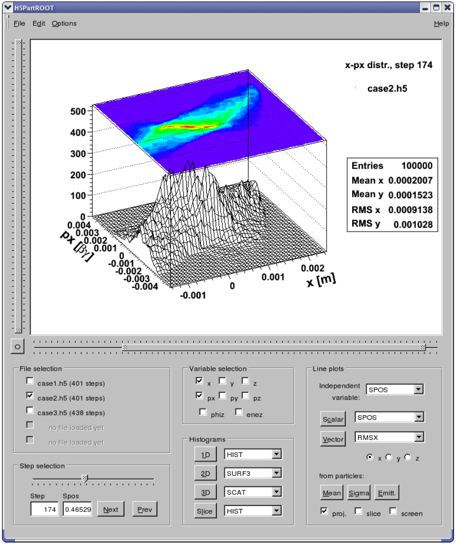
Software Architecture



- **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/**

Parallel I/O (H5hut) & Postprocessing (H5root)





Comparing Simulations with Reality - Schottky Scan

$$\phi_{eff} = \phi_W - \sqrt{\frac{eE(x,t)}{4\pi\varepsilon_0}}$$

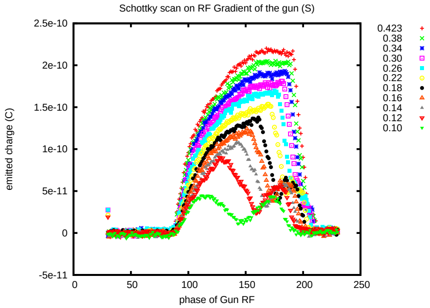
$$E(x,t) = E_{rf}(\not{x},t) + E_{sc}(x,t)$$

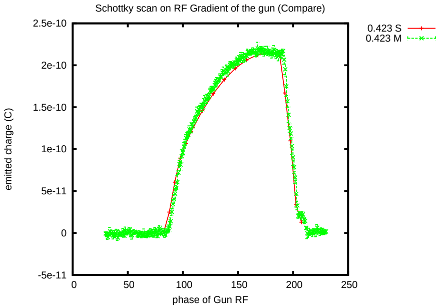
$$I_{emit} = \mu L_I (h\nu - \phi_{eff})^2$$

- Initial conditions: laser energy, laser profile, W of materal (Cu)
- Problem: find renormalization constant μ for a given nominal charge

Comparing Simulations with Reality - Schottky Scan

- Solution: iterative scheme to find μ (non-linear problem)





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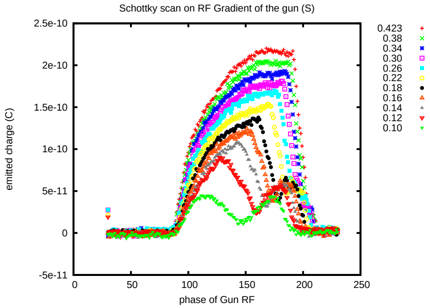

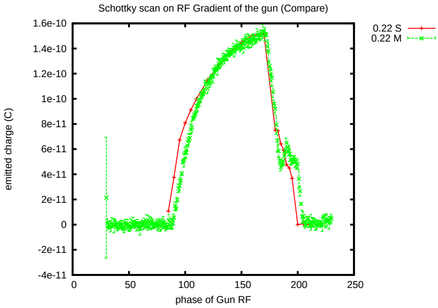

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