Large Scale Computing: Progress report

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Main tasks

- TRACK updates
  - The TRACKv37 version is in web-site now
    http://www.phy.anl.gov/atlas/TRACK/Trackv37/
  - H-minus stripping (residual gas, static & RF magnetic fields, black-body radiation) is fully incorporated as a Monte-Carlo process
  - Trajectories of secondary particles produced by an internal target inside a solenoid
  - New version TRACKv38 includes DTLs,CCLs
- P-TRACK: is being updated to version v38, is not yet available on web-site
- Parallel electromagnetic solvers: collaboration with John DeFord (STAR-ANALYST)
  - Application for STTR
- Collaboration attempt with SLAC computer simulation group was not successful

Objectives of the STTR

- The development of efficient parallel implementations of thermal and structural finite-element solvers within the Analyst DFEM solver library. These implementations will be designed for use on Terascale and Petascale parallel computers, with particular focus on the solution of very large (>100M element) problems on the 1 Petaflop BG/P at Argonne National Laboratory. The new solvers will augment the existing parallel electromagnetic capabilities in the commercial Analyst software package, leveraging comprehensive support for finite-element modeling that includes automated meshing, visual and numerical post-processing, design optimization, and Python-based scripting. By combining massively parallel support for electromagnetics, thermal, and structural analysis into a single package, virtual prototyping of accelerator components will be possible at an unprecedented level of detail and accuracy.

Recent work on BD simulations and code development

- End-to-end simulations of the new AEBL driver linac
  - Paper at PAC-2007
- Design of the 17 MeV/u, q/A=1/3 Light Ion Injector for AEBL (upgrade)
- GANIL (France): physics design and end-to-end simulations new heavy-ion injector for SPIRAL-2
- ANL/FNAL collaboration:
  - implementation of H-minus stripping process into the TRACK code, stripping simulations (SNS, FNAL-HINS)
  - Lattice for the 8-GeV linac, “Project X”

Papers

- J. Xu, P. Ostroumov and J. Nolen,

  "*A Parallel 3D Poisson Solver for Space Charge Simulation in Cylindrical Coordinates*" accepted for publication in **Computer Physics Communications**

I. Status of the PTRACK code

- Upgrade according to the changes in serial code (Brahim, Vladislav)
- Developing manual, publish on the website, copyright

II. Multiphysics simulation for cavity optimization

- Geometry optimization using MWS (Peter)
- Multiphysics simulation by MWS+ProE+ANSYS (Geoff, Joel)
- Frequency shift and tuning (Peter)
- Multipacting simulation by ANALYST (Ivan)

III. Parallel version of ANALYST

- Port the parallel version of ANALYST on BG/L (Ben)
- Apply it for cavity eigenvalue simulations (AEBL cavities) (Peter, Ivan)
- Improving the scaling of parallel direct solver---dfem (John)

IV. Design and optimization of the coupler

- Magnetic- and electric- coupling (Peter)
- Thermal analysis (on going)

