Advanced Computational Electromagnetics 3D Parallel (ACE3P)

ACE3P Webinar

November 19, 2025

Presented by:

Mohamed Othman – Introduction to ACE3P

Lixin Ge – Workflow on NERSC Perlmutter

David Bizzozero – Parametric and Optimization workflow using *lume-ace3p*

SLAC NATIONAL ACCELERATOR LABORATORY

Stanford University | U.S. DEPARTMENT OF ENERGY

Welcome to the ACE3P Webinar!

Housekeeping & Recording:

- This webinar is being recorded.
- The recording and all presentation materials will be published online after the webinar.

How to Ask Questions:

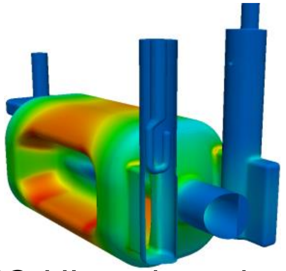
- **During the webinar:** Please use the Q&A linked in the Zoom chat.
- **For community discussion:** Join our Slack Channel: #ace3p-user
- **For technical support:** Email us at ace3p-developer@slac.stanford.edu

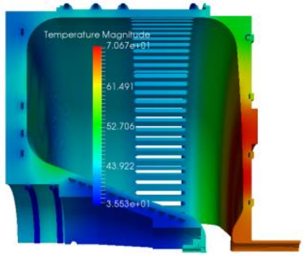
ACE3P for Scalable Multiphysics Modeling

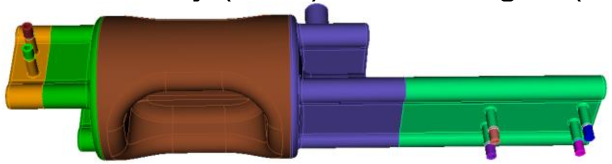
- **ACE3P**, developed at SLAC, is a comprehensive suite of *conformal, high-order, C++/MPI based parallel finite-element (FE) multiphysics codes* including electromagnetic (EM), thermal and mechanical capabilities.
  - Based on *curved high-order finite elements* for high-fidelity modeling
  - Implemented on *massively parallel computers* for increased memory (problem size) and speed
  - Software infrastructure facilitates linking to third-party numerical libraries (with GPU capabilities)

ACE3P (Advanced Computational Electromagnetics 3P)

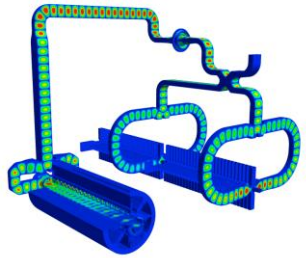
Frequency Domain:	**Omega3P**	**– Eigensolver (damping)**
	S3P	**– S-Parameter**
Time Domain:	**T3P**	**– Wakefields and Transients**
Particle Tracking:	**Track3P**	**– Multipacting and Dark Current**
EM Particle-in-cell:	**Pic3P**	**– RF guns & space charge effects**
Multi-physics:	**TEM3P**	**– EM, Thermal & Mechanical analysis**
Static Particle-in-cell:	**Gun3P**	**– DC guns & space charge effects**

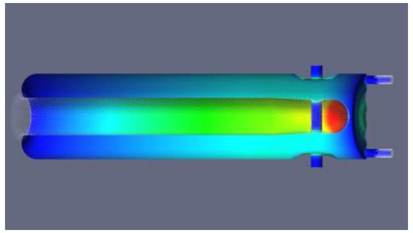

LHC-HL crab cavity (HEP)

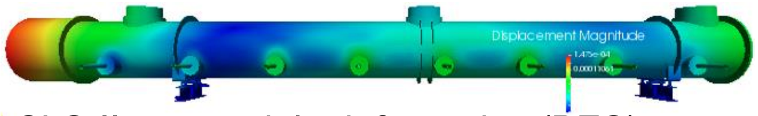

LCLS-II gun (BES)


EIC crab cavity (NP)


SPEAR3 kicker wakefield using moving window (BES)


CLIC wakefield (HEP)


FRIB multipacting (NP)


LCLS-II cryomodule deformation (BES)

