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# OPAL and FEMAXX - Parallel & Open Source Codes for Precise Particle Accelerator Modeling

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# Outline

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1. Context of this Talk
2. Why not (yet) using a GPU?
3. Inside the Boxes
4. Plans for the Future

# Developer/User Model of OPAL and FEMAXX

- OPAL (Object Oriented Parallel Accelerator Library)
  - particle tracking with 3D space charge
  - linear and circular machines
  - MAD based input language
- FEMAXX (Finite Element Eigenmode Solver)
  - real and complex solver
  - large structures

**The Common Theme of the Codes**

- Open Source Codes
- Heavily student & user based development
- MPI based, weak scaling up to $\approx 10k$ cores on relevant & challeging problems

How can we make use of the new technologies (crazy concurrency, memory hierarchies) in a "community code"?

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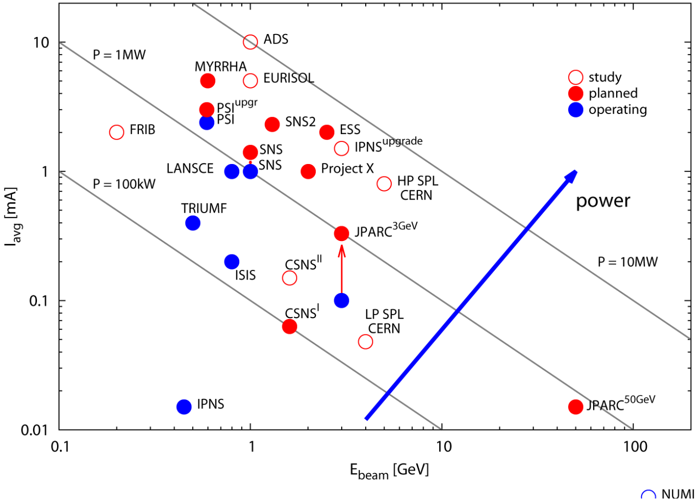
# Science Driver - One Argument

## Why Precise Beam Dynamics Simulations?



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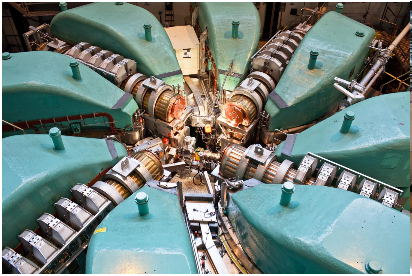
## Why Precise Beam Dynamics Simulations?

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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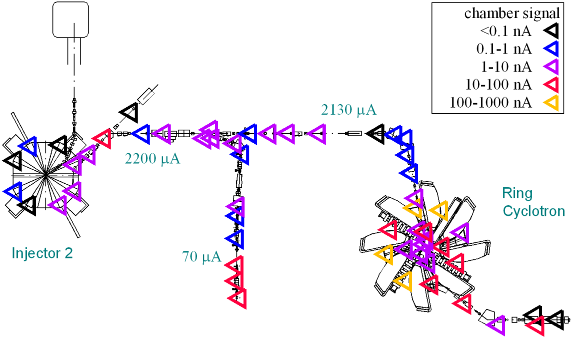

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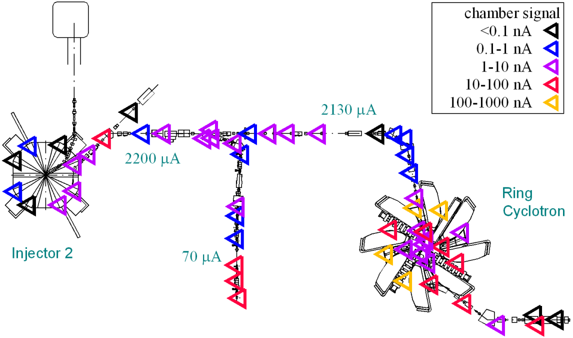

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# Science Driver - One Argument

# 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: $10^{-4} \ldots 10^4$ (m) $\rightarrow \mathcal{O}(1e5)$ integration steps
  - $v \ll c \ldots v \sim c$
  - Large (complicated structures)
  - Neighboring bunches
- Multiphysics
  - Particle mater interaction: monte carlo
  - Secondary particles i.e. multi specis

**Advanced ~~Computing~~ Modeling for Accelerators**

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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# Outline

# Why not (yet) GPU

History

- Connection Machine (Thinking Machines CM-2 .. 5) out of business: 1994:
  - was HPC leader ...
  - Lisp*,C* and "non standard" architecture/HW
- IBM Road Runner LANL
  - what would you do with a cell-code today ?