Cavity optimizations

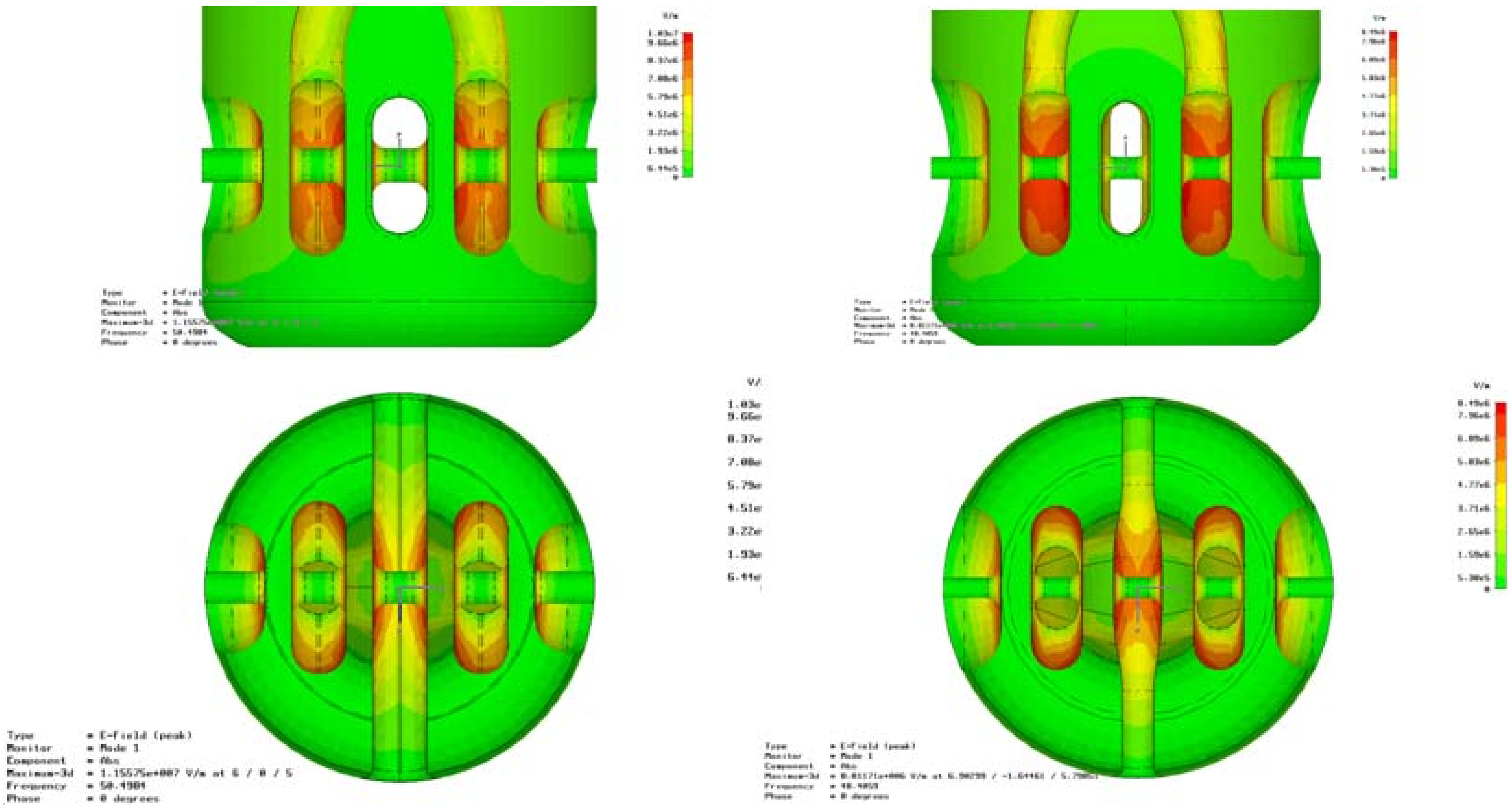


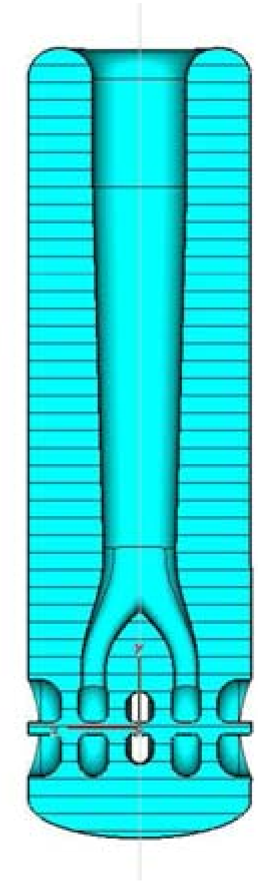
Figure. Surface electric field distribution in (x, z) and (y, z) planes.
The preliminary design (on the left) and optimized design (on the right).

Cavity optimizations

Table. Main electrodynamics parameters of 4G-QWRS given for E_{ACC} =1 MV/m.

