Advances in Accelerator Modeling with Parallel Multi-Physics Code Suite ACE3P

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OUTLINE

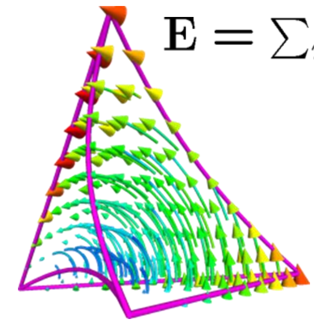
- **Parallel Multi-Physics Code Suite ACE3P**
- **Nonlinear RF Eigensolver in Omega3P**
- **Moving window for pulse propagation in T3P**
- **Mechanical Eigensolver in TEM3P**
- **Hybrid MPI+OpenMP Programing in Track3P**
- **Summary**

Parallel Multi-Physics Code Suite ACE3P

ACE3P is a comprehensive set of parallel multi-physics codes

- Based on *high-order curved finite elements* for high-fidelity modeling
- Implemented on *massively parallel computers* for increased problem size and speed

$\mathbf{E} = \sum_i x_i \mathbf{N}_i$



Curved finite element

NERSC Cori: Cray XC40

- 632,672 compute cores
- 1 PB of memory
- peak performance of 29.5 Pflops/sec

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**

Toward Virtual Prototyping for RF Accelerator Design and Optimization!

RF Eigensolver Omega3P Capabilities

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

$F(\lambda)x = 0$

λ (= k^2) the eigenvalue,
x the eigenvector
k the wave number

- Lossless Cavity
- Cavity w/ Lossy Materials

$Kx = k^2Mx$

Real/Complex eigenvalue problem

- Cavity w/ SIBC
- Cavity w/ WG ports (one cutoff)

$Kx + ikWx = k^2Mx$

$Kx + i\sqrt{k^2 - k_c{}^2}Wx = k^2Mx$

Quadratic eigenvalue problem

- Cavity w/ WG ports (multi-modes)

Nonlinear eigenvalue problem*

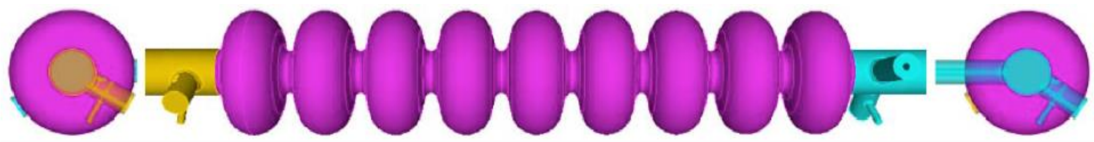
$$Kx + i\sqrt{k^2 - \left(k^c\right)^2}W^{TEM}x + i\sum_m \sqrt{k^2 - \left(k_m^c\right)^2}W_m^{TE}x + i\sum_m \frac{k^2}{\sqrt{k^2 - \left(k_m^c\right)^2}}W_m^{TM}x = k^2Mx$$

** Roel Van Beeumen, “Parallel algorithms for solving nonlinear eigenvalue problems in accelerator cavity simulations”, invited talk on Oct. 23*

8-Cavity TESLA TTF Cryomodule (CM)

- The HOMs above the beampipe cutoff need to be investigated in a CM;
- The last pair of 3rd dipole band may provide unwanted transverse kick to the beam because of their higher transverse R/Q.

