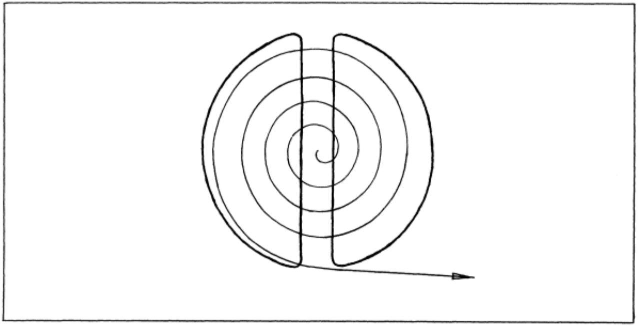
Accelerator Modeling and Advanced Simulation (AMAS) - Past, Present & Future

A. Adelmann

February 8, 2018

Different Views on Accelerators ...

curtesy of D.L. Judd (LBL)



THE CYCLOTRON AS SEEN BY THE INVENTOR

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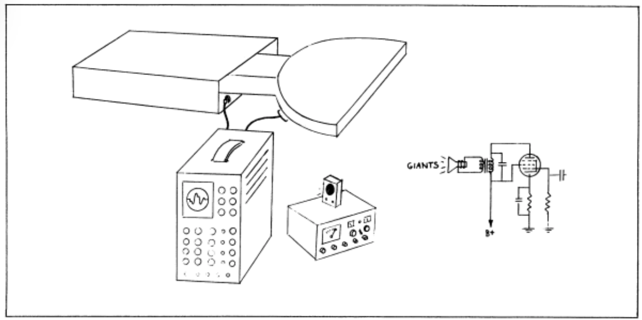

THE CYCLOTRON AS SEEN BY THE ELECTRICAL ENGINEER

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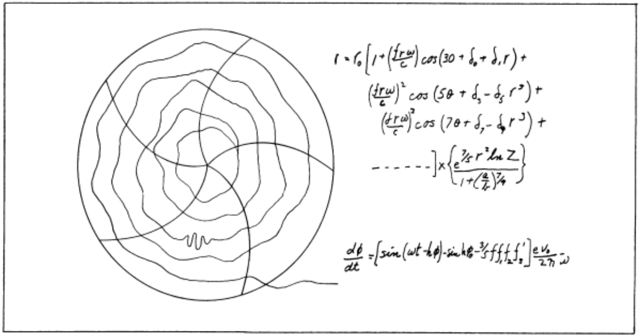

THE CYCLOTRON AS SEEN BY THE THEORETICAL PHYSICIST

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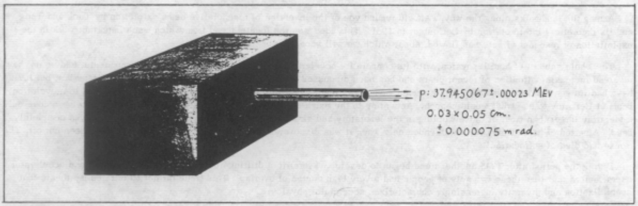

THE CYCLOTRON AS SEEN BY THE EXPERIMENTAL PHYSICIST

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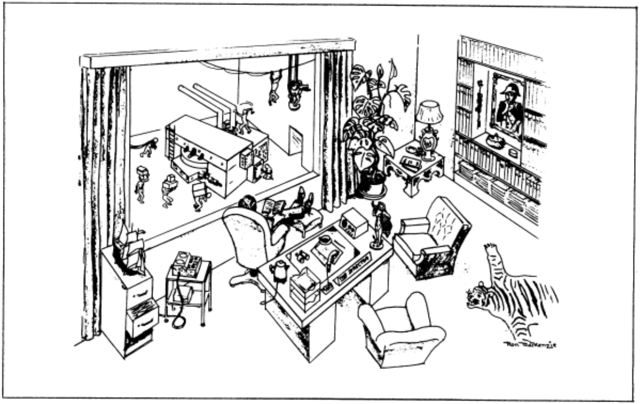


THE CYCLOTRON AS SEEN BY THE LABORATORY DIRECTOR

Mission of AMAS

Bridging the gap between qualitative and quantitative modelling by combining and extending the latest development in:

- Accelerator-Physics
- Numerical- Modelling and
- High Performance Computing.

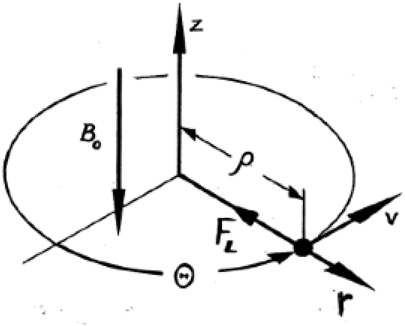
The AMAS group conducting research in the area of accelerator system simulation, participates in educational efforts (PAM-1 & PAM-1 ETH), maintains/establishes national and international collaboration.
The AMAS group applies the developed methods to PSI's existing and future machines and to cutting edge international projects.

Outline

The Principe of Charged Particle Accelerators

- guide the particles
- accelerate the particle(s)

$$\frac{m_0 v^2}{\rho} = qvB_0$$



- Revolution time $t = \frac{2\pi\rho}{v} = \frac{2\pi m_0}{qB_0}$
- t is not a function of Energy if $\beta \ll c$
- Cyclotron frequency $\omega_c = \frac{2\pi}{t}$
- Constraint $\omega_{rf} = n\omega_c$
- $\Delta E = qU_{\sim}$
- have neglected all the fun ...
  - dimensions
  - coulomb repulsion
  - radiation
  - collisions
  - spin
  - ...

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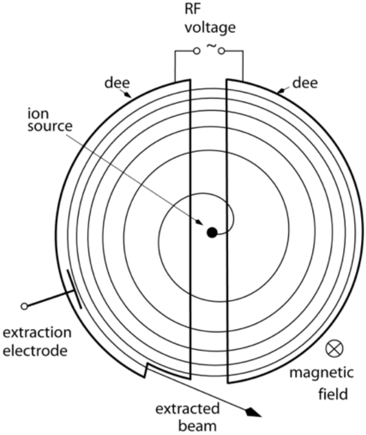

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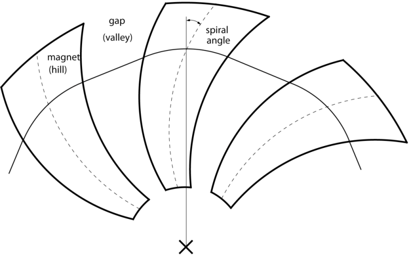

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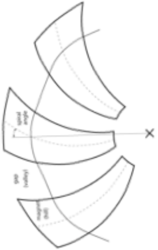

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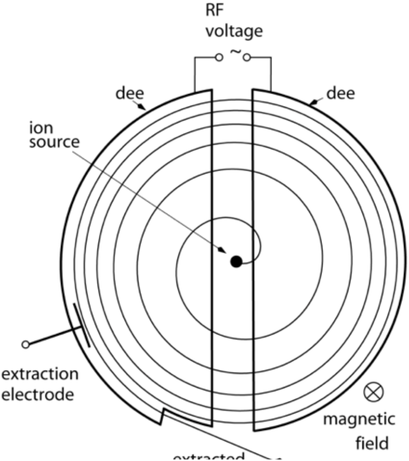