ACE3P Modules and Capabilities

Omega3P *(Frequency domain)*

- Eigenmodes in lossless, lossy, periodic or externally loaded cavities
- Mode damping in dielectric and ferrite materials
- Linear, quadratic and nonlinear eigensolvers
- Absorbing and PML boundary condition

T3P *(Time domain)*

- Transient and wakefield from source excitation
- Moving window technique for broadband pulse and short beam propagation
- Absorbing and PML boundary conditions for far fields
- Impedance boundary condition for thin coating and lossy conductor walls
- Complex materials: nonlinear and dispersive
- User-specified pulse excitation

S3P *(Frequency domain)*

- S-parameters of rf components and open structures
- Dielectric, dispersive and ferrite materials
- Effects due to surface impedance on conductor walls
- Absorbing and PML boundary condition
- Boundary condition for thin coating layer

Pic3P *(Time domain)*

- Self consistent particle-in-cell (PIC) modeling of beam-cavity interactions in space-charge dominated devices
- User-specified particle emission model

Gun3P *(Static)*

- DC gun modeling at steady state
- Space-charge limited emission
- Electrostatic solver
- Magnetostatic solver
- Particle tracking in external and self static fields

Track3P *(Particle tracking)*

- Particle tracking code in external rf and static fields
- Multipacting and dark current in rf cavities and components
- Surface physics for field and secondary emissions
- Enhancement counter for multipacting

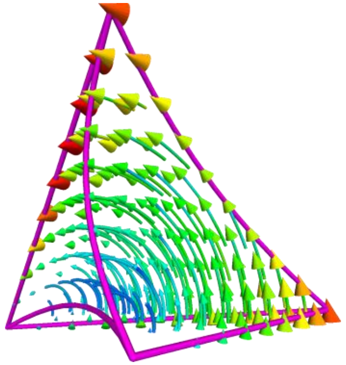
TEM3P *(Multiphysics)*

- Integrated EM, thermal and mechanical effects
- Non-linear thermal and electrical conductivities
- Convective boundary conditions
- Shell elements for surface coating
- Mechanical eigensolver and harmonic solver
- Transient analysis

Computational Electromagnetics in ACE3P

In ACE3P, the electric field $\mathbf{E}$ is expanded into vector basis functions, which are discretized using curved tetrahedral high-order Nedelec-type finite elements

Maxwell Equations



- Omega3P - *In frequency domain*

$$\nabla \times \left(\frac{1}{\mu}\nabla \times \vec{\mathbf{E}}\right) - k^2\epsilon\vec{\mathbf{E}} = 0 \ on \ \Omega$$

- T3P - *In time domain*

$$\nabla \times \left(\frac{1}{\mu}\nabla \times \vec{\mathbf{E}}\right) + \sigma\frac{\partial\vec{\mathbf{E}}}{\partial t} + \epsilon\frac{\partial^2\vec{\mathbf{E}}}{\partial t^2} = -\frac{\partial\vec{\mathbf{J}}}{\partial t}$$

- Track3P uses E and B from Omega3P or S3P for particle tracking

$$\frac{d\vec{p}}{dt} = e\left[\vec{E} + \frac{1}{c}\left(\vec{v} \times \vec{B}\right)\right] \qquad \vec{p} = m\gamma\vec{v} \qquad \gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

Mathematical formulation in finite element

- Omega3P - Eigenvalue problem for eigenvalue k^2 and eigenvector x

$$\mathbf{E} = \sum_i x_i \mathbf{N}_i$$
$$\mathbf{K}\mathbf{x} = k^2\mathbf{M}\mathbf{x}$$

where

$$\mathbf{K}_{ij} = \int_\Omega (\nabla \times \mathbf{N}_i) \cdot \frac{1}{\mu}(\nabla \times \mathbf{N}_j)\, d\Omega$$
$$\mathbf{M}_{ij} = \int_\Omega \mathbf{N}_i \cdot \epsilon\mathbf{N}_j\, d\Omega$$

- T3P - Newmark-β scheme for time stepping to solve

$$\vec{\mathbf{E}}(\vec{\mathbf{r}}) = \sum_i \frac{\partial}{\partial t} x_i \vec{\mathbf{N}}_i(\vec{\mathbf{r}})$$