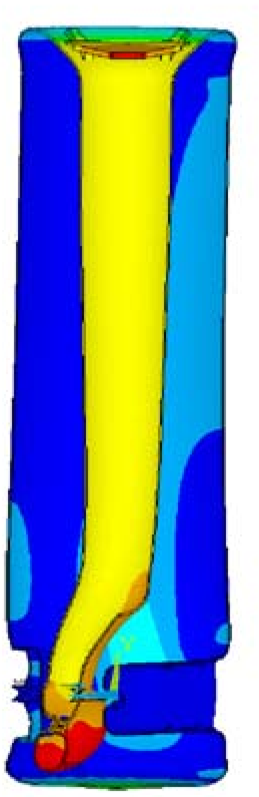
Parameter	Units	ATLAS	Type-I	Type-II	Type-III	Type-IV
Mesh-points		385K	626K	2M	2M	2M
E_{PEAK}	MV/m	5.04	3.76	3.41	3.48	3.61
B_{PEAK}	Gauss	117	42	43	55	48
Length, L_c	cm	24.638	17	26	26	26.4
W	mJ	221	72	150	118	149
G	Ω	13.8	11.5	18.1	25.1	20.9
R/Q_0	Ω	900	1309	1486	1254	1298
β_G		0.025	0.017	0.026	0.038	0.031
Height	cm	110.5	139.5	131.3	80.8	107.3
Diameter	cm	30.48	23.54	37.0	37.0	37.0

Multiphysics simulations



MWS

ProE



ANSYS

- ✓ Two meshes:
  - > RF mesh in the cavity
  - > Structural mesh in Nb shell
- ✓ First RF analysis on un-deformed geometry
- ✓ Then structural analysis
- ✓ Update RF mesh to deformed geometry
- ✓ At last RF analysis on deformed geometry

Structural analysis using ANSYS

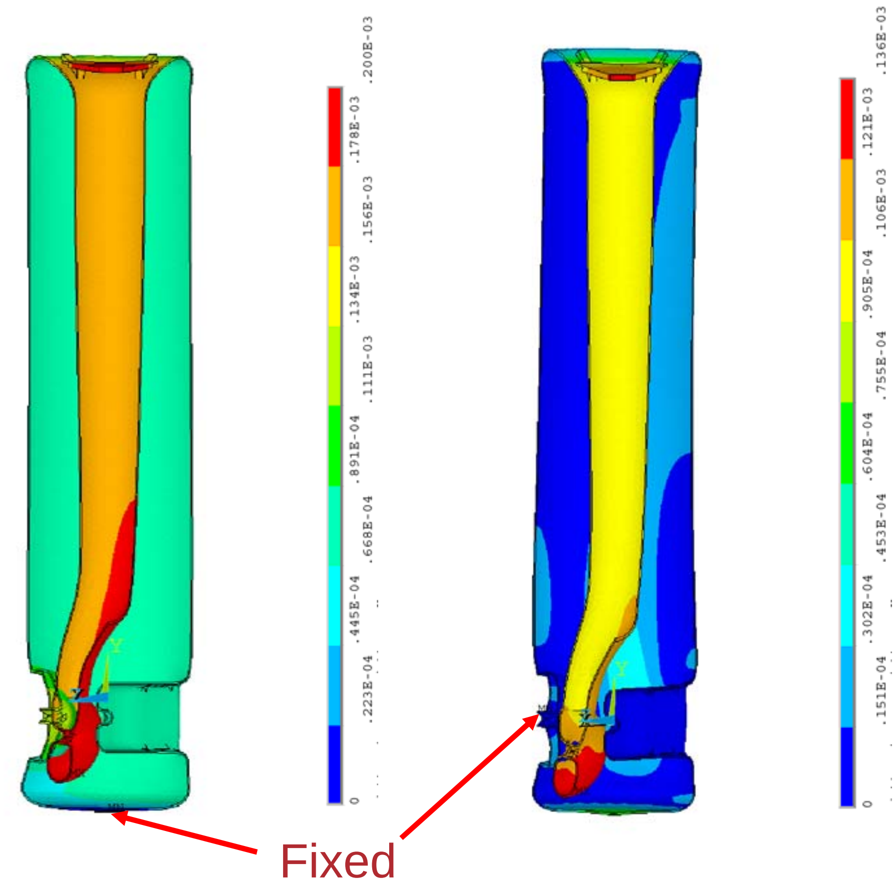


Figure. ANSYS results of deformed geometries for the case 1 (on the left) and case 2 (on the right).

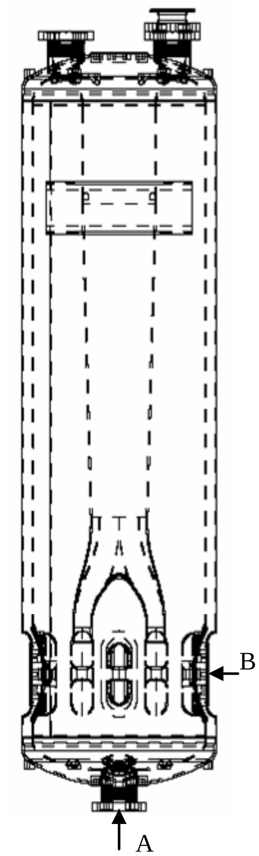


Figure. Cross section of the type-II cavity in the SS jacket.