# Why not (yet) using a GPU?

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## Lessons Learned

- For a complex multi-physics code it is a big investment
- However, with the advent of languages such as CUDA etc. the risk is somewhat smaller.
- There is still the question, if the future, we really wants to deal with heterogenous architectures ...

# Outline

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# 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

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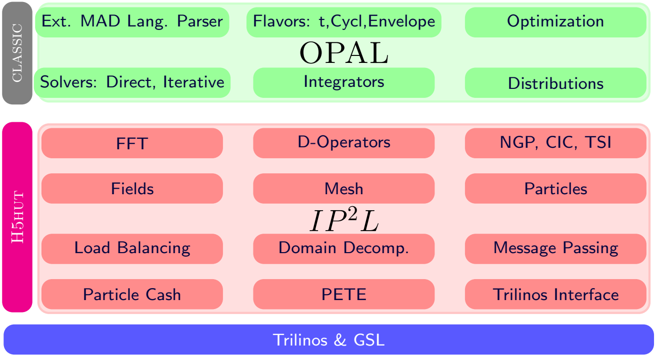
# OPAL Architecture




- **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/**

# Maxwell's Equation in the Electrostatic approximation

Field Maps &
Analytic Models

Electro
Magneto
Optics

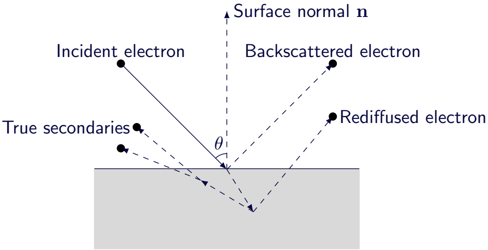
$$\nabla \cdot \boldsymbol{E}_{sc} = \rho/\varepsilon_0 = \nabla \cdot \nabla \phi_{sc}$$
$$\Delta \phi_{sc} = -\frac{\rho}{\varepsilon_0}$$
& BC's

N-Body
Dynamics

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

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

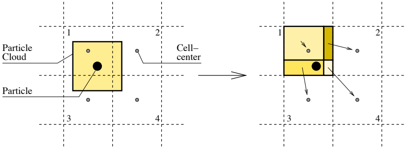



- Phenomenological- don't involve secondary physics but fit the data.
- Model 1 developed by M. Furmann and M. Pivi
- Model 2 (Vaughan) is easier to adapt to SEY curves

# A fast Direct FFT-Based PIC Poisson Solver

Solving for $\phi$ 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/grid-points.

1. Let $\Omega$ be spanned by a Cartesian structured mesh of $l \times n \times m$ with $l = 1 \ldots M_x$, $n = 1 \ldots M_y$ and $m = 1 \ldots M_z$. The mesh size is a function of time: $h_x(t), h_y(t)$ and $h_z(t)$.
2. Discretize $\rho \to \rho_h$ and $G \to G_h$ on a regular grid (PIC).




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

# A fast Direct FFT-Based PIC Poisson Solver

- ▷ Assign (scatter) all particles charges $q_i$ to nearby mesh points to obtain $\rho$
- ▷ Lorentz transform to obtain $\rho$ in beam rest frame $\mathbf{S}_{beam}$.
- ▷ Use FFT on $\rho$ and $G$ to obtain $\widehat{\rho}$ and $\widehat{G}$
- ▷ Determine $\widehat{\phi}$ on the grid using $\widehat{\phi} = \widehat{\rho} \cdot \widehat{G}$
- ▷ Use inverse FFT on $\widehat{\phi}$ to obtain $\phi$
- ▷ Compute $\mathbf{E} = -\nabla\phi$
- ▷ Lorentz back transform to obtain $\mathbf{E}_{sc}$ and $\mathbf{B}_{sc}$ in laboratory frame $\mathbf{S}_{lab}$
- ▷ Interpolate (gather) $\mathbf{E}$, $\mathbf{B}$ at particle positions $\mathbf{x}$ from $\mathbf{E}_{sc}$ and $\mathbf{B}_{sc}$

Charge assignment and electric field interpolation are related to the interpolation scheme. If $e_i$ is the charge of a particle, we can write the density at mesh point $\mathbf{k}_m$ as