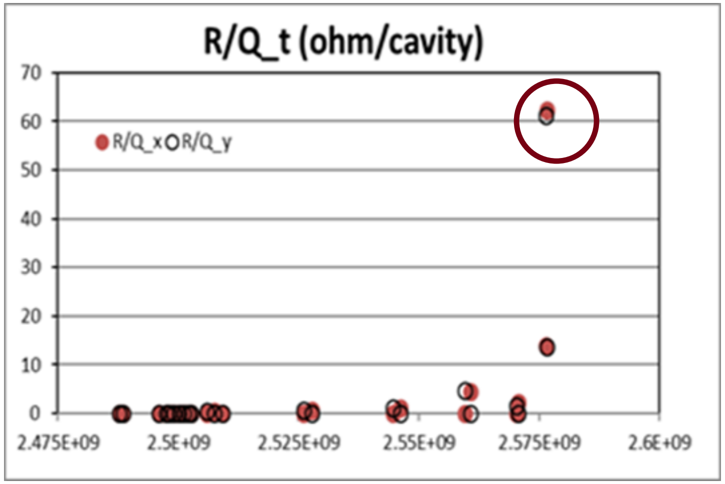
TESLA Cavity



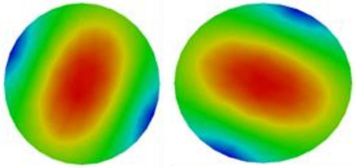
R_beampipe=39mm,
Fc(dipole)=2.2GHz,
Fc(mono)=2.9GHz

$$F(\lambda) = K - \lambda M + i\lambda W^{TEM} + i\sqrt{\lambda - k_1^2}\, W_{11}{}^{TE} + i\sqrt{\lambda - k_2^2}\, W_{11}{}^{TE}$$

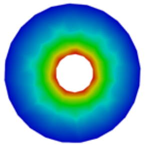
8-Cavity CM for XFEL/LCLS-II



3rd dipole band



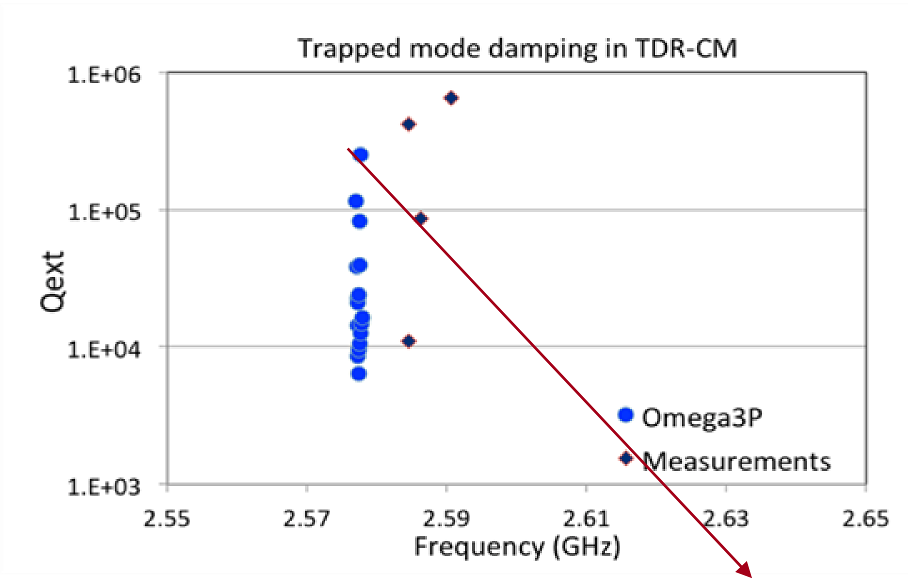
2 Beampipe ports:
TE11 Fc1=Fc2=2.2525GHz



16 HOM coupler ports: ABC

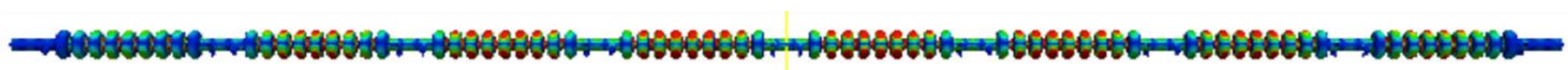
The Trapped Mode Damping in TTF CM

- Determining the trapped mode damping needs to solve a nonlinear eigenvalue problem;
- The trapped mode damping factors calculated using Omega3P agree well with the measurements at DESY;



Omega3P simulation parameters –

- ~3M curved mesh elements,
- ~ 20M DOFs,
- 960 cores on NERSC Edison,
- 1min per mode