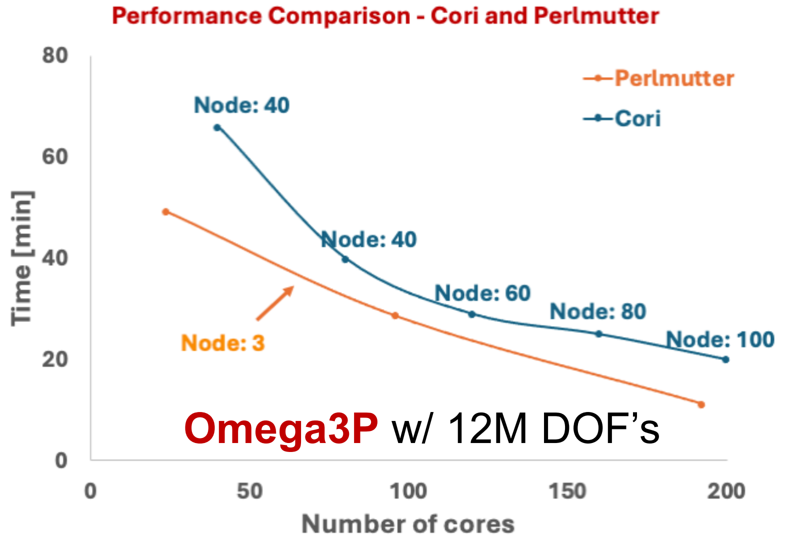
$$\mathbf{M}\frac{1}{c^2}\frac{\partial^2\mathbf{x}}{\partial t^2} + (\mathbf{R} + \mathbf{Q})\frac{1}{c}\frac{\partial\mathbf{x}}{\partial t} + \mathbf{K}\mathbf{x} = \mathbf{f}$$

- Track3P - Use Boris scheme or Runge-Kutta method for time integration.

High Performance Computing (HPC) at Ever Increasing Speed and Scale

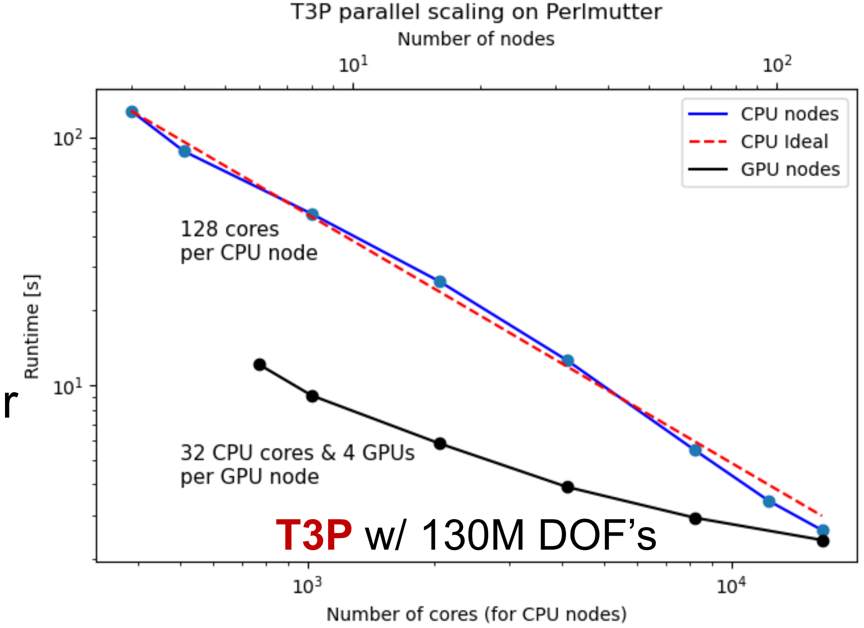
Perlmutter: Cray EX

- 3072 CPU-only nodes with a total of 196,608 cores
- 1536 GPU accelerated nodes
- 2.2 petabytes of memory