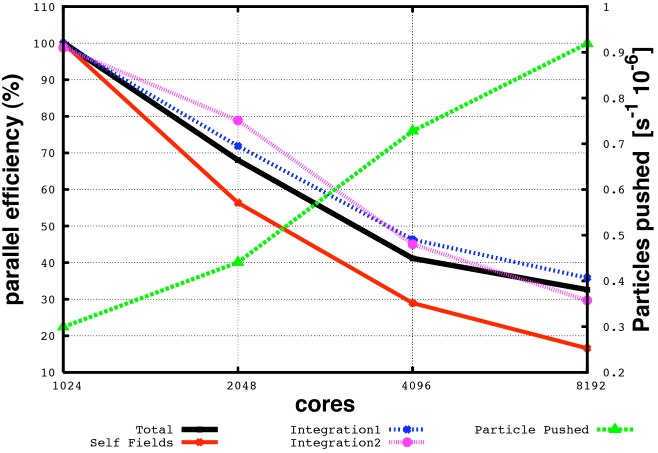
$$\rho(\mathbf{k}_m)^D = \sum_{i=1}^{N} e_i \cdot W(\mathbf{q}_i, \mathbf{k}_m),\ m = 1 \ldots M \qquad (1)$$

where $W$ is a suitably chosen weighting function.

# A fast Direct FFT-Based PIC Poisson Solver

## OPAL Parallel Scaling on Cray XT5 (FFT Solver)

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

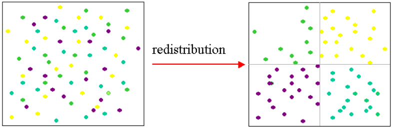


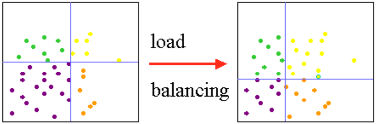
# A fast Direct FFT-Based PIC Poisson Solver

## Load Balancing

Logically we can divide OPAL into three sections:

1. Initialisation: create distribution and set-up accelerator
2. Initial Load balancing using *spatial layout*
3. Tracking
    1. If necessary, dynamic load balancing



# Iterative Poisson Solver SAAMG-PCG

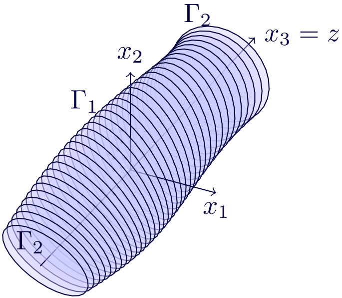
## Boundary Problem

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

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

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

- $\Omega \subset \mathbb{R}^3$: simply connected computational domain
- $\varepsilon_0$: the dielectric constant
- $\Gamma = \Gamma_1 \cup \Gamma_2$: boundary of $\Omega$
- $d$: distance of bunch centroid to the boundary




$\Gamma_1$ is the surface of an

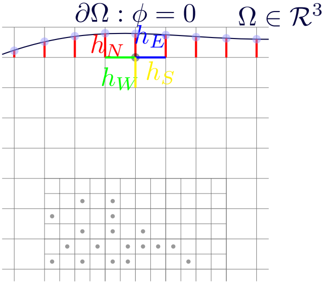
1. elliptic beam-pipe
2. arbitrary beam-pipe element

# Iterative Poisson Solver SAAMG-PCG cont.

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

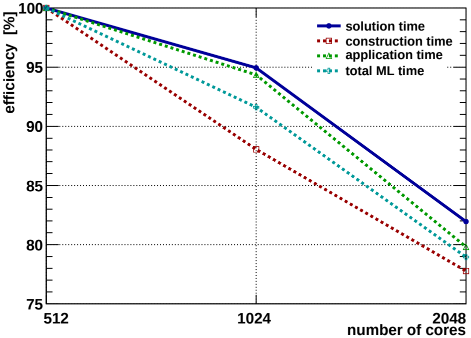
$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

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




- solve anisotropic electrostatic Poisson PDE with an iterative solver
- 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

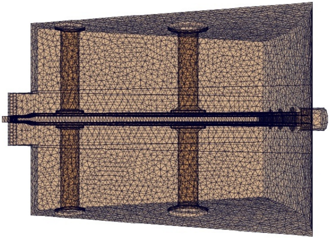


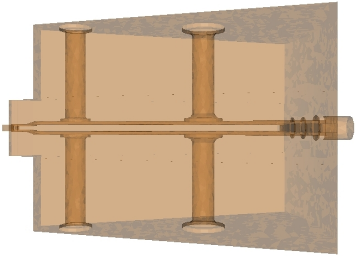

[A. Adelmann, P. Arbenz, et al.]