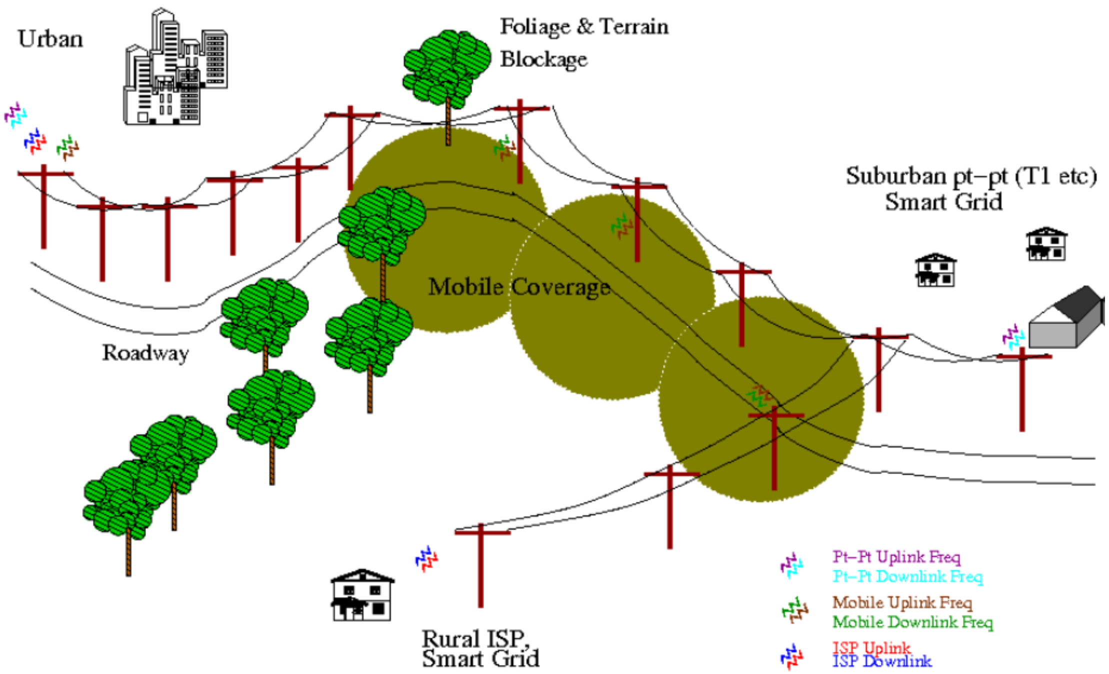


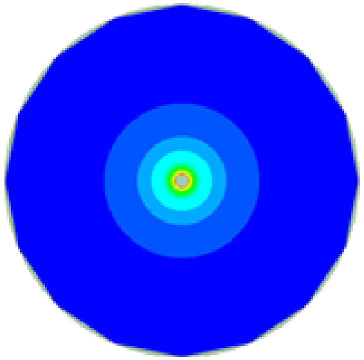
The trapped mode's E-field in TTF CM from Omega3P

The simulated frequencies are shifted to lower values due to cavity imperfection;

Time-Domain Solver T3P

- T3P is used to simulate low-loss surface TM0 wave propagating on a overhead power line for the last-mile information transmission solution for 5G network;
- New moving window for pulse power propagation and surface impedance boundary condition (SIBC) model for thin dielectric coating have been implemented;



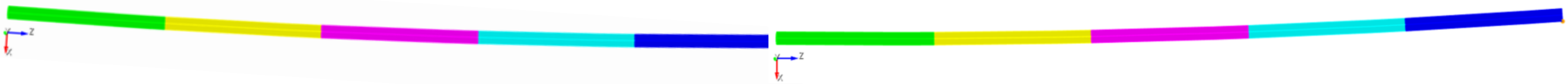


Sommerfeld TM0 mode

Real-world industrial applications through HPC!