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Electron Cloud Interaction

(Electron Cloud Effects)

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Particle Matter Interaction - I

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

(Parallel Plate Benchmark)

Particle Matter Interaction - II

(Dark Current in Electron Sources)

Non Linear Interaction

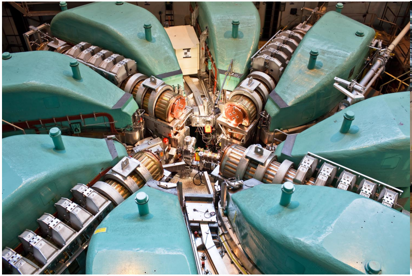
ETH prize for excellent MSc. project, P. Berger 2015

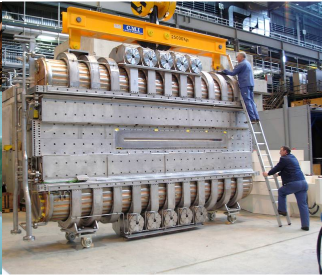
(Coasting Beam with Space Charge)

Modelling Challenges PSI

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





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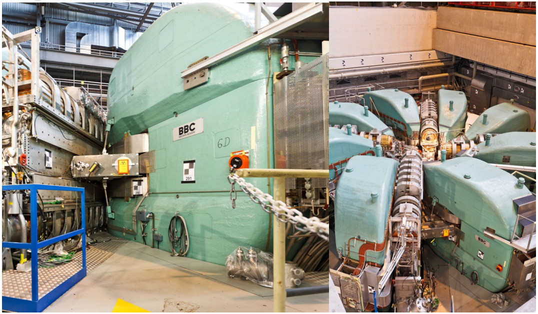

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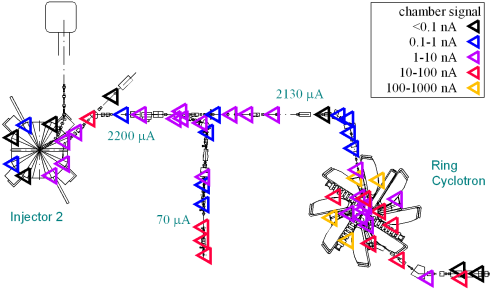

Uuups

For this Discussion: Modelling Challenges

Challenge: **understand and mitigate halo**

Q: How do we create a precise beam dynamics simulation model

- for large structures
- to enable S2E simulations with realtime aspects

Outline

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FEMAXX overview

Joint project PSI/ETH (Prof. P. Arbenz ETHZ)

- Solves 3D electric field vector wave equation
- Finite element method (FEM) with unstructured tetrahedral mesh
- Model arbitrary geometry or material property
- The parallel nature allows us to model largest structures

Compute electromagnetic fields in accelerator cavities, i.e. some of the lowest eigenfrequencies and corresponding eigenfields.

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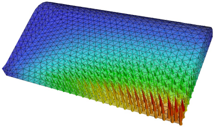

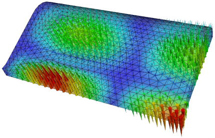

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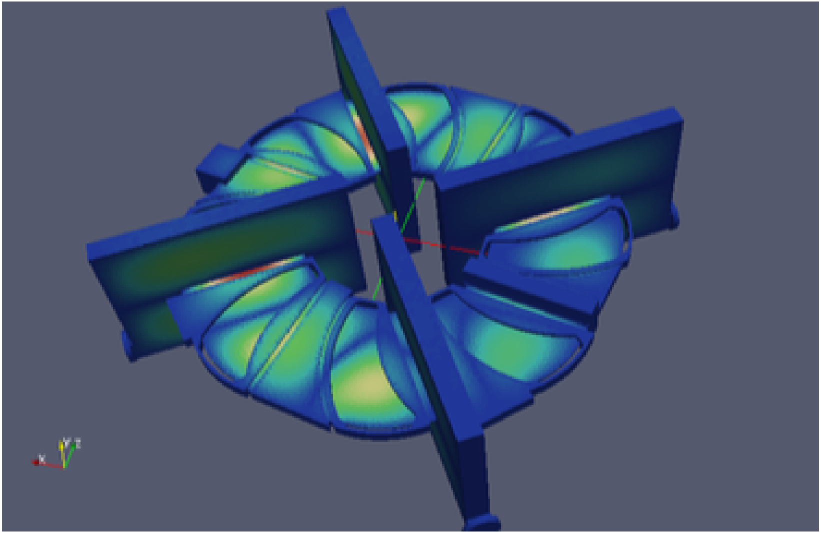
The Full PSI-Ring



Available Solvers

Eigensolver	Problem Type	Application
JDSYM	Generalized real symmetric EVP	lossless resonant cavities [R. Geus, ETH Ph.D Thesis]
JDQZ	Generalized non -Hermitian & quadratic EVP	dielectric & ohmically lossy material [H. Guo, ETH Ph.D Thesis (2012)]
NLJD	Nonlinear EVP	cavities with finite conductivity [H. Guo, ETH Ph.D Thesis (2012)]

The OPAL Developer Team

Ch. Metzger-Kraus S. L. Sheehy V. Rizzoglio (*) D. Winklehner U. Locans P. Xiaoying

J. Snuverink A. Gsell M. Frey (*) S. Russel Y. Ineichen

Ch. Rogers Ch. Wang A. Adelmann

OPAL is open source ...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A. Adelmann

OPAL V.2.0 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 released

- Common features
  - 3D space charge
  - particle Matter Interaction (protons)
  - multi-objective optimisation
  - from e, p to Uranium (q/m is a parameter)

1. OPAL-T
   - OPAL-T with time as the independent variable, can be used to model beamlines, rf-guns, injectors
   - many more linac features like auto-phasing, wake fields, 1D CSR
2. OPAL-CYCL (+ FFAG's)
   - neighbouring turns
   - time integration, 4th-order RK, LF, adaptive schemes [M. Toggweiler, AA, et al. (2014)]
   - find matched distributions with linear space charge
   - spiral inflector modelling with space charge

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Vlasov-Poisson Equation

Addressing the multi scale challenge

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.