- 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

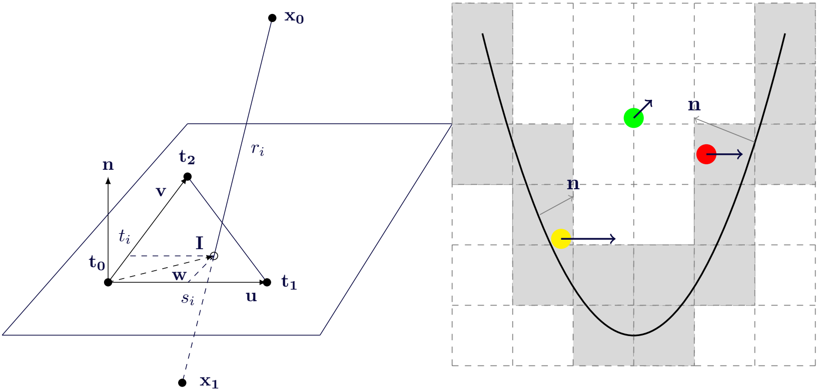
# 3D Geometry Handling Capability of OPAL

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





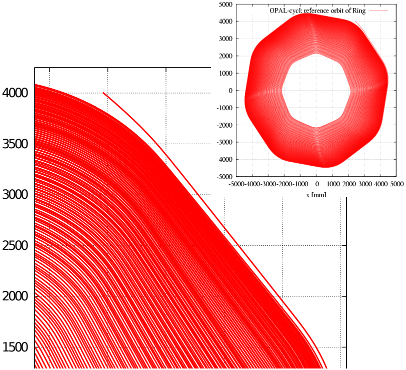
- Triangle-line segment intersection
- Boundary bounding box to speedup the collision tests
- We can handle arbitrary structure as long as it is closed

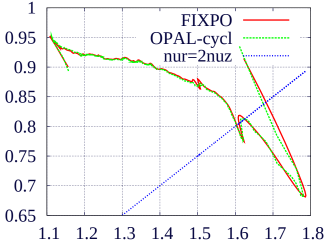



[C. Wang, A. Adelmann, et al.]

# PSI 590 MeV Ring - last 8 turns @ 2.2 mA

- 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



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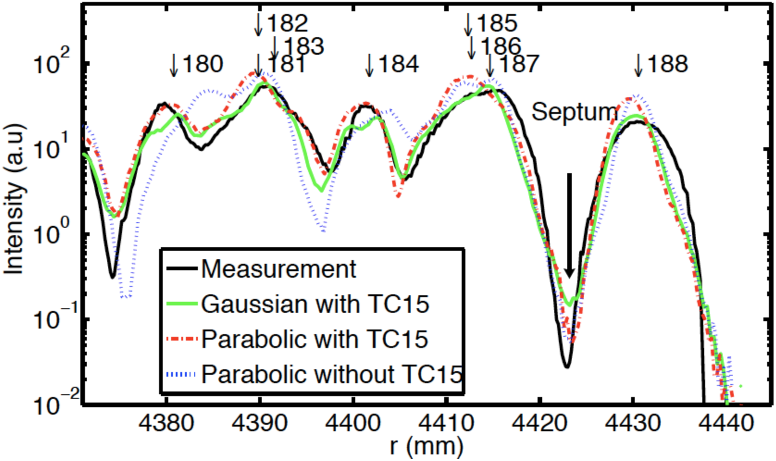


[Y. Bi, A. Adelmann, et al.]

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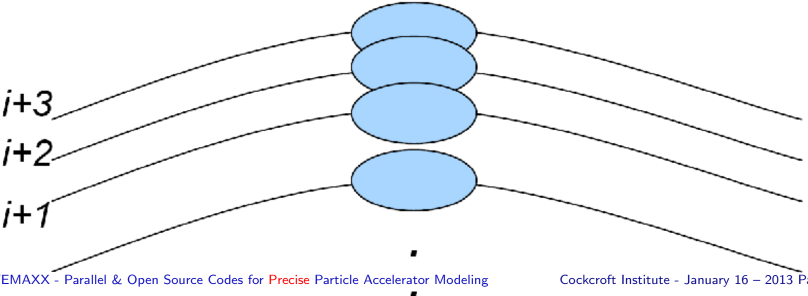
# Neighboring Bunch Effects- Multi Bunch Model