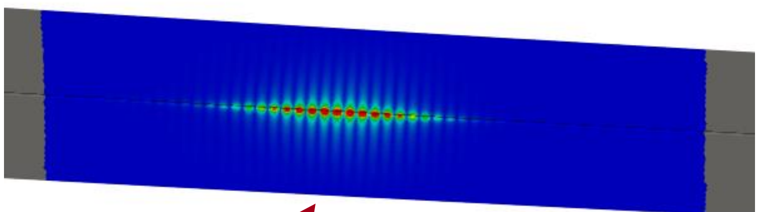
Courtesy of Glenn Elmore

Surface Wave Propagation on an Overhead Power Line

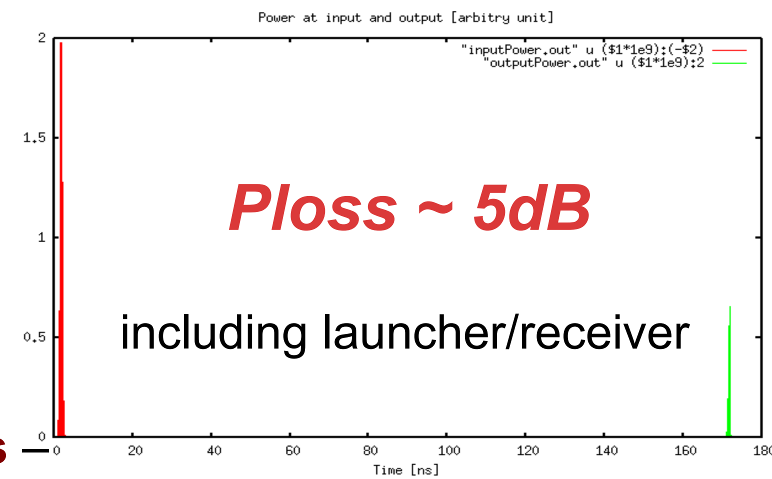


50m wire mesh generated through mesh merging tool

SIBC for lossy dielectical coating model on metal for rain fall on the wire



Moving window for pulse propagation



T3P simulation parameters

- ~ 50M mesh elements, 2nd order basis function
- 3200 cores on NERSC Edison,15 hours for 50m long distance

Snapshots of TM0 propagation on 50m wet wire sag from T3P

Multi-Physics TEM3P Capabilities

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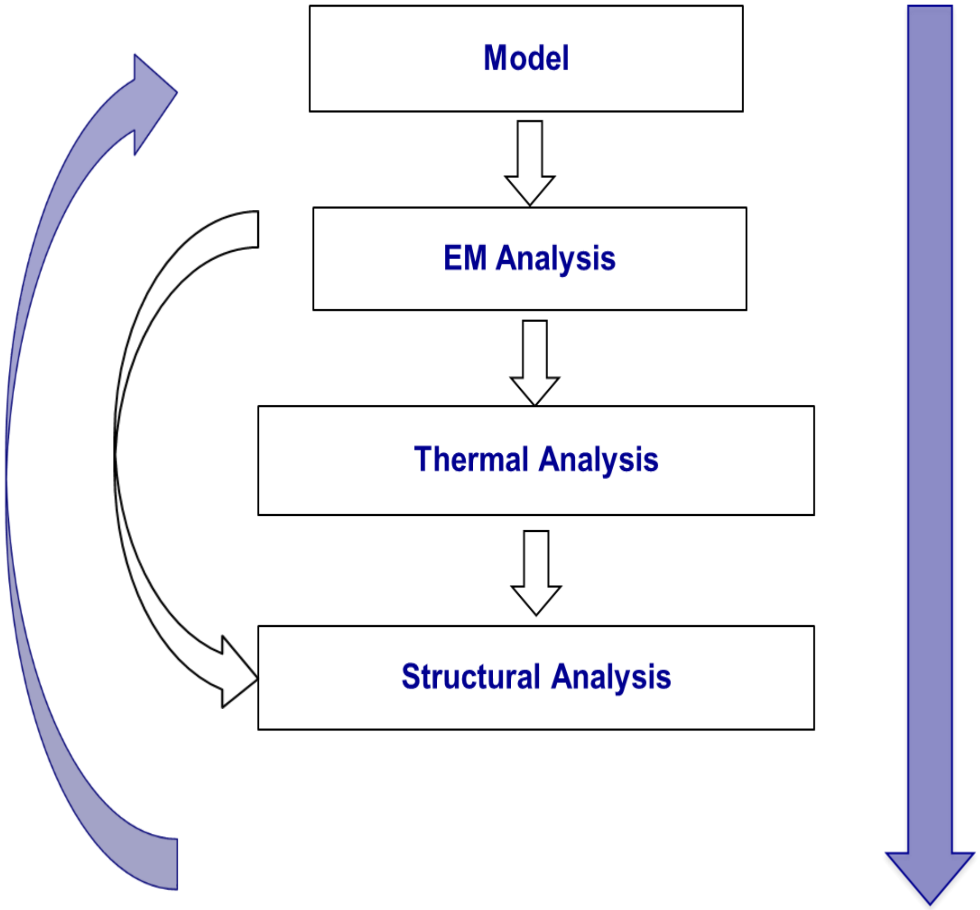
TEM3P: integrated electromagnetic, thermal and mechanical effects