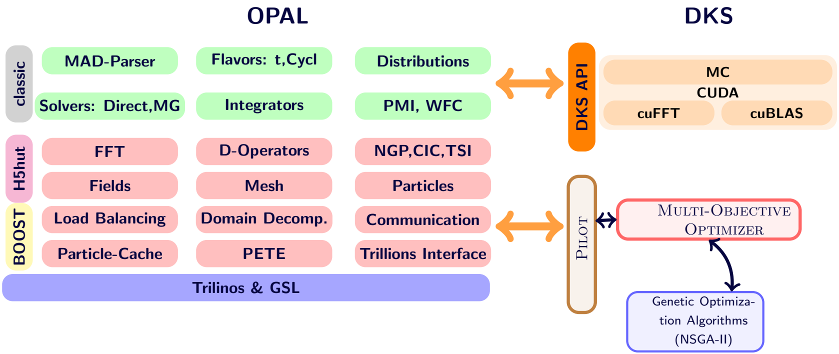
$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \frac{q}{m}(\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t)) \cdot \nabla_v f = 0. \qquad (2)$$

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 (later)
- change M during simulation (many different field solver instances)
- change Δt adaptively [M. Toggweiler, AA, et al. (2014)]
- modern computational architectures (later)

Software Architecture

MPI based + HW accelerators + Optimiser



DKS in a Nutshell I

[A. Adelmann, U. Locans, et al., CPC **207** (2016)],[U. Locans, AA, et al., CPC **215** (2017)]

Dynamic Kernel Scheduler (DKS) is a slim software layer between host application and hardware accelerator

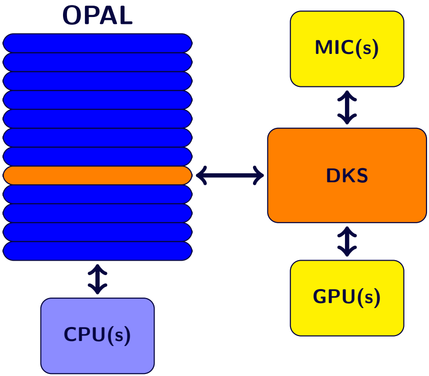
- Ease the use of hardware accelerators (GPUs and Intel MICs)
- Fully OO (C++) using CUDA, OpenCL and OpenMP to handle device specific code
- The host application remains portable and adapt better to new hardware that comes available
- Separating the hardware specific code from host application
- Software investment protection - no device code in host application

DKS in a Nutshell II

[A. Adelmann, U. Locans, et al., CPC **207** (2016)],[U. Locans, AA, et al., CPC **215** (2017)]

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 jet available)



Example 1: A Direct FFT-Based Poisson Solver

Assume you know G the Green's function

The solution of the Poisson's equation

$$\nabla^2\phi = -\rho/\varepsilon_0,$$

for the scalar potential, ϕ can be expressed as:

$$\phi(x,y,z) = \int\int\int dx'dy'dz'\rho(x',y',z')G(x-x',y-y',z-z'), \quad (3)$$

where G is the Green function and ρ is the charge density.
Discretisation of Eq. (3) on a grid with cell sizes h_x, h_y and h_z leads to:

$$\phi_{i,j,k} = h_x h_y h_z \sum_{i'=1}^{M_x}\sum_{j'=1}^{M_y}\sum_{k'=1}^{M_z} \rho_{i',j',k'} G_{i-i',j-j',k-k'}, \quad (4)$$

The solution of Eq. (4) can be obtained using FFT based convolution:

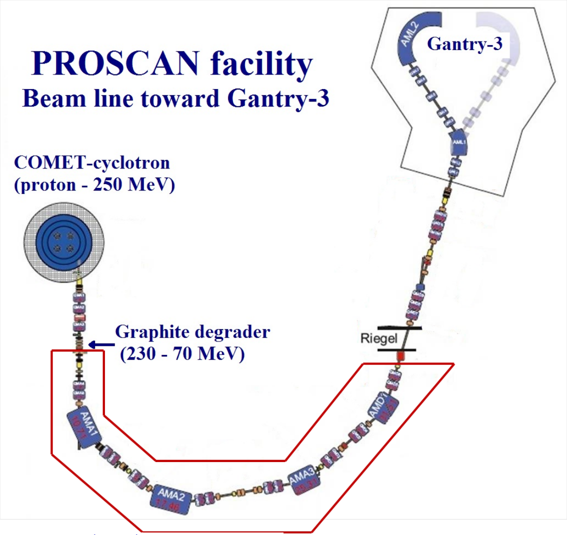
$$\phi_{i,j,k} = h_x h_y h_z \ \mathsf{FFT}^{-1}\{(\mathsf{FFT}\{\rho_{i,j,k}\}) \otimes (\mathsf{FFT}\{G_{i,j,k}\})\}$$

FFT Poisson solver - results

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

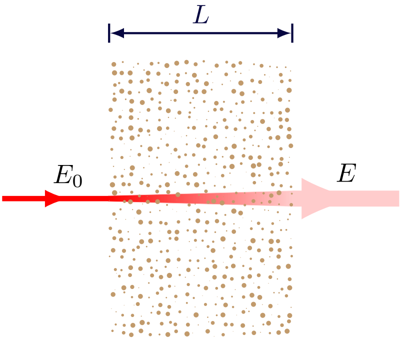
FFT size	DKS	Total time (s)	OPAL speedup	Solver t (s)	Solver speedup
64x64x32	no	324.98		22.53	
	K20	**311.17**	×**1.04**	**7.42**	×**3**
	K40	**293.7**	×**1.10**	**7.32**	×**3**
128x128x64	no	434.22		206.73	
	K20	**262.74**	×**1.6**	**32.15**	×**6.5**
	K40	**245.08**	×**1.8**	**25.87**	×**8**
256x256x128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

Example 2: Degrader for proton therapy



Example 2: Degrader for proton therapy

- The PSI COMET cyclotron deliver a proton beam at a fixed energy of 250 MeV. For proton therapy it is necessary to decrease the particle energy with in the range of 70 - 250 MeV
- A degrader is a slab of matter 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



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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

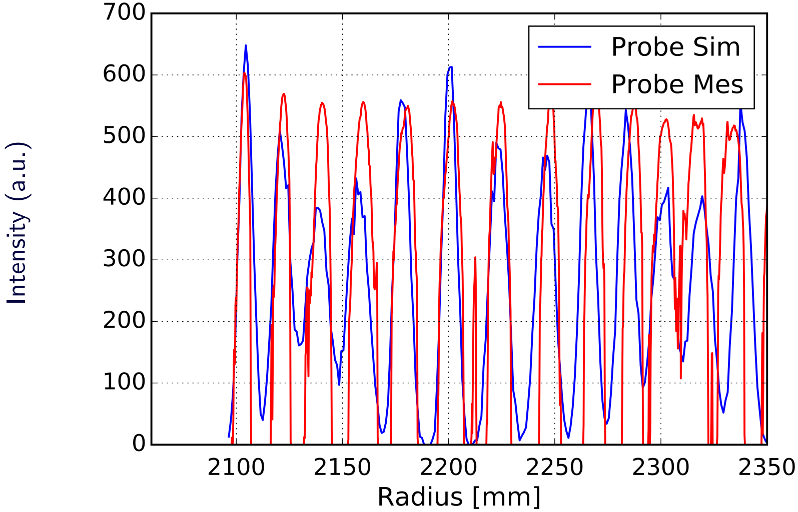
Particles	DKS	t_{degr} (s)	Degrader speedup	t_{integ} (s)	Integration speedup
10^5	no	20.30		3.46	
	MIC	**2.29**	**×8**	**0.89**	**×4**
	K20	**0.28**	**×72**	**0.15**	**×23**
	K40	**0.19**	**×107**	**0.14**	**×24**
10^6	no	206.77		34.93	
	MIC	**5.38**	**×38**	**4.62**	**×7.5**
	K20	**1.41**	**×146**	**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), Y. Ineichen, AA, et al. (2014)]