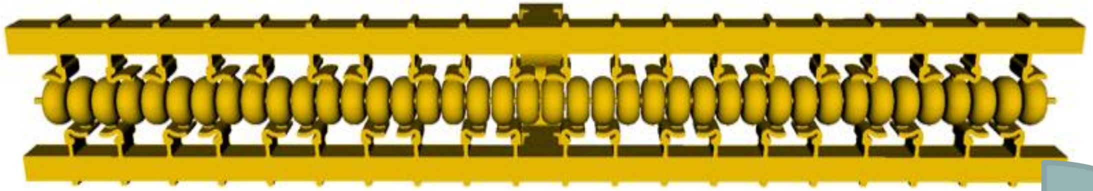
Numerical libraries used in ACE3P

- Libraries in linear algebra, linear solver, eigensolver, partitioning and data format
  - BLAS, LAPACK, ScaLAPACK
  - MUMPS, SuperLU, PETSc
  - ARPACK
  - ParMetis, Zoltan
  - Netcdf, HDF5
- Interfaced to PETSc GPU backend for linear/nonlinear solver
- OpenMP adopted for CPU threads and GPU offload

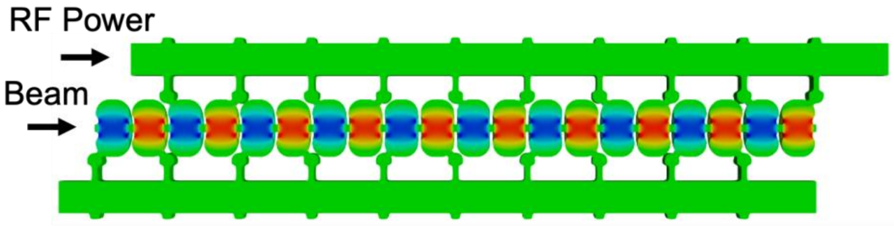


High Fidelity Simulation Enables Virtual Prototyping of Accelerator Structures

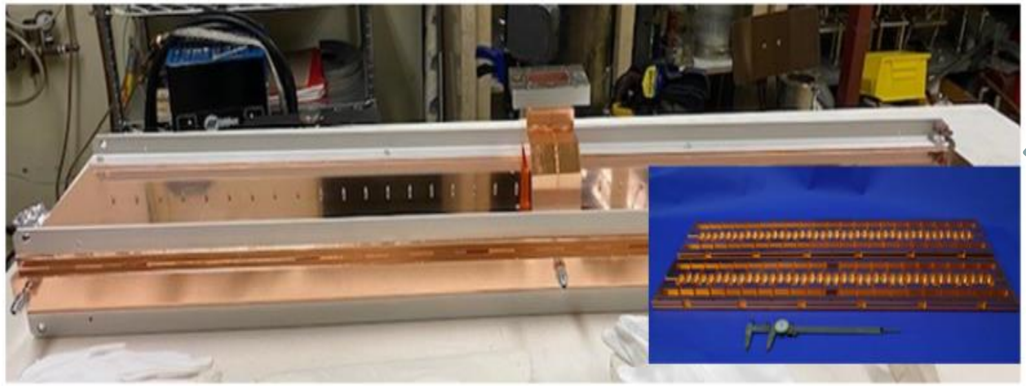
Full C3 rf accelerator system simulation to save labor-intensive modifications



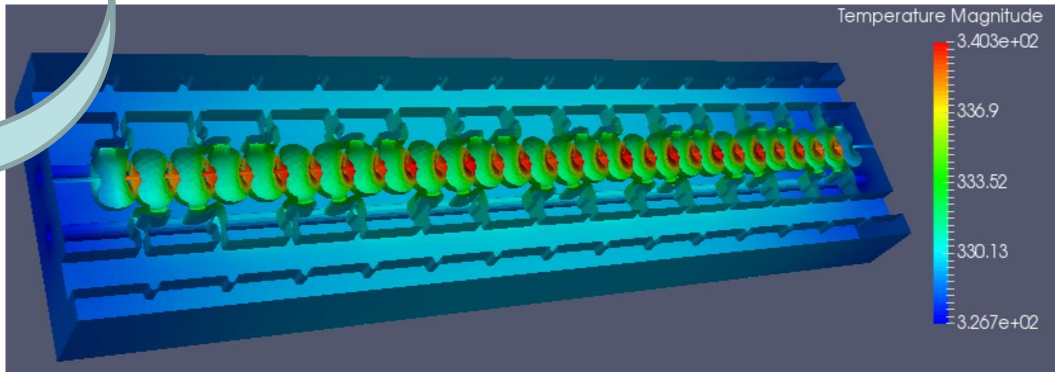
One meter (40-cell) C-band accelerator design