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

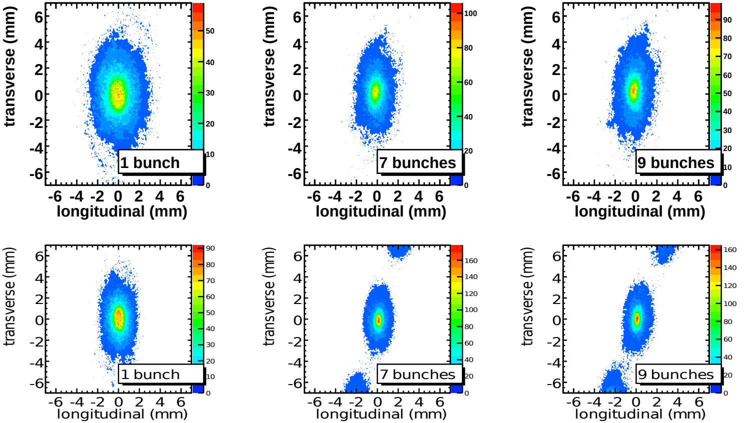
- Full 3D
- Energy bins & re-binning
- Large grids needed



# Neighboring Bunch Effects- Multi Bunch Model

Single bunch and multiple bunches at turn 80 and 130

PSI 590MeV Ring




[J. Yang, A. Adelmann, et al.]

# Dark Current & Multipacting Simulations

(Dark Current)

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# Outline

# FEMAXX overview

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

- 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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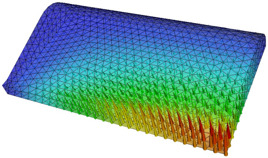

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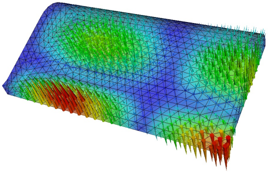


Compute electromagnetic fields in accelerator cavities, i.e. some of the lowest eigenfrequencies and corresponding eigenfields.

# Available Solvers

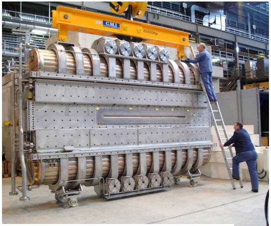
| Eigensolver | Problem Type | Application |
|---|---|---|
| JDSYM | Generalized real symmetric EVP | lossless resonant cavities [R. Geus] |
| JDQZ | Generalized non-Hermitian & quadratic EVP | dielectric & ohmically lossy material [H. Guo] |
| NLJD | Nonlinear EVP | cavities with finite conductivity [H. Guo] |

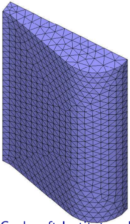
# Mathematical model of JDSYM

- We are interested in the resonant behaviour of a cavity $\Omega$, thus we work in frequency domain
- Reformulating Maxwell's equations, eliminating $\mathbf{H}$ and using a time harmonic ansatz for $\mathbf{E}(\mathbf{x}, t)$ we obtain

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

  $\mathbf{e}(\mathbf{x})$ is the amplitude of the eigenfield at location $\mathbf{x}$.
- Tetrahedral meshes, exploiting symmetries





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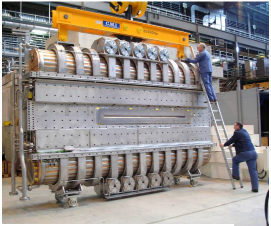


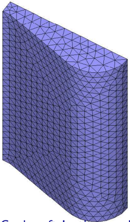

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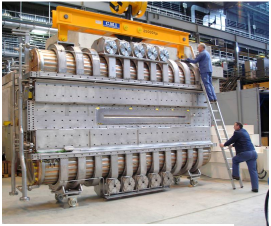
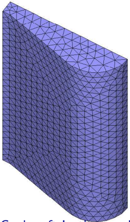


# Mathematical model of JDSYM

## FEM discretisation

We use the weak formulation proposed by Kikuchi (1987)

$$\begin{aligned}
&\underline{\text{Find } (\lambda, \mathbf{e}, p) \in \mathbb{R} \times H_0(\mathbf{curl}; \Omega) \times H_0^1(\Omega)} \\
&\underline{\text{such that } \mathbf{e} \neq \mathbf{0} \text{ and}} \\
&\text{(a)} \quad (\nabla \wedge \mathbf{e}, \nabla \wedge \mathbf{\Psi}) + (\nabla p, \mathbf{\Psi}) \\
&\qquad\qquad = \lambda(\mathbf{e}, \mathbf{\Psi}), \qquad \forall \mathbf{\Psi} \in H_0(\mathbf{curl}; \Omega) \\
&\text{(b)} \quad (\mathbf{e}, \nabla q) = 0, \qquad \forall q \in H_0^1(\Omega)
\end{aligned} \tag{2}$$

Here, $p$ is a Lagrange multiplier.