- Access to **all** OPAL statistics data as objectives
- Access to **all** OPAL varialbles as design variables
- Specify the MOOP in the OPAL input file
- Finds Pareto optimal solutions (NSGA-II)
- No tight coupling to parallelisation mechanism
- No tight coupling to optimisation algorithm
- Runs smoothly with 10000 cores and hopefully more

PSI Ring - Turnmatching



Iterative Poisson Solver SAAMG-PCG

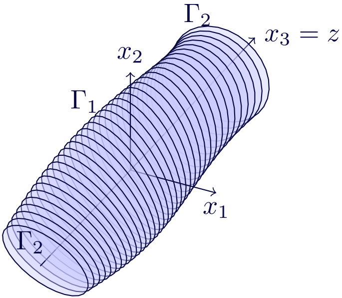
Boundary Problem

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

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

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

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

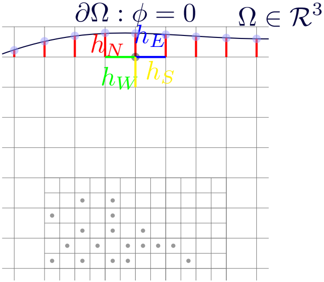
1. elliptic beam-pipe
2. arbitrary beam-pipe element

Iterative Poisson Solver SAAMG-PCG cont.

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

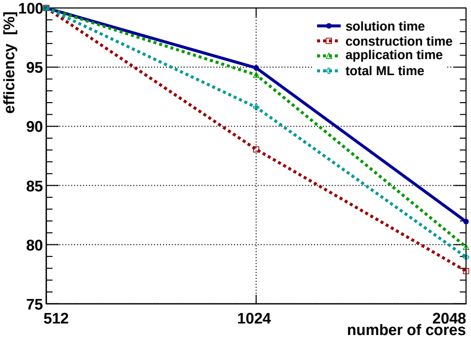
$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

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



- solve anisotropic electrostatic Poisson PDE with an iterative solver
- accuracy ε is a parameter
- reuse information available from previous time steps
- achieving good parallel efficiency
- irregular domain with “exact” boundary conditions
- easy to specify boundary surface

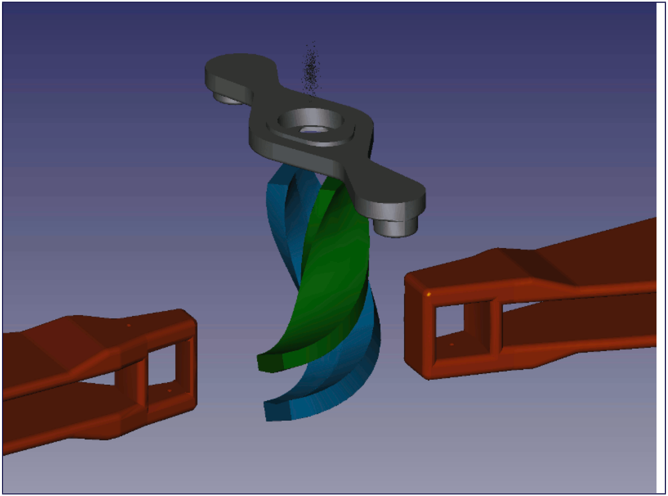
SAAMG-PCG Parallel Efficiency



[AA et al., JCP, **229** 12 (2010)]

- obtained for a tube embedded in a $1024 \times 1024 \times 1024$ grid
- construction phase is performing the worst with an efficiency of 76%
- influence of problem size on the low performance of the aggregation in ML

IsoDAR Inflector



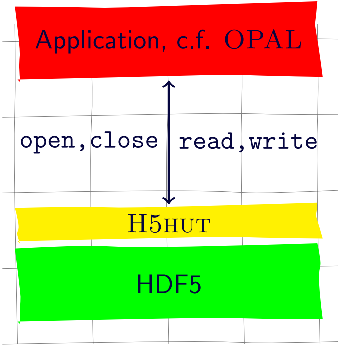
Data Analytics

(Coasting Beam with Space Charge)

H5hut in a Nutshell

H5hut is a slim API on top of HDF5. Developed in collaboration with LBL, H5hut is made available as an open-source library to various communities: particle accelerator, plasma & climate.

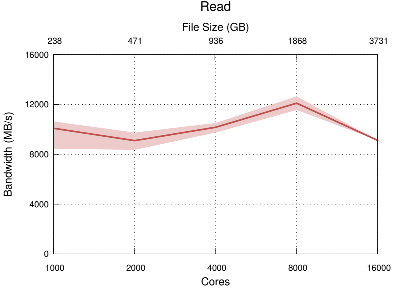
- H5hut provides abstraction for
  - n-dimensional particles
  - n-dimensional scalar and vector fields
  - triangle based surface representation
- H5hut hides the complexity of (parallel) HDF5 and at the same time provides maximum I/O performance.
- OPAL is using H5hut

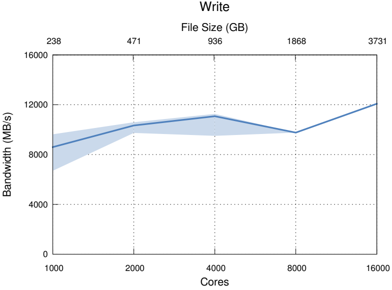


`http://www-vis.lbl.gov/Research/H5hut/` & A. Gsell (PSI)

Performance: Results

Synthetic H5Block weak scaling study



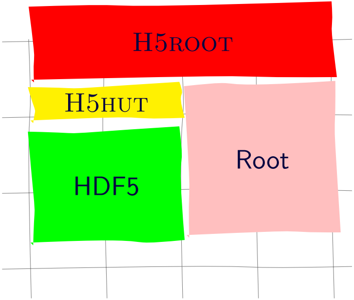


- Weak scaling to 16,000 cores on Franklin and 3.7TB of data.
- Read times include a halo exchange, to transmit a ghost region of cells among neighboring blocks.
- The solid line shows the mean bandwidth, shaded region minimum and maximum.

H5ROOT in a Nutshell

H5ROOT efficiently analyses the largest amount of data resulting from particle accelerator simulations. H5ROOT was originally developed by TS and is continuously kept up to date with the root development and slightly enhanced.