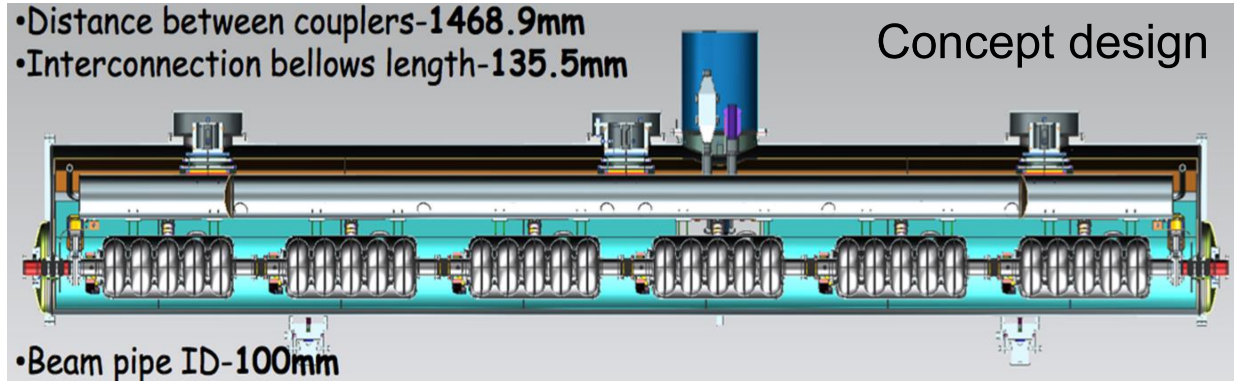
- Thermal analysis including
  - Conduction & convection BCs
  - Non-linear thermal conductivity
  - Non-linear convection BCs
  - Shell elements for surface coating

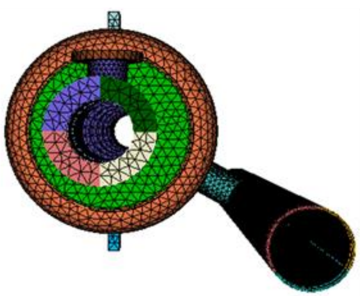
- Mechanical analysis including
  - Lorentz force detuning
  - Static structural analysis
  - **Mechanical eigenmodes**