Frequency shift and tuning

Table. ANSYS simulation results for frequency detuning due to 10^5 Pa helium pressure.

Mode number	1 (operational)	2	3
Initial frequency (MHz)	48.297	159.113	289.212
Frequency shift, case 1 (kHz)	-13	-3	25
Frequency shift, case 2 (kHz)	-5	1	22

Table. ANSYS simulation results for frequency tuning with mechanical tuner (case 1).

Mode number	1 (operational)	2	3
Initial frequency (MHz)	48.297	159.113	289.212
Frequency shift, pressure is applied (kHz)	1	5	20
Frequency shift, no pressure (kHz)	15	8	-6

Pulling force of 1120 N has been applied symmetrically at beam pipe at point B

Multipacting simulation

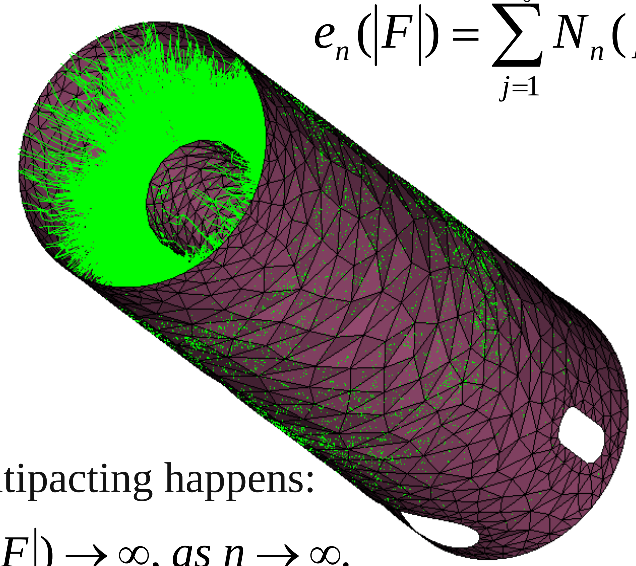
Total number of electrons after the k^{th} impact is the yield function: $\delta(x_k^j, \varphi_k^j)$

Total number of electrons due to a single electron launched after n impacts:

$$N_n(p_0) = \prod_{k=1}^{n} \delta(x_k, E_k)$$

Enhance Counter Function:

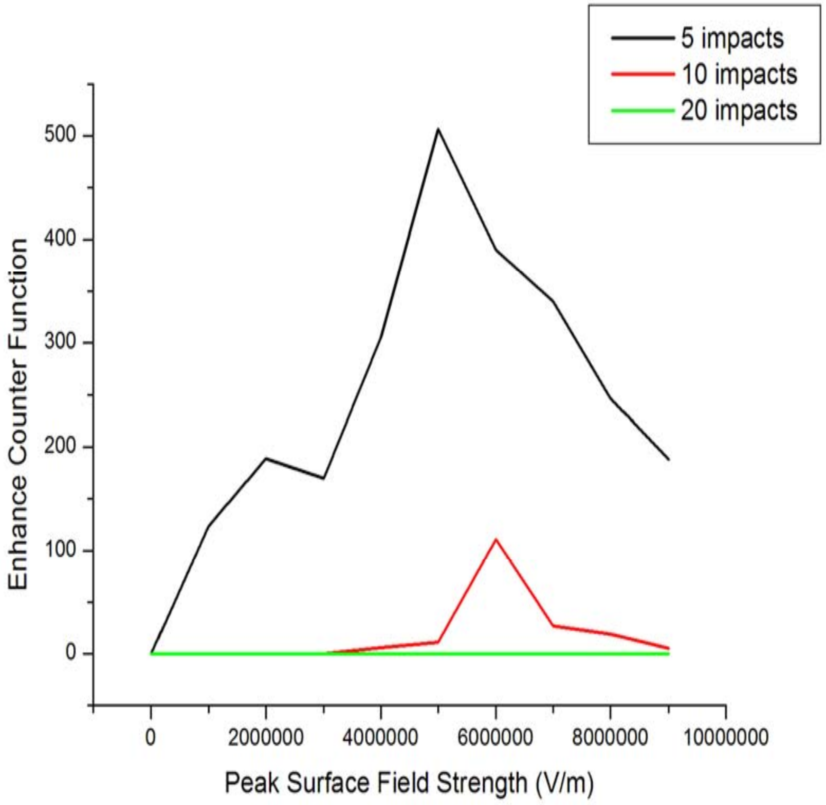
$$e_n(|F|) = \sum_{j=1}^{N_0} N_n(p_0^j)$$