- H5ROOT provides GUI and scripting capabilities
- H5ROOT inherits the performance and functionalities of
    - root
    - H5HUT
- Roger is based to $\sim$ 80 % H5ROOT



`http://amas.web.psi.ch/tools/H5root/index.html`

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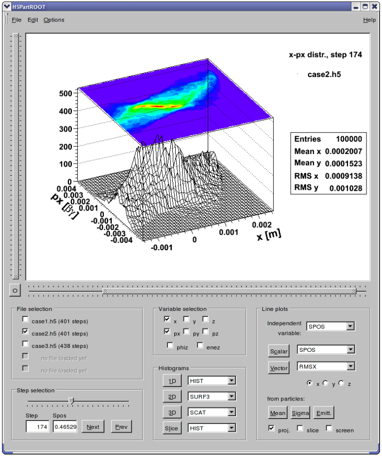
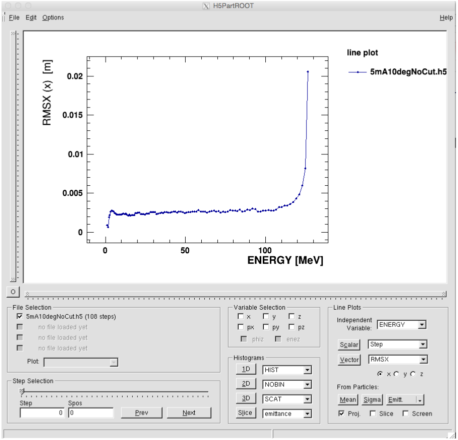
H5ROOT Sample Panels

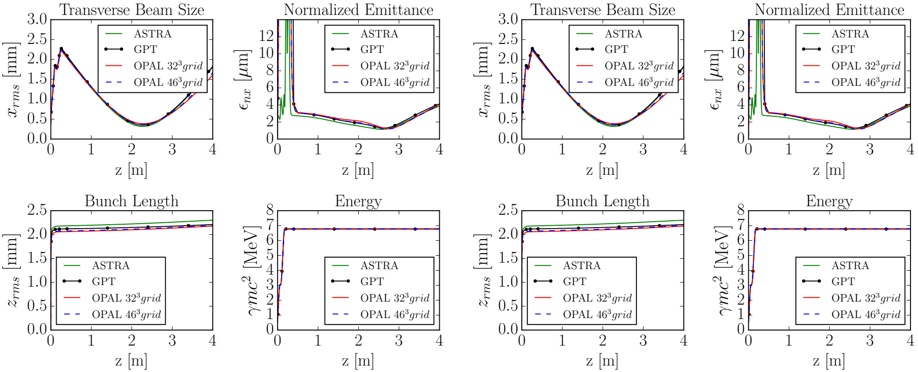




Benchmarking

AWA-Gun Code Comparison - N. Neveu (ANL & IIT)

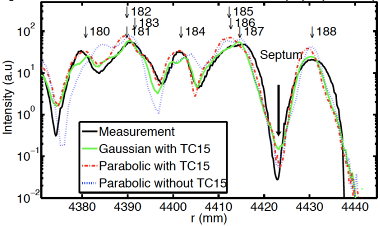
All codes matched within 5%.
Well below measurement thresholds at AWA.



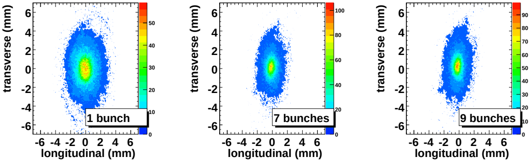
Outline

A Selection of Past Achievements

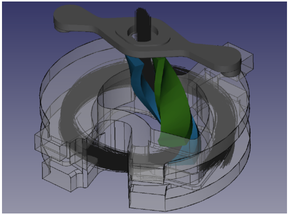
Precise high intensity cyclotron modelling
[Y. Bi, AA, et al., PR-AB **14**(5) (2011)]



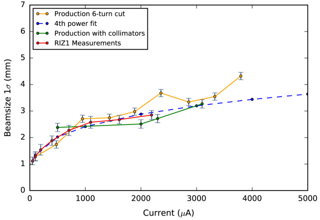
Neighbouring bunch modelling
[J. Yang, AA, et al., PR-AB **13**(6) (2010)]



3D Simulations of a Cyclotron Spiral Inflector
[Winklehner D, AA, et al., PR-AB **20**(12) (2017)]



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



A Selection of Past Achievements

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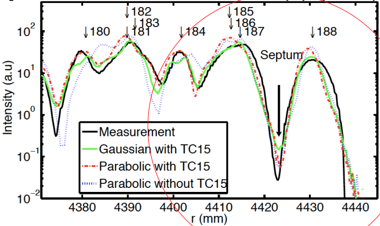
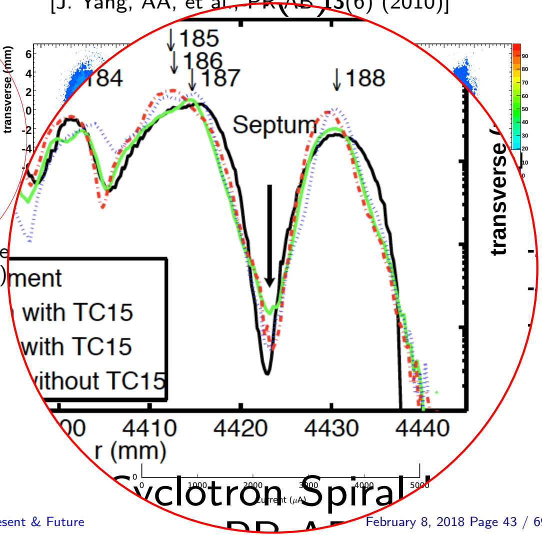


Neighbouring bunch modelling
[J. Yang, AA, et al., PR-AB **13**(6) (2010)]



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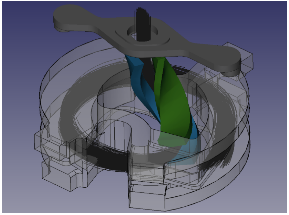
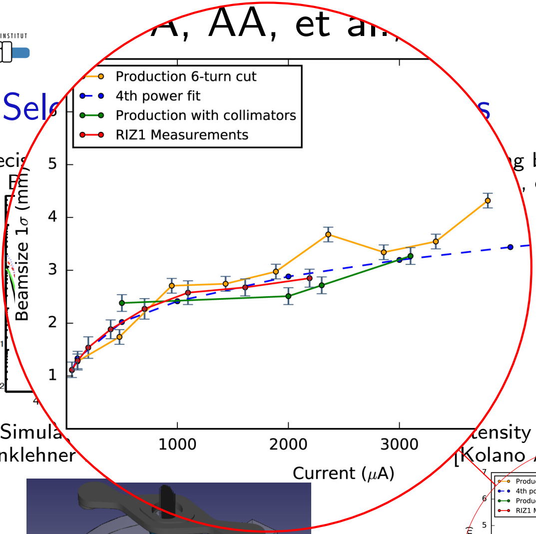
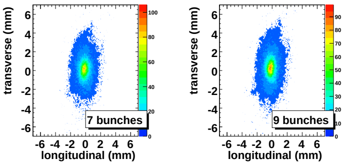


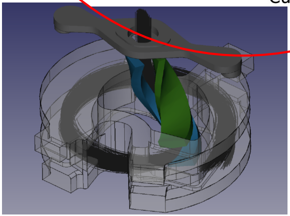
A Sele... s



Precis... g bunch modelling
[Y. B... , et al., PR-AB **13**(6) (2010)]