# Mathematical model of JDSYM

## FEM discretisation

We discretize the field $\mathbf{e}$ in (2) by quadratic edge elements proposed by Nédélec (1980) and the Lagrange multiplier $p$ by quadratic node elements. This yields a large sparse constrained matrix eigenvalue problem of the form

$$A\mathbf{x} = \lambda M\mathbf{x} \qquad C^T\mathbf{x} = \mathbf{0}. \tag{3}$$

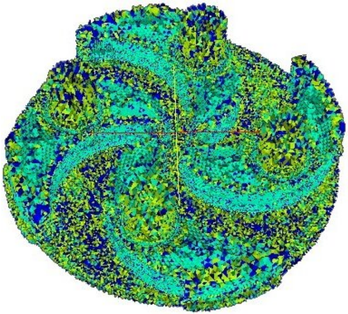
where $A$ is symmetric positive semidefinite and $M$ is symmetric positive definite. $C$ has full rank. The number of columns of $C$, i.e. the number of constraints, is about one eighth of the order of $A$ and $M$! However, with this peculiar finite element discretization we have

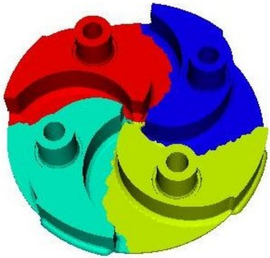
$$C^T\mathbf{x} = \mathbf{0} \iff \mathbf{x} \perp_M \mathcal{N}(A). \tag{4}$$

This means that the eigenvalues of (3) are equal to the positive eigenvalues of

$$A\mathbf{x} = \lambda M\mathbf{x}. \tag{5}$$

# Mesh partitioning using ParMETIS





## Purpose

- Load balancing: Each processor gets the same number of tetrahedra
- Minimise solver communication: Minimise the size of the interprocessor boundary
- Crucial for efficient parallel execution

## Implementation

- ParMETIS: Parallel library for graph partitioning
- Heuristic multilevel algorithm
- Parallel I/O with H5hut

# Parallel solver algorithms using Trilinos framework

## Solver algorithms

### Distributed objects

Distributed matrices and vectors provided by Epetra.

### Inner solver

Parallel implementation of the QMRS iterative linear solver.

### Eigensolver

Parallel implementation of Jacobi-Davidson method (JDSYM), R. Geus

### Preconditioners

- Incomplete factorisation (IFPACK)
- Algebraic Multigrid (ML & SuperLU)

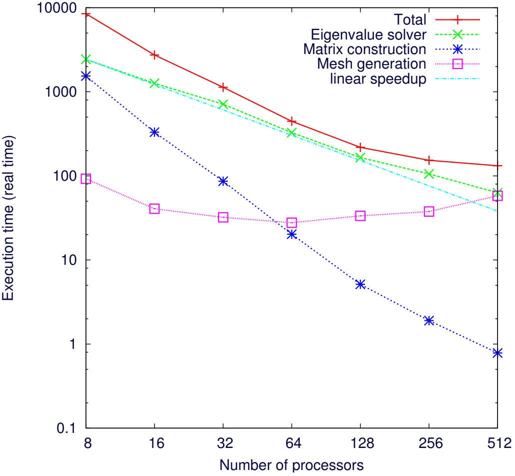
# Experimental results obtained on Cray XT3 (Horizon)

## What was computed

- 5 lowest eigenvalues with eigenvectors of the COMET cavity
- 1st order elements used
- $LDL^T$ preconditioner
- 1.4 million DOFs
- Post-processing not included