Multipacting happens:

$e_n(|F|) \to \infty, as\ n \to \infty.$

$$p_0^j = (x_0^j, \varphi_0^j) \in \Omega \times [0, 2\pi], \quad j = 1, 2, \cdots, N_0.$$



Collaboration with FNAL

Scaling problem of ANALYST on BG/L

- Direct solver can not be run on BG/L, as it requires large mount of memory.
- Only iterative solver can be run on BG/L.
- The scaling of current iterative solver is not so good on small number of processors (<=32), and becomes very bad on thousands of processors (>=1024).
- For iterative solver, better preconditioners should be implemented.

Figure. Scaling of iterative solver

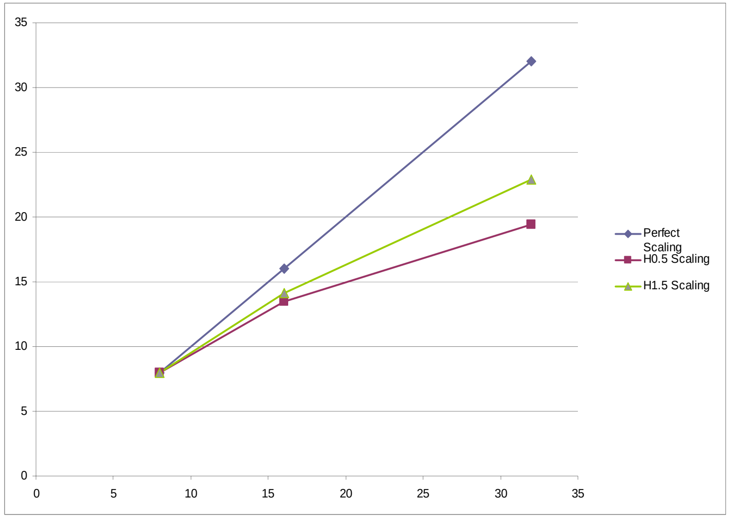


Table. Timing of parallel ANALYST on BG/L

Processor	Base	Elements	Nodes	Time (s)
32	h0.5	2032120	385270	16041
64	h1.0	2032120	385270	24673
32	c1.0	2032120	385270	27366
1024	h1.0	9656519	1743509	86400

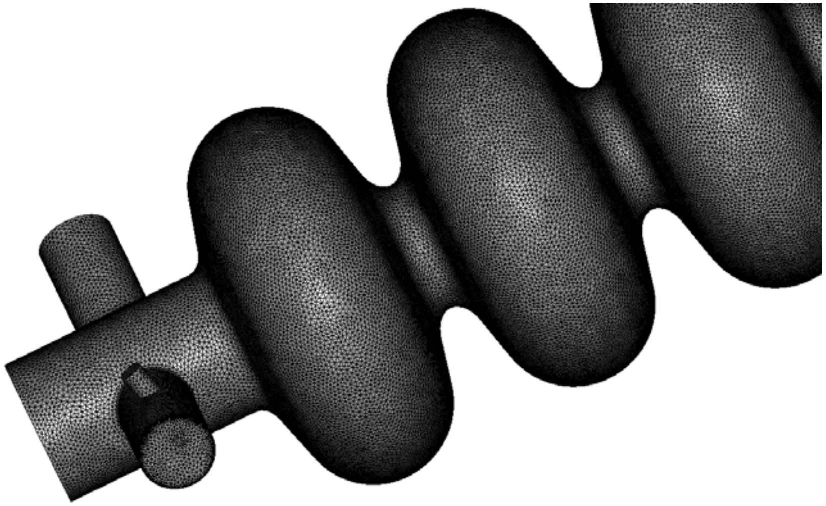
Problems of ANALYST on BG/L

- Because of small memory available on BG/L nodes, porting and scaling of ANALYST requires more efforts.
- Large scale computing brings challenges not only on scaling, but also on meshing, I/O, visualization and also post-processing.
- Right now ANALYST performs serial I/O, which is slow and not robust. This requires much more memory on root processor.
- Multifrontal method for direct LU solver in ANALYST:

1. Preprocessing
2. Matrix Reorder to reduce fill
3. Subdivision of large Frontal Matrix (Poor scaling)
4. Symbolic Factorization (Serial)
5. Numerical Factorization (Poor scaling)
6. Backward solving (Poor scaling)
7. Postprocessing (Serial)

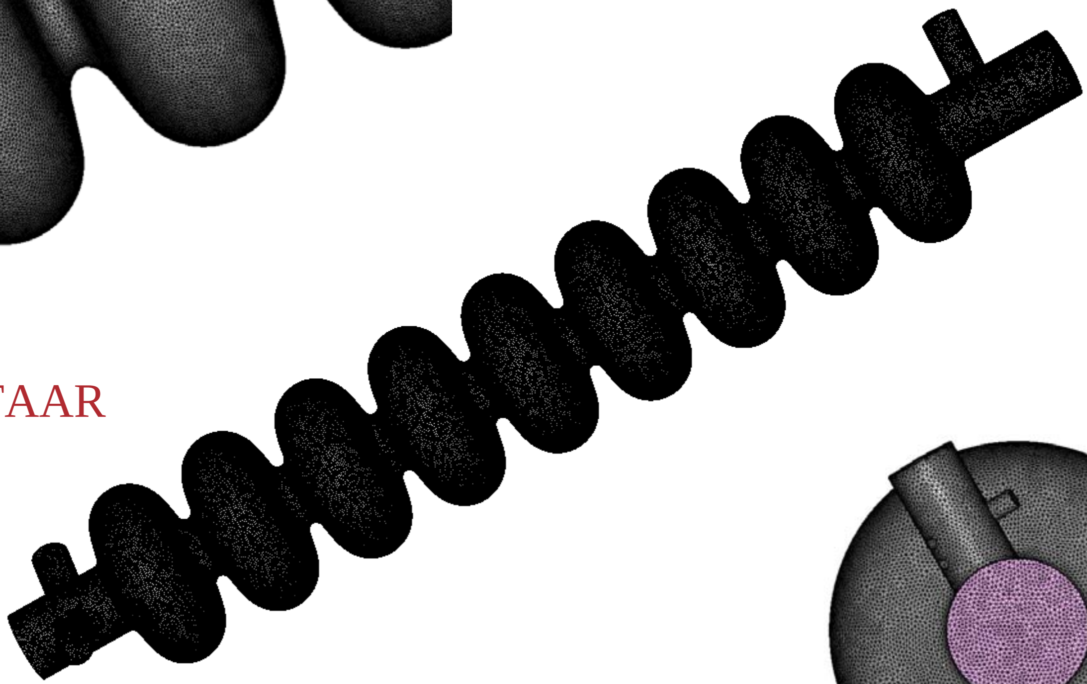
Collaboration with STAAR

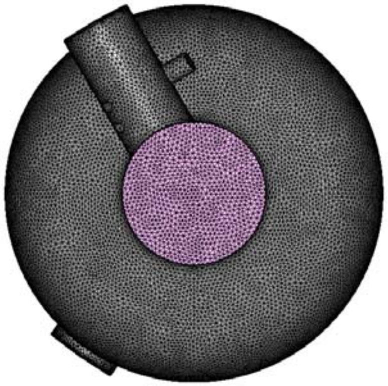
Simulation of the ILC cavity on BG/L with 1024 processors