E field from Omega3P



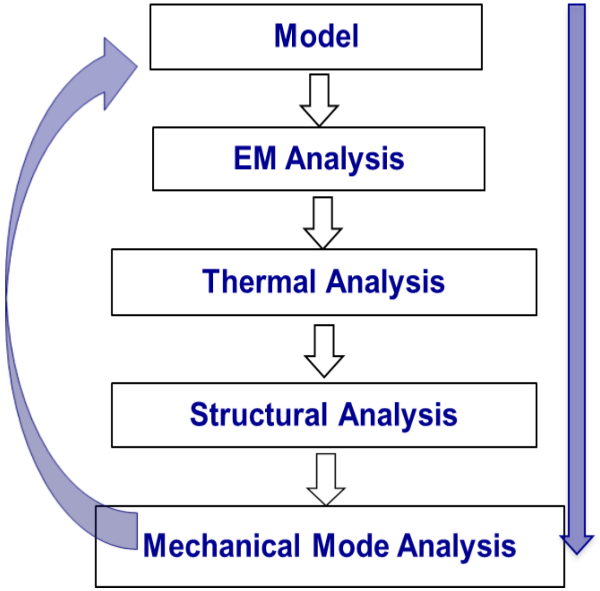
Prototype structure

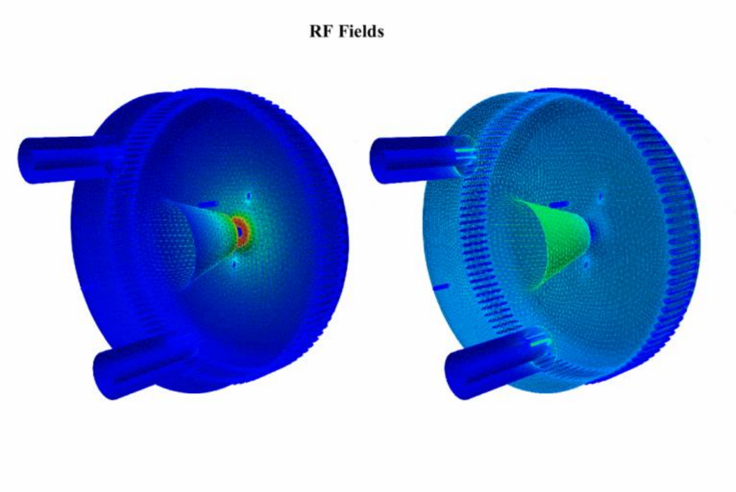


Temperature field from TEM3P

Omega3P simulation: 2.8 M mesh elements, 19 M DOFs, ~1-2 nodes, one mode/min on NERSC Perlmutter

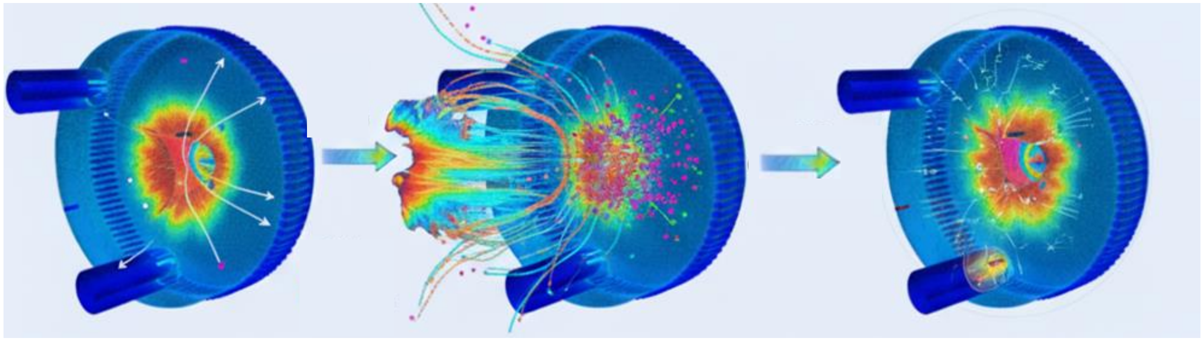
Multiphysics Modeling – Components to Systems