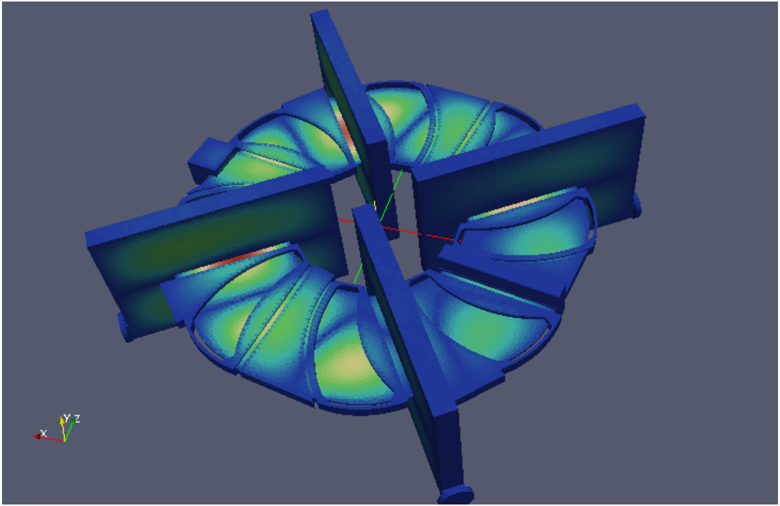
## Observations

- The code scales well to large number of cpus
- Computation takes only 4 minutes on 512 cpus
- Enables shape optimization



# Glow Discharge in the PSI ring

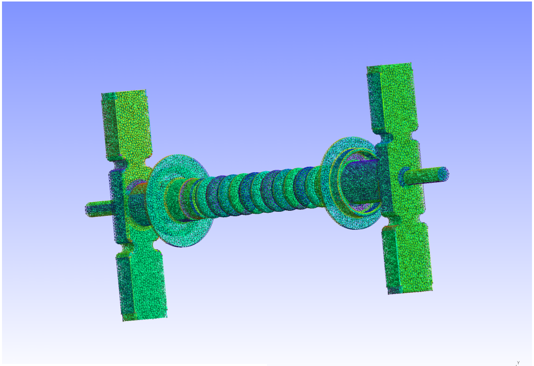
This problem needs it all ... (not solved yet)



# Outline

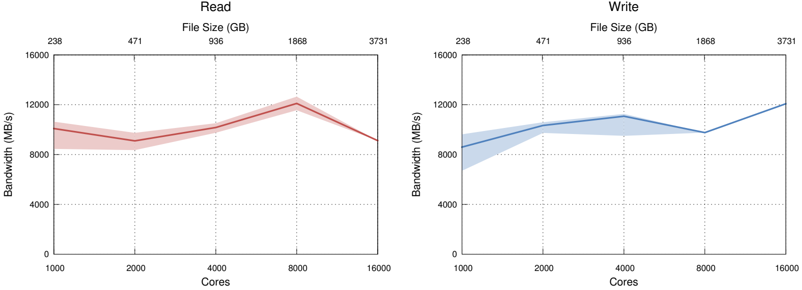
# Aim of H5hut

- H5Part, H5Block & H5Fed [M. Howison, A. Adelmann, et al.]
- Handle very large files (16k cores Franklin, 3.7TB)
- Platform independent processing of the same data
- integrated into state of the art analysis & visualization tools (Visit, ParaView & Root)



# Performance: Results

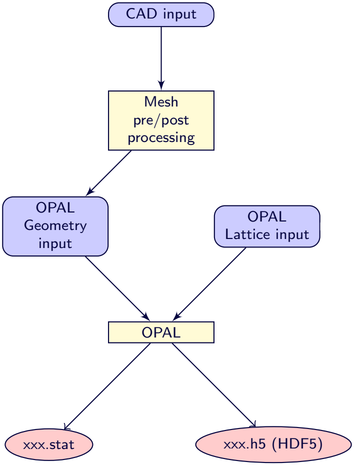
Synthetic H5Block weak scaling study

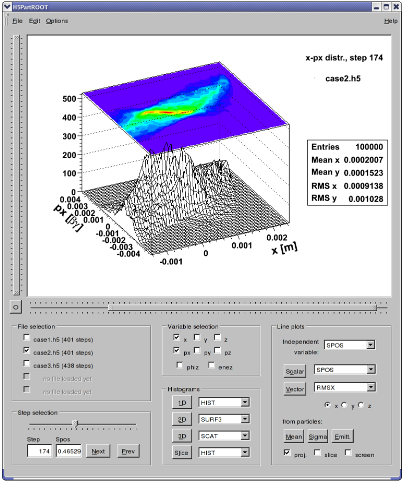



- Weak scaling to 16,000 cores on Franklin and 3.7TB of data.
- Read times include a halo exchange, to transmit a ghost region of cells among neighboring blocks.
- The solid line shows the mean bandwidth, shaded region minimum and maximum.

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

[T. Schietinger A. Adelmann, et al.]