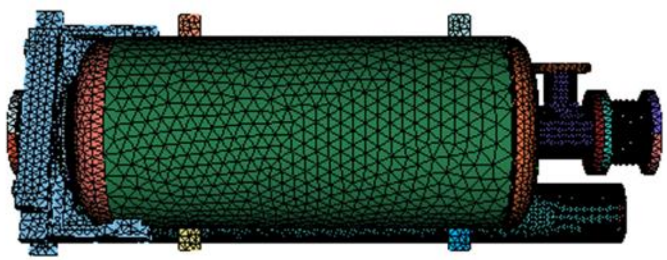


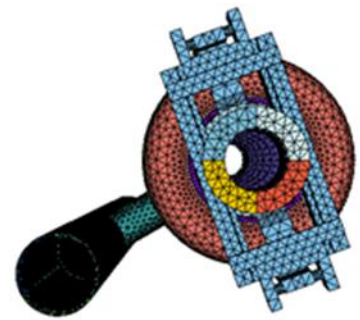
PIP-II ß=0.92 650MHz CM

Collaborate with FNAL
T. Nicol and V. Yakovlev

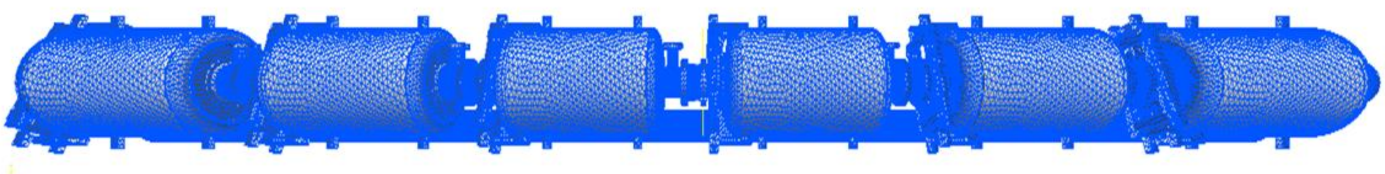








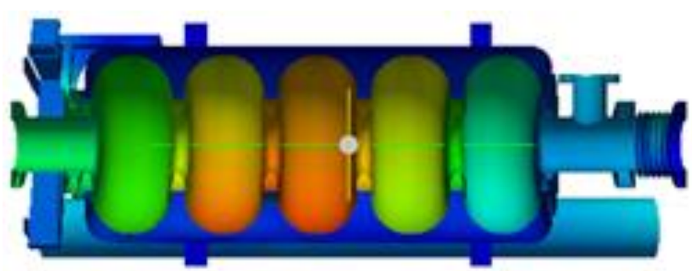
Single cavity meshes



CM meshes through mesh merging tool

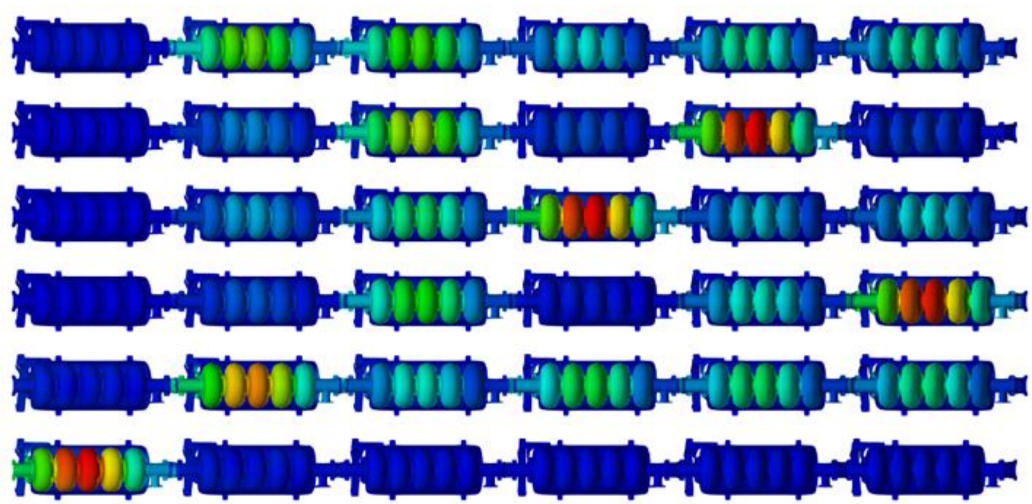
Mechanical Mode Simulations

- The mode frequencies in a CM differ from those in a single cavity;
- If one cavity is vibrated by external force, the other cavities might be detuned due to the mechanical mode excitation.
- The longitudinal modes have transverse displacement components due to HGR pipes and tuner which destroy the geometry symmetry;



F=111.28Hz

longitudinal mode in a single cavity



Longitudinal modes in CM from TEM3P

TEM3P simulation parameters –
- ~ 4.3M mesh elements, ~26M DOFs
- 320 cores on NERSC Cori, ~ 1min per mode

Particle Tracking Code Track3P

Track3P provides accurate and efficient multipacting and dark current simulation:

- *High-resolution EM fields:* Load RF fields calculated from other ACE3P modules
- *High-fidelity geometry representation:* Allow realistic modeling of particle emission on curved cavity wall
- *Large scale simulation:* Allow solving large scale problems through HPC
- *Versatile postprocessing:* Provide convenient ways to analysis MP & DC activities.