Goal: Extract 3D fields on fine mesh in the presence of coupler

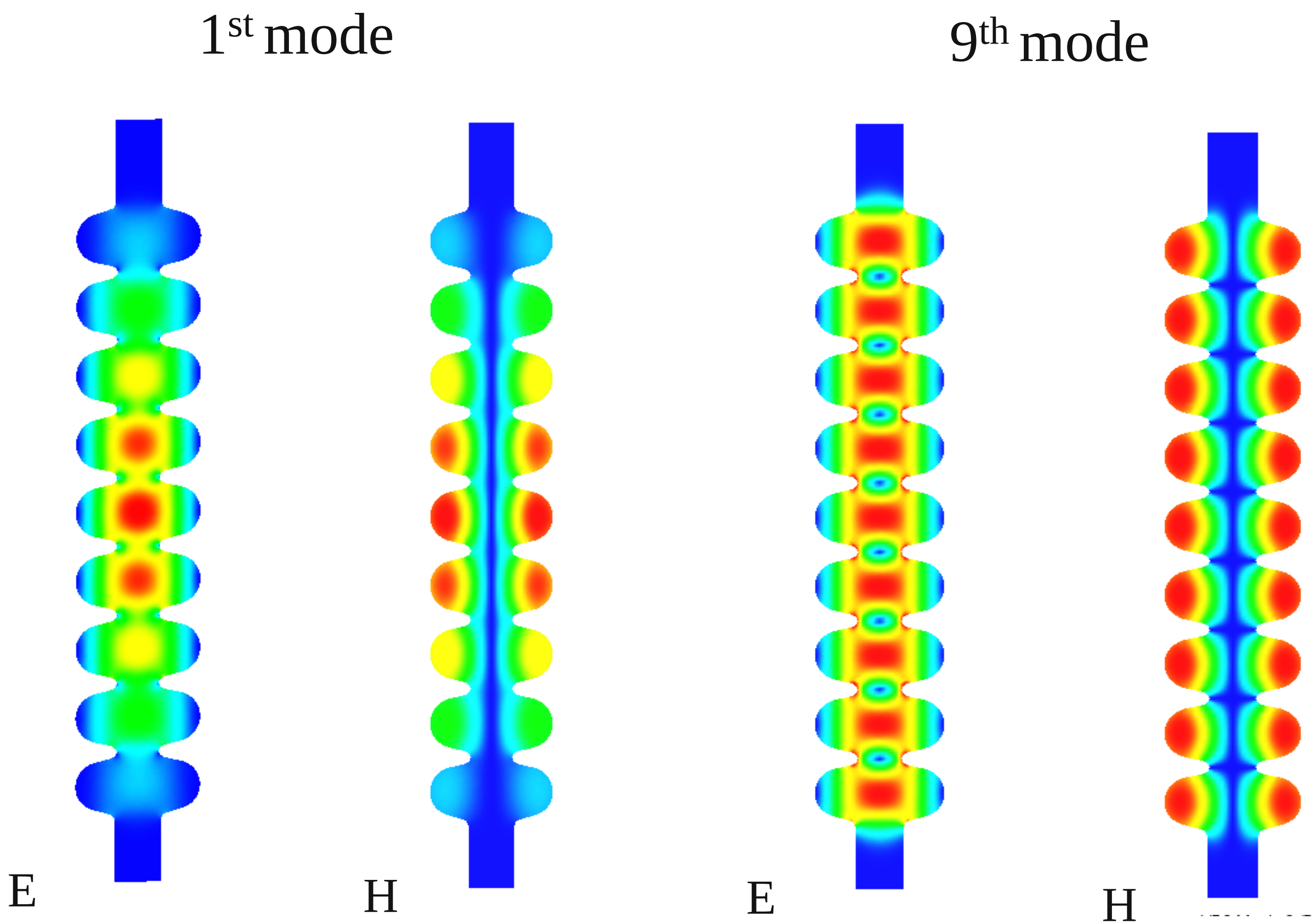
Collaboration with STAAR





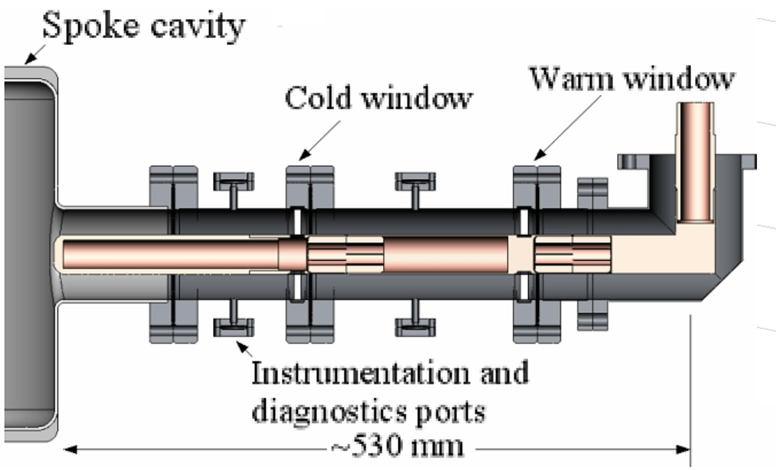
Global mesh has 1743509 nodes and 9656519 elements.