# Outline

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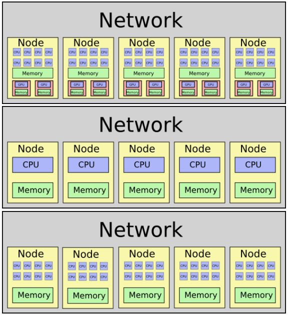
# Hardware & Software Development is not *working for us*




## Facts

- Heterogenous Many-Core Architecture (CPU/GPU)
- MPI (OpenMP) based software stack
- Watt/FLOP is very important

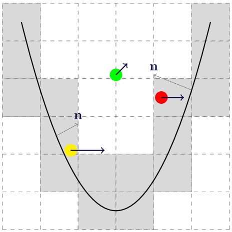
## Works well ...

if you have an isolated Kernel that needs to be optimized

# A Complex Application: OPAL

$$\mathbf{Ax} = \mathbf{b}$$

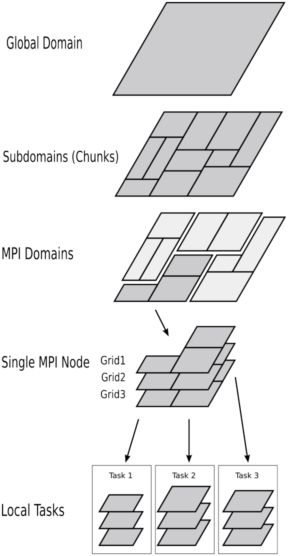
+




- PDE & Monte-Carlo
- Complicated boundary conditions
- Adaptivity

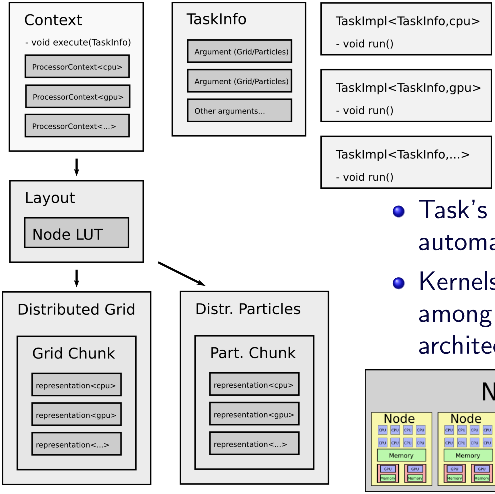
## This does not fit per se ...

- complicated data structures (not Array)
- need good load balancing → dynamic data structures

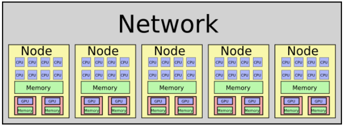


# A Parallel Hybrid Particle Mesh Framework

A prototype exists (ETH BSc Thesis *A Parallel Hybrid Particle Mesh Framework*, J. Progsch)




- Task's can be distributed automatically
- Kernels can be specialized among heterogenous architectures



# A new Architecture that avoids one level of complexity!

Lets have a look at a very simple but powerful (new) architecture - Intel Xeon/PHI (MIC):


- it is a x86-compatible co-processor (60 cores)
- multi-threaded
- can compile my existing SW-Stack out of the box

- The Xeon Phi 5110P will be capable of 1.01 teraflops of double precision floating point instructions
- 320GB/sec memory bandwidth
- 225 W (The latest Green500 list announced the National Institute for Computational Sciences "Beacon" system as the world's most energy-efficient supercomputer)

# Conclusions

- Using the High Performance Computing (HPC) technology will enable us to speedup computations while increasing the accuracy of the used models
- HPC is an enabler of new modeling capabilities: 3D space charge & secondary effects in large structures & EVP in large and complicated structures
- State-of-the-art numerical methods and adequate **software technology** are mandatory
- New Major Capabilities for OPAL in the near future are:
  - Multiobjective Optimization (Ph.D ETH/PSI/IBM to be defended in 1Q 2013) [Y. Ineichen, A. Adelmann, et al.] PRACE Award 2013
  - Adaptive Mesh Refinement (PSI-FELLOW post doc start 1. March 2013)
  - FFAG modeling capabilities (Ch. Rogers & S. Sheehy)
- Active OPAL collaborations with CIAE, LANL, Cornell, LBL, Rutherford and ETH
- OPAL & FEMAXX are open software tools, please join!

The OPAL & FEMAXX framework combines essential factors

- physics modeling
- numerical mathematics and
- high performance computing
- multidisciplinary community efforts (open source)

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

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