3D Simula... [Winklehner



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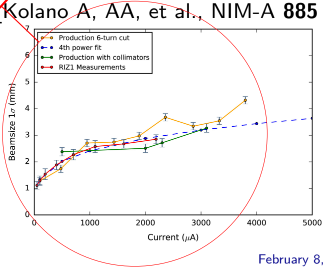
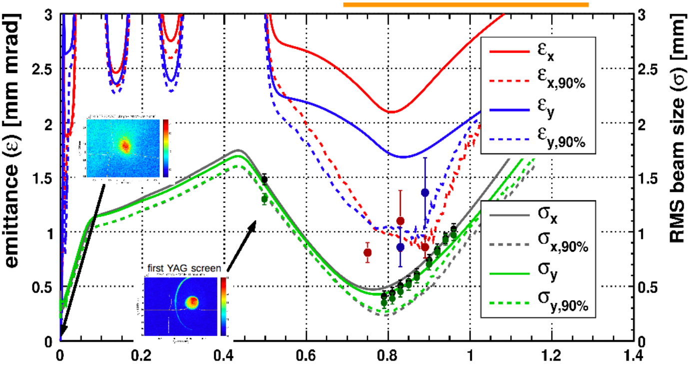
[Kolano A, AA, et al., NIM-A **885** (2018)]



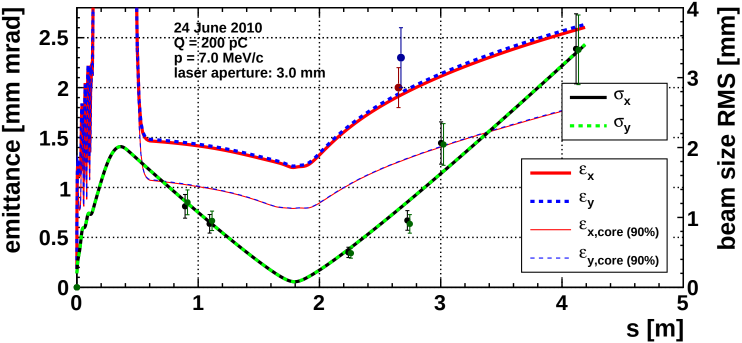
PSI 500-kV Low-Emittance Electron Source

[T. Schietinger et.al. (2008)]



The SwissFEL Injector Test Facility Gun

[T. Schietinger et.al., (2010)]

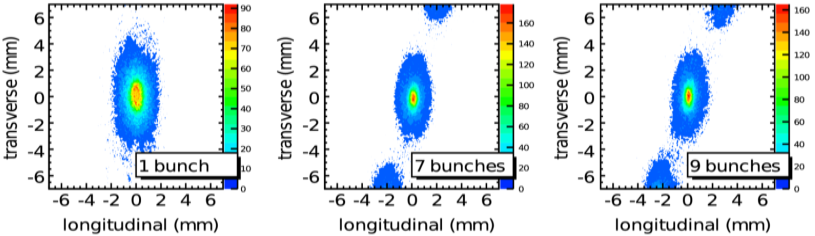


Outline

M. Frey: Precise Simulations of Multi Bunches in High Intensity Cyclotrons

SNF project 200021_159936

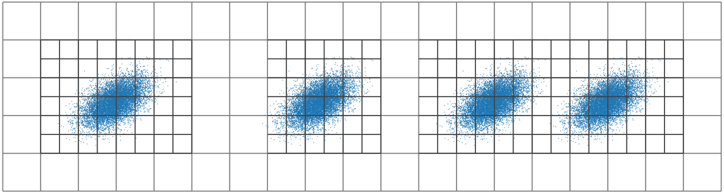
- Neighbouring bunch effects occur in case of small turn separation for high intensity cyclotrons (see paper [J. Yang, AA, et al., PR-AB **13**(6) (2010)])



M. Frey: Precise Simulations of Multi Bunches in High Intensity Cyclotrons

SNF project 200021_159936

- **Requirements:**
  - Solving large-scale N-body problems of $\mathcal{O}(10^9 \ldots 10^{10})$ particles coupled with Maxwell's equations
  - Particle-in-Cell with extremely fine mesh of $\mathcal{O}(10^8 \ldots 10^9)$ grid points
- **Bottlenecks:**
  - Waste of memory and resolution in regions of void
- **Solution:**
  - Block-structured adaptive mesh-refinement



M. Frey: Precise Simulations of Multi Bunches in High Intensity Cyclotrons

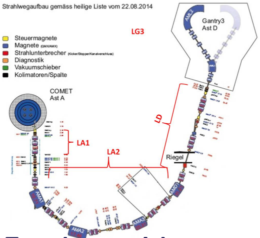
SNF project 200021_159936

- **Software:**
  - OPAL (for physics)
  - AMReX (for grids, formerly: BoxLib) (`https://ccse.lbl.gov/AMReX`)
- **Hardware:**
  - Piz Daint at CSCS

Taken from `https://www.cscs.ch/computers/piz-daint/`

BD model of the transport line towards Gantry 3

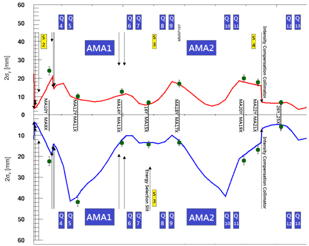
[Rizzoglio V, AA, et al., PR-AB **20**(12) (2017)]



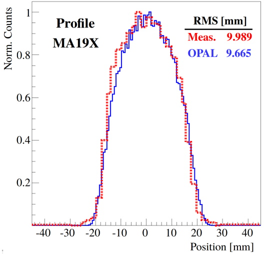
- linear and non-linear transport
- particle-matter interaction
- benchmark against several measurements
- optimization of the beam line (transmission)
- support the commissioning of the Gantry 3

Model results

Envelope with measurements



Measured beam profile



Monte Carlo simulation in OPAL: graphite degrader

PROSCAN degrader

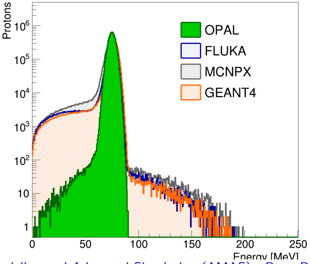
6 movable wedges of graphite

Particle-matter interaction

- simplfied geometry: 6 slabs
- energy loss: Bethe-Bloch equation
- elastic multiple Coulomb scattering: Moliere theory
- single elastic scattering: Rutherford theory
- no inelastic scattering

OPAL benchmark against...

3 fully integrated Monte Carlo codes:



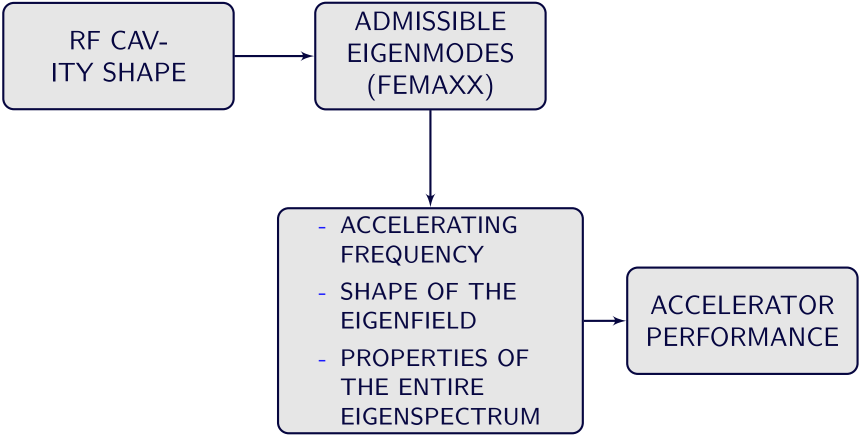
Range measurements with a water tank

Reference (MeV)	OPAL (MeV)	Measurem. (MeV)
230	231.69	231.20 ± 0.17
190	192.10	191.61 ± 0.16
150	152.13	152.05 ± 0.16
70	73.66	73.88 ± 0.17