Launch Electrons

- **Kinetic energy, angle**
- **Location, phase, field level, …**

Track particles in electromagnetic fields

- **Determine impact positions**
- **Generate secondary electrons**
- **Continue tracking for a specified No. of RF cycles**
- **Field emission**

Postprocess

- **Determine "resonant" trajectories**
- **Construct MP susceptible zone**
- **Faraday Cup**

Hybrid Programing Model for Track3P

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MPI based "embarrassing parallelized"

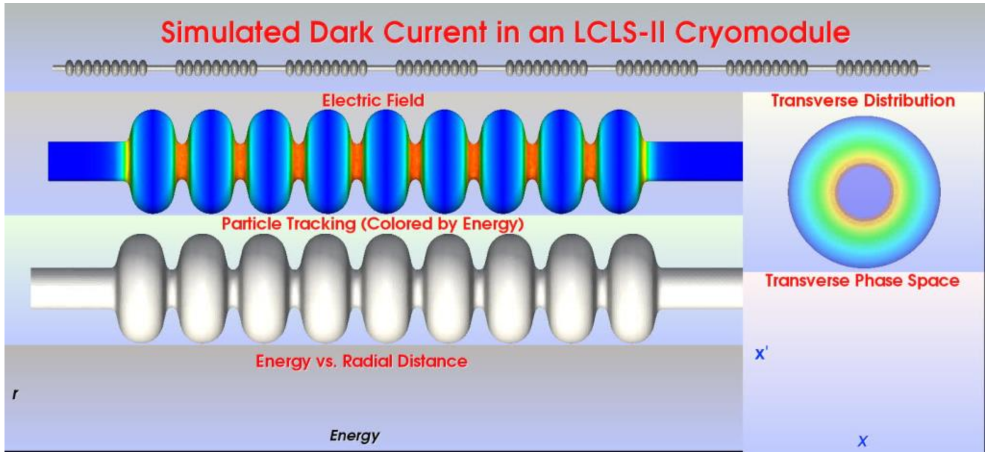
- *Whole mesh & fields are on each processor,*
- *Particles uniformly distributed on each processor*
- *No communication between processors*
- *For large problem, more memory on each processor is required.*
- *Some processors might be idle*

Hybrid model – MPI+OpenMP for Particle Tracking

- MPI across nodes and OpenMP within nodes
- OpenMP for particle tracking
- No idle threads: speed up particles tracking
- OpenMP shared memory model on the nodes: improve memory use efficiency

Dark Current Simulations in LCLS-II CM

Operating mode in LCLS-II CM from Omega3P



Field emitted dark current in cavities simulated from Track3P

Track3P parameters:

- ~1.5M mesh elements, ~ 10M DOFs, mesh and fields can not fit in each processor
- 4 MPI tasks/node, 24 threads/node
- 4 times speed up

