AI for RF Technology

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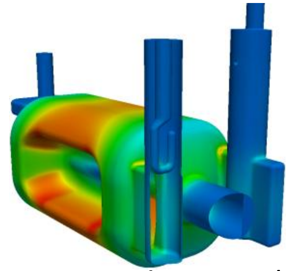
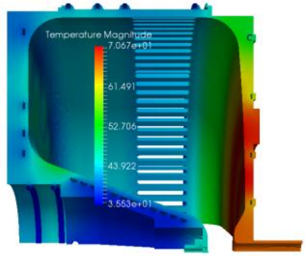
ACE3P for Multi-Physics Accelerator and RF Modeling

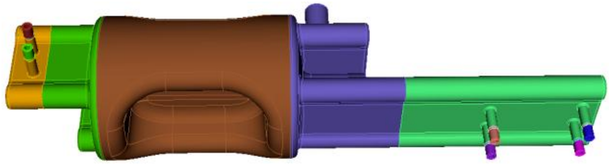
- **ACE3P**, developed at SLAC, is a comprehensive suite of *conformal, high-order, C++/MPI based parallel finite-element (FE) multiphysics codes* including electromagnetic (EM), thermal and mechanical capabilities.
  - Based on *curved high-order finite elements* for high-fidelity modeling
  - Implemented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

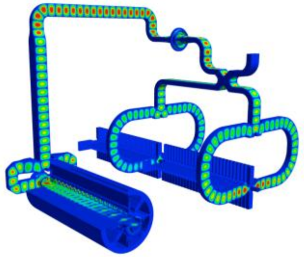
ACE3P (Advanced Computational Electromagnetics 3P)

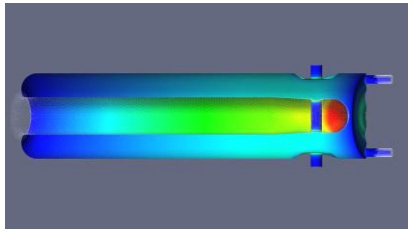
Frequency Domain:	**Omega3P**	**– Eigensolver (damping)**
	S3P	**– S-Parameter**
Time Domain:	**T3P**	**– Wakefields and Transients**
Particle Tracking:	**Track3P**	**– Multipacting and Dark Current**
EM Particle-in-