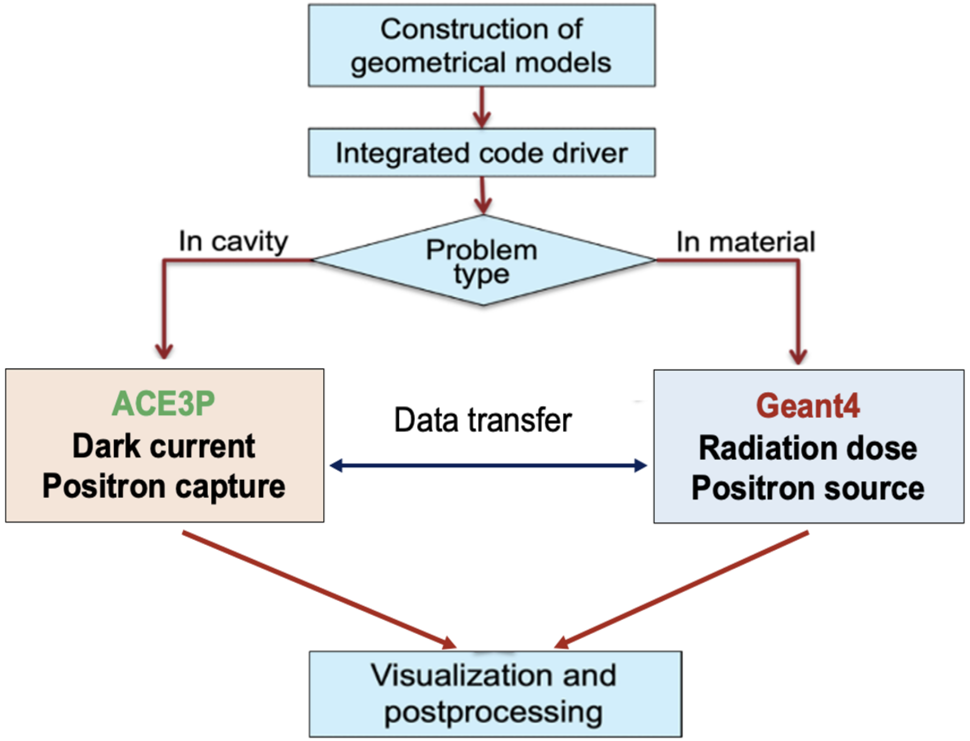


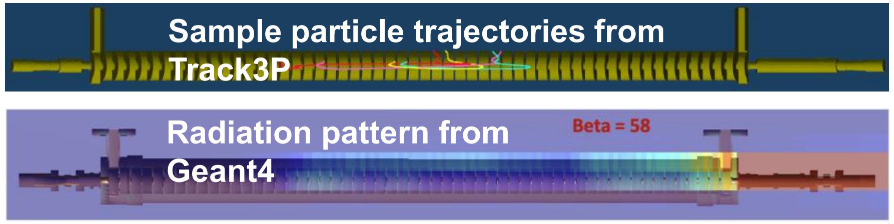
Integration of multiphysics (ACE3P) and beam dynamics (IMPACT)

Eigenmode and S-parameters *Beam Dynamics* *Thermal analysis*



ACE3P multiphysics analysis





Integration of EM (ACE3P) and radiation transport (Geant4)