Summary

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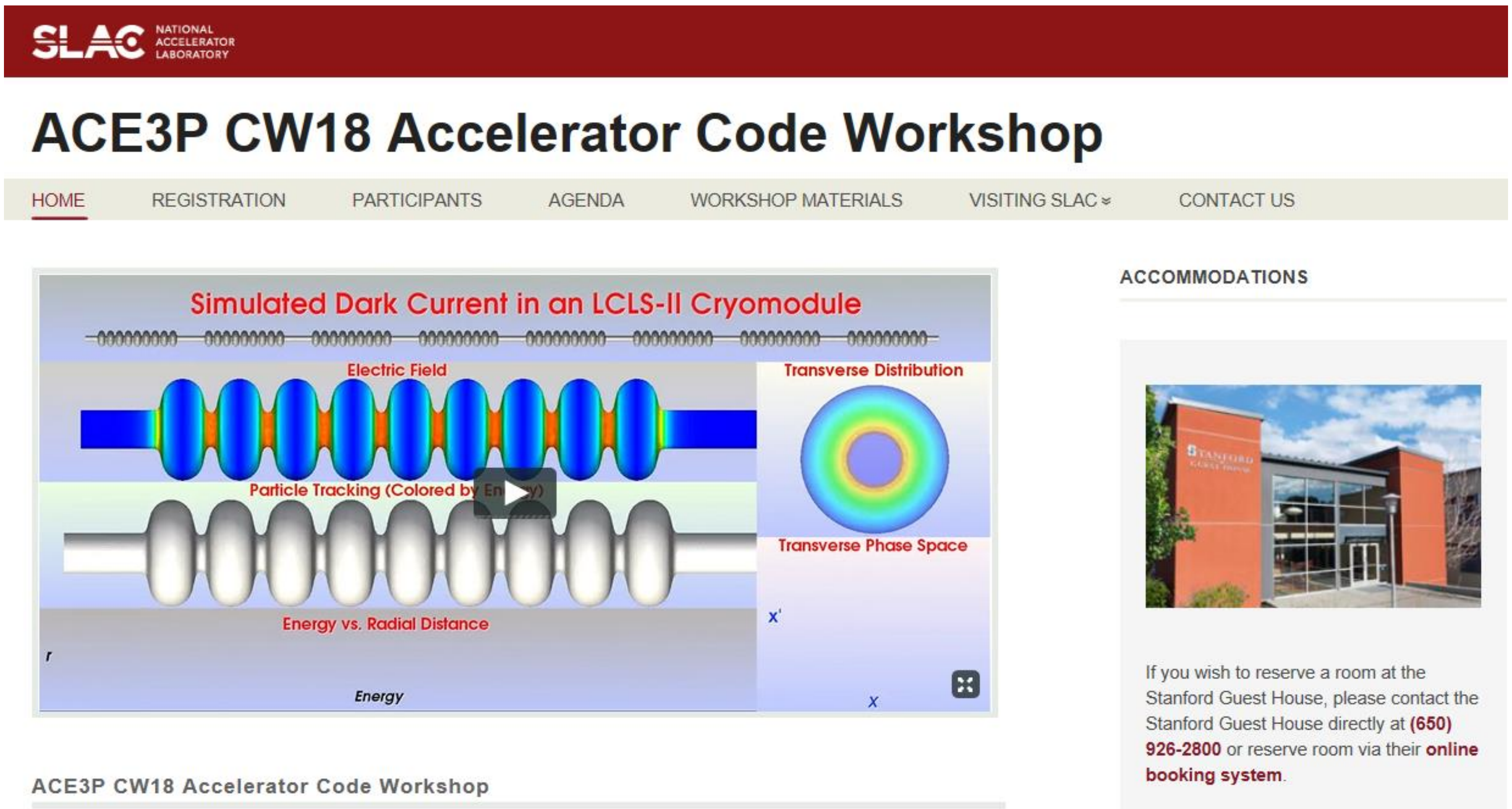
- A nonlinear eigensolver has been implemented in the eigensolver module Omega3P to enable accurate determination of damping factors of resonant modes above the beampipe cutoff frequency in LCLS-II SRF CM;
- Surface impedance model for thin dielectric coating on metal plus moving window scheme implemented in time-domain module T3P enables to simulate low loss surface wave propagating on a single wire over 50m long distance under a realistic environment;
- A newly developed mechanical eigensolver in the multi-physics module TEM3P has allowed the determination of mechanical modes in Fermilab PIP-II high beta 650 MHz CM;
- A hybrid MPI+OpenMP parallel programing has been developed in the particle tracking module Track3P to speed up dark current simulation in LCLS-II linac by factor of 4.

ACE3P User Community

Learn more on modeling capabilities of ACE3P at
ACE3P CW18 Accelerator Code Workshop, Nov. 5 to 9, 2018
https://conf.slac.stanford.edu/cw18/



Welcome collaboration with us!