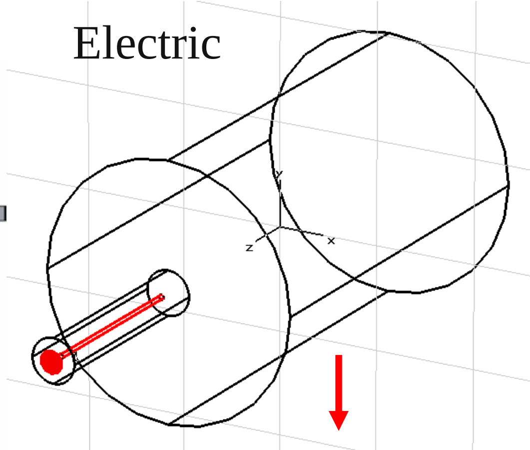
ILC 9-cell cavity E- and H-fields

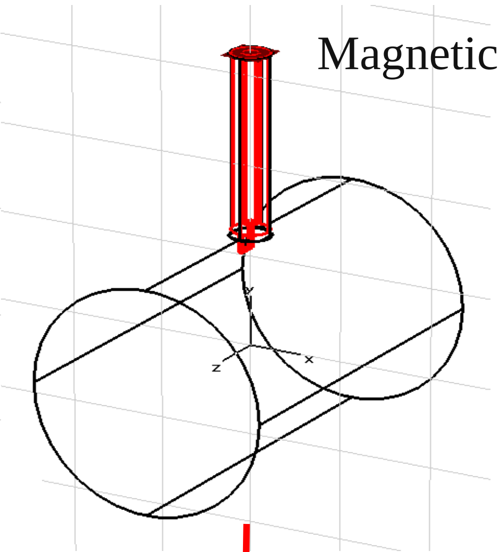


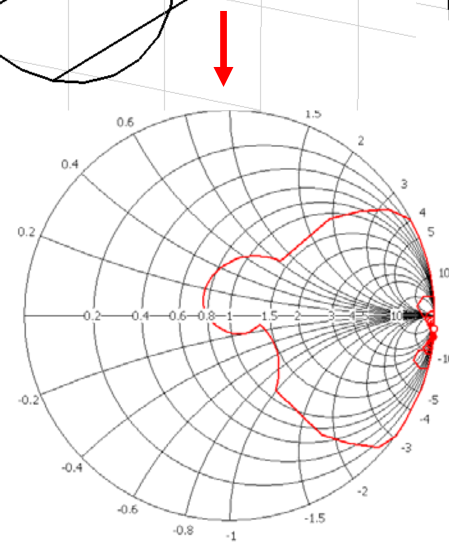
Base c1.0, 2032120 Elements and 385270 Nodes

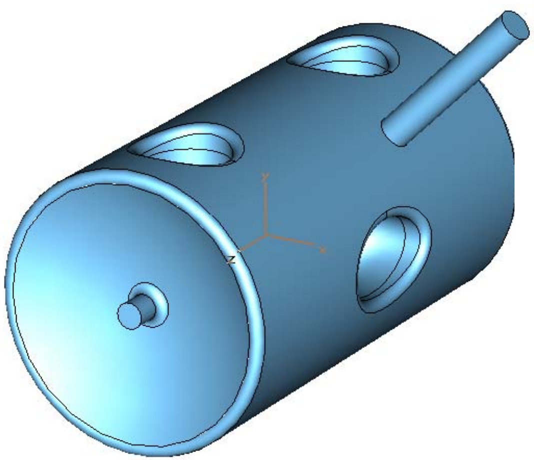
Design and optimization of coupler

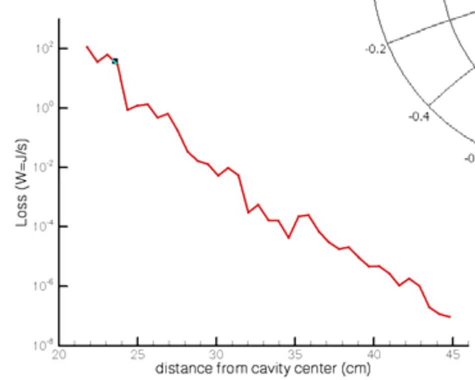












S-Parameter
Smith Chart