Part I: ACE3P Simulation Workflow

Cubit

Geometry and Mesh Generation

⇩ **Mesh**

ACE3P Modules

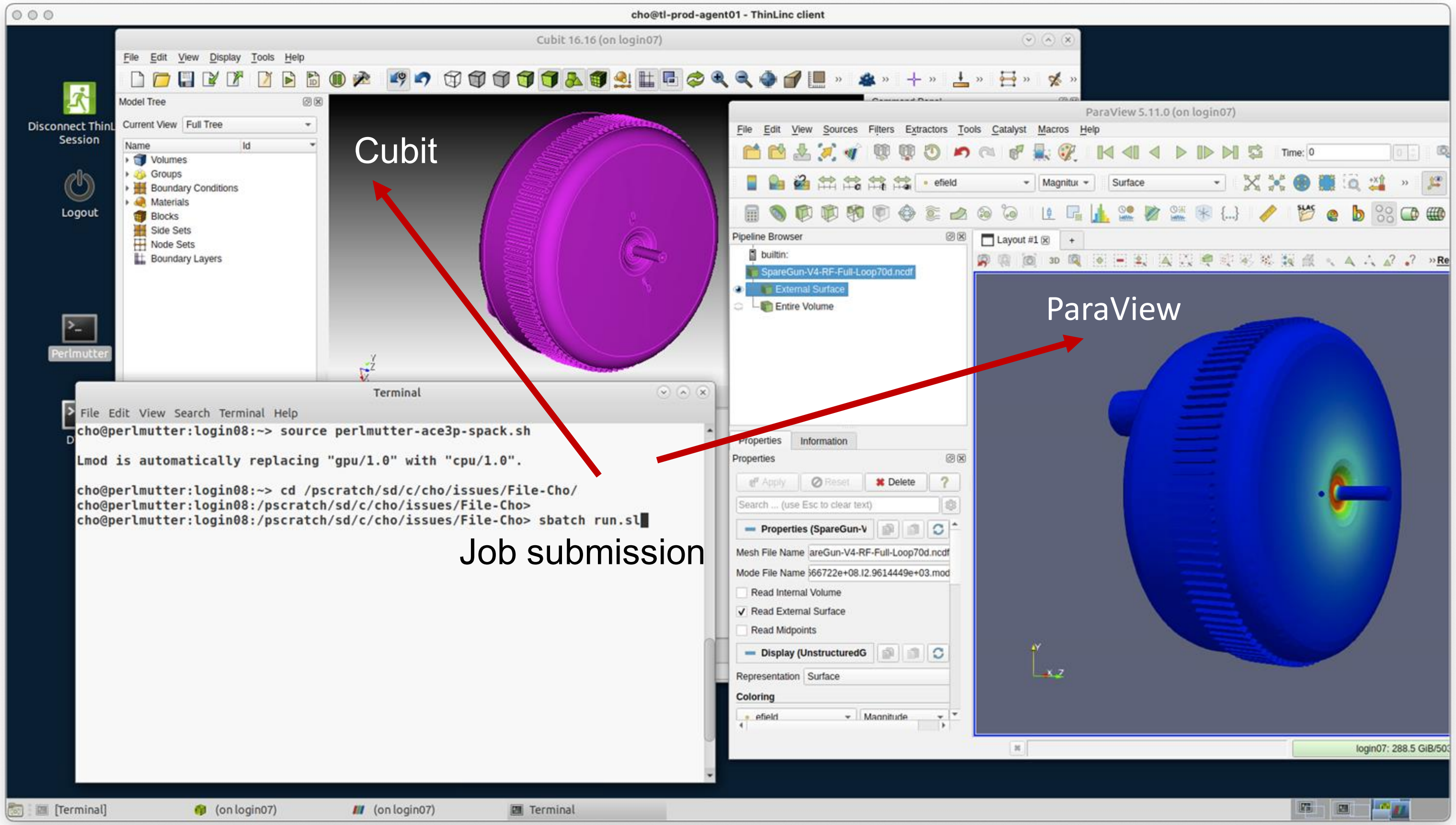
Omega3P Eigensolvers	**TEM3P** Multi-physics (thermal & mechanical)
S3P S-parameters	**Track3P** Particle Tracking
T3P/Pic3P Wakefields/PIC	**Gun3P** Static PIC

⇩ **Results**

ParaView

Data Visualization and Postprocessing

ThinLinc remote desktop at NERSC - Simulation workflow entirely on Perlmutter without the need for data transfer



See Lixin Ge's presentation

Part II: ACE3P Parametric Design and Optimization

ACE3P
Simulation

- CUBIT journal file
- ACE3P input file
- Postprocess input File (optional)
- Runtime settings (MPI cores, etc.)