Discrepancy around 0.2%

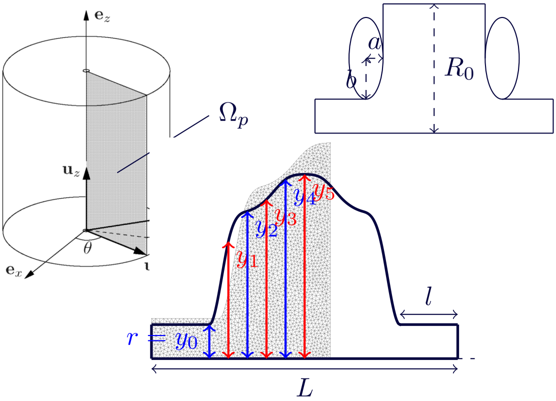
Marija Kranjčević: Multiobjective optimization of RF cavities shapes

Collaboration with Prof. P. Arbenz (ETH), [Y. Ineichen, ETH Ph.D Thesis (2013)]



Shape optimization of RF cavities

1. parameterizing the cross section Ω_p[1] of axisymmetric cavities



[1] Sketch taken from Diss. ETH No. 16243.

Shape optimization of RF cavities

2. defining goals
   - target frequency
   - maximizing the quality factor
   - maximizing the shunt impedance
   - etc.

3. using optimization algorithms to find the parameters of cavity shapes that fulfil the given goals

Future AMAS Research Directions

- PSI HIPA
  - Ring flat top cavity [N.J. Pogue, AA, et al., NIM-A **828** (2016)], [N.J. Pogue, AA, et al., NIM-A **821** (2016)]
  - Detailed understanding of halo development
- ACHIP
  - Numerical modelling of QFEL (R. Ischebeck, PSI)
- Reduced order models (OPAL related)
  - Machine learning
  - polynomial chaos based [arXiv:1509.08130]
  - particle core models
- Numerical Methods
  - collisions (OPAL related)
  - fast randomised iteration (largest EV problems)
- International Collaborations
  - High power cyclotron for sterile neutrino search (MIT)
  - High power cyclotron/linac for ADS (Cern, CIAE & Riken)
  - Modelling of advanced accelerator schemes AWA (ANL)
  - OPAL open source collaboration (PSI leading house)

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

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[J. Qiang, et.al] IPAC 2007, `10.1109/PAC.2007.4441024`

[Rizzoglio V, AA, et al., PR-AB **20**(12) (2017)] Rizzoglio, V., Adelmann, A. et al., Phys. Rev. AB **20**(12) 124702 (2017)

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Backup

Collisions I

Motivation

1. model emission of ultra cold electrons
2. understand Coulomb scattering (Borsch effect) [J. Qiang, et.al]
3. do we have to worry about it in next generation machines?
4. model non Gaussian tails (high intensity hadron machines)

In [J. Qiang, et.al] we wrote:

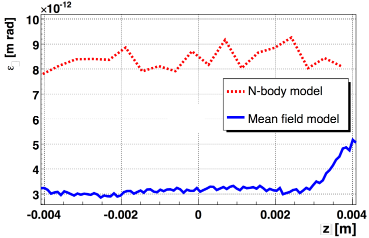
- Nano-tips with high acceleration gradient around the emission surface have been proposed to generate high brightness beams.
- However, due to the small size of the tip $r = 10\,\text{nm}$, the charge density near the tip is very high even for a small number of electrons.
- The stochastic Coulomb scattering near the tip can degrade the beam quality and cause extra emittance growth and energy spread.

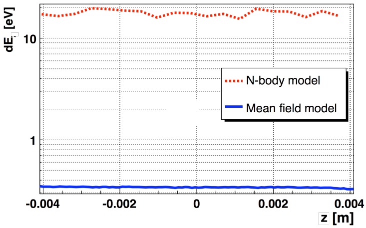
Collisions II

Motivation

Using a brute force N^2 summation we obtained the following observations:

- slice emittance over the bunch length $\times\ 2$ higher
- energy spread $\times\ 100$ higher





Collisions III

Motivation

The

$\mathrm{P^3M}$ = **P**article-**P**article + **P**article-**M**esh

is a efficient way to accomplish this task.

- high resolution from PP part: $\mathcal{O}(K^2), K \ll N$, $1/(\boldsymbol{x} - \boldsymbol{x'} + \varepsilon)$
- good performance from PM part: $\boldsymbol{\Phi}(\boldsymbol{x}) = \int G(\boldsymbol{x}, \boldsymbol{x}')\rho(\boldsymbol{x}')d^3\boldsymbol{x}'$
- adjustable influence of Coulomb collisions by fixing K in choosing r_c

Opens up the possibility of S2E beam simulations with *adjustable* Coulomb interaction

Disorder Induced Heating

Problem Setup

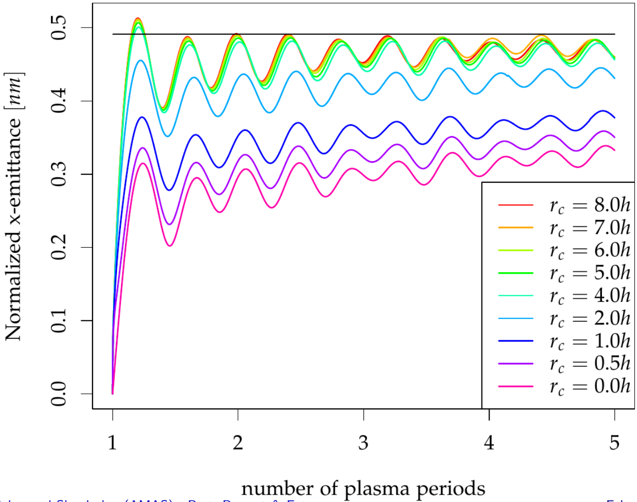
Loosely connected to LBL UED parameters:

- spherical, cold beam of radius $R = 17.7400\,\mu m$ and charge $Q = 25\,fC$
- constant focusing applied
- cubical domain with edge length $L = 100\,\mu m$
- $\mathrm{P}^3\mathrm{M}$ simulation over 5 plasma periods
- boundary conditions: open in x, y periodic in z
- $M = 256^3$
- r_c varying from $0\,\mu m$ to $3.1250\,\mu m$
- $N = \mathcal{O}(10^7)$
- $P_{core} = 128$
- simulation over 1000 time-steps