LUME
Environment

- Python script interface
- General workflow settings

Simulation inputs

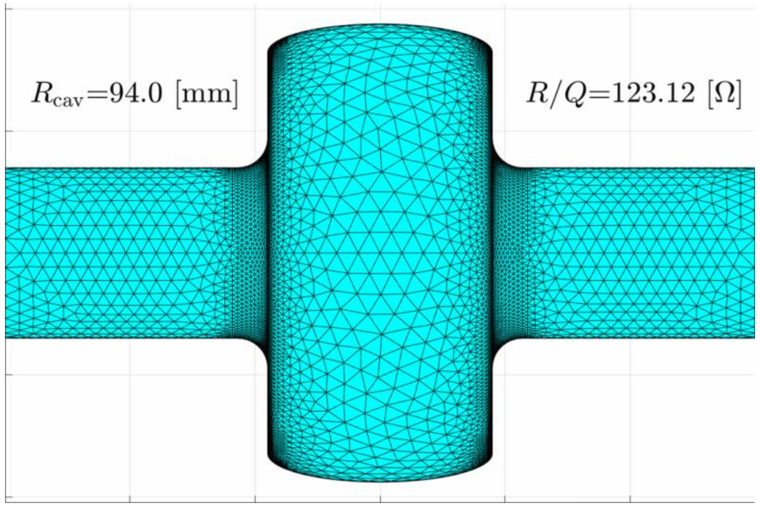
Dictionary-based communication

Simulation outputs

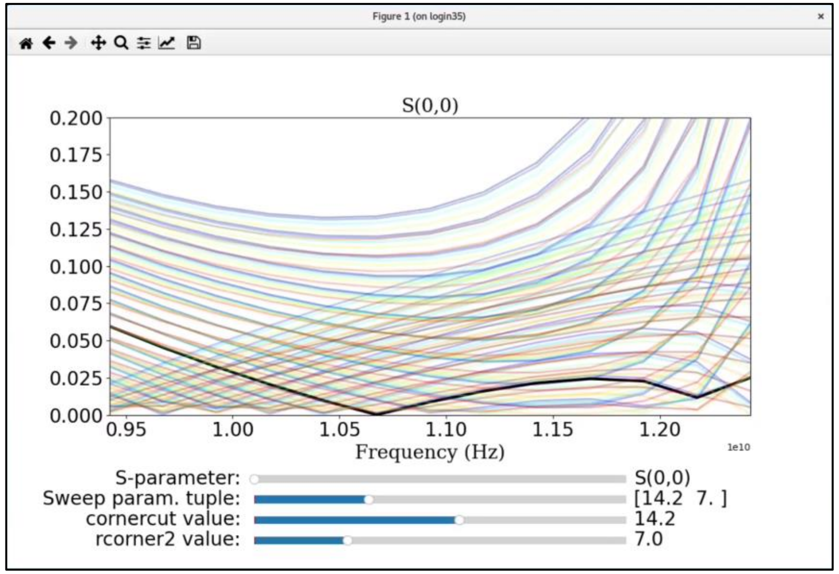
Xopt
Optimization

- Parameters
- Objectives
- Constraints
- Optimization settings
- Function callbacks for ACE3P/CUBIT

See David Bizzozero's presentation



Omega3P shape optimization



S3P S-parameter optimization

List of Resources for ACE3P

- Examples and command syntax are found in here
  https://confluence.slac.stanford.edu/spaces/AdvComp/pages/240264211/Materials+for+CW23

- On NERSC Perlmutter
  - Load ace3p simulation environment
    `source $CFS/ace3p/perlmutter/CPU/perlmutter-ace3p-spack.sh`
  - Load parametric and optimization environment (LUME)
    `conda activate $CFS/ace3p/software/lume-ace3p`
  - ACE3P examples location
    `$CFS/ace3p/lume-ace3p/examples`
    `$CFS/ace3p/cw23/examples`

- For community discussion: Join our Slack Channel: #ace3p-user
- For technical support: Email us at ace3p-developer@slac.stanford.edu