Goal compute T^f

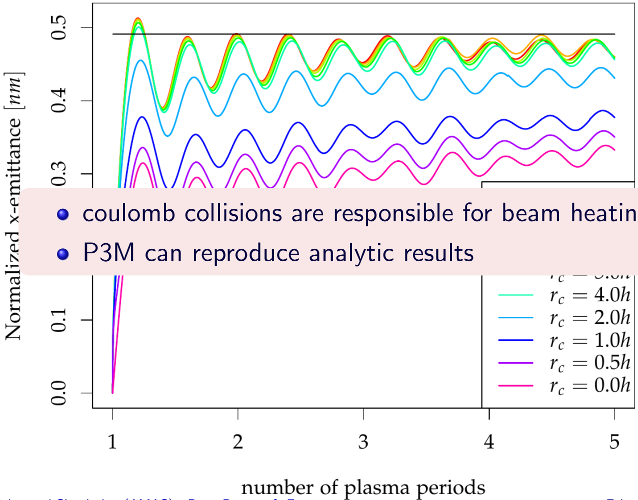
Disorder Induced Heating

Simulation Results MSc. thesis B. Ulmer



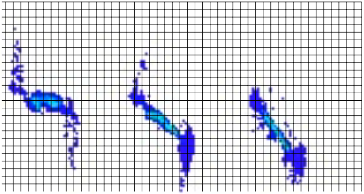
Disorder Induced Heating

Simulation Results MSc. thesis B. Ulmer

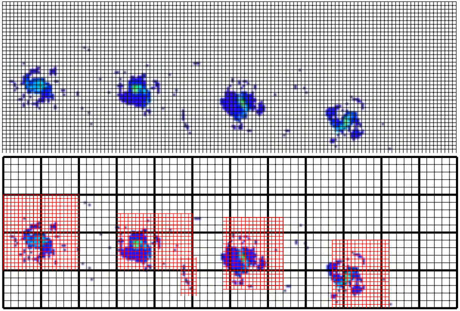


- coulomb collisions are responsible for beam heating!
- P3M can reproduce analytic results

AMR and OPAL-CYCL



- Boxlib based AMR
- PhD. project SNF funded
- Focus on PSI-Ring neighboring bunch interaction & UQ [arXiv:1509.08130]



FFT Poisson solver and DKS

CUDA implementation of FFT Poisson solver in DKS

- **cuFFT:** The Nvidia CUDA Fast Fourier Transform library is used to compute FFT and inverse FFT
- **CUDA Streams:** Separate CUDA streams are used to overlap data transfer and kernel execution
  - Stream for transferring ρ to GPU memory and calculating $\widehat{\rho}$
  - Stream for calculating G and $\widehat{G}$
- **CUDA IPC:** CUDA Inter-process communication is used to share device memory between multiple MPI processes
- **CUDA MPS:** CUDA Multi-Process Service is used to optimize sharing of device resources between multiple MPI processes

Future implementations

- **OpenCL:** based on same principles as CUDA, FFT implementation needed
- **Intel MIC:** Intel MKL library used for FFT, streams and memory sharing principles necessary to achieve asynchronous execution and sharing of one device among multiple MPI processes

Dynamic Kernel Scheduler concept - example code

```
//DKS base class handles communication and task execution on device
DKSBase dks;
dks.setAPI(API_NAME); //optional (OpenCL, CUDA, OpenMP)
dks.setDevice(DEVICE_NAME); //optional (-gpu, -mic)

//allocate memory on device and write data
void *mem_ptr;
mem_ptr = dks.allocateMemory<Complex_t>(DATA_SIZE, NULL);
dks.writeData<Complex_t>(mem_ptr, DATA_ARRAY, DATA_SIZE);

//execute FFT or IFFT
if (direction == 1) {
  dks.callFFT(mem_ptr, DIMENSIONS, DIM_SIZE);
} else {
  dks.callIFFT(mem_ptr, DIMENSIONS, DIM_SIZE);
  dks.callNormalizeFFT(mem_ptr, DIMENSIONS, DIM_SIZE);
}

//read data and free memory
dks.readData<Complex_t>(mem_ptr, DATA_ARRAY, DATA_SIZE);
dks.freeMemory<Complex_t>(mem_ptr, DATA_SIZE);
```

Dynamic Kernel Scheduler concept - example code

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dks.readData<Complex_t>(mem_ptr, DATA_ARRAY, DATA_SIZE);
dks.freeMemory<Complex_t>(mem_ptr, DATA_SIZE);
```

Dynamic Kernel Scheduler concept - example code

```
//DKS base class handles communication and task execution on device
DKSBase dks;
dks.setAPI(API_NAME); //optional (OpenCL, CUDA, OpenMP)
dks.setDevice(DEVICE_NAME); //optional (-gpu, -mic)

//allocate memory on device and write data
void *mem_ptr;
mem_ptr = dks.allocateMemory<Complex_t>(DATA_SIZE, NULL);
dks.writeData<Complex_t>(mem_ptr, DATA_ARRAY, DATA_SIZE);

//execute FFT or IFFT
if (direction == 1) {
  dks.callFFT(mem_ptr, DIMENSIONS, DIM_SIZE);
} else {
  dks.callIFFT(mem_ptr, DIMENSIONS, DIM_SIZE);
  dks.callNormalizeFFT(mem_ptr, DIMENSIONS, DIM_SIZE);
}

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Linear Space Charge Map

- Space charge Hamiltonian (Baumgarten, PhysRevSTAB.14.114201)

$$H_{sc} = -\frac{K_x}{2}x^2 - \frac{K_y}{2}y^2 - \frac{\gamma^2 K_z}{2}z^2,$$

with space charge strengths K_x, K_y and K_z. This leads to

$$M_{sc}(s) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ K_x s & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & K_y s & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & K_z \gamma^2 s & 1 \end{pmatrix}.$$

Mathematical model of JDSYM

- Reformulating Maxwell's equations, eliminating $\mathbf{H}$ and using a time harmonic ansatz for $\mathbf{E}(\boldsymbol{x}, t)$ we obtain

$$\begin{aligned} \mathbf{curl}\,\mathbf{curl}\,\boldsymbol{e}(\boldsymbol{x}) - \lambda\boldsymbol{e}(\boldsymbol{x}) &= 0 \quad \forall \boldsymbol{x} \in \Omega, \quad \lambda = \omega^2/c^2 \\ \nabla \cdot \boldsymbol{e}(\boldsymbol{x}) &= 0 \quad \forall \boldsymbol{x} \in \Omega \\ \boldsymbol{e}(\boldsymbol{x}) \times \boldsymbol{n}(\boldsymbol{x}) &= \mathbf{0} \quad \forall \boldsymbol{x} \in \Gamma \end{aligned}$$

  $\mathbf{e}(\mathbf{x})$ is the amplitude of the eigenfield at location $\mathbf{x}$.
- Discretization using tetrahedral meshes and Nédélec elements
- Exploiting symmetries, BC: $\mathbf{e} \times \mathbf{n} = \mathbf{0}$ or $\mathbf{e} \cdot \mathbf{n} = 0$
- We use the weak formulation proposed by Kikuchi (1987) and discretize using quadratic edge elements proposed by Nédélec (1980). This yields a large sparse constrained matrix eigenvalue problem of the form

$$A\mathbf{x} = \lambda M\mathbf{x} \qquad C^T\mathbf{x} = \mathbf{0}. \tag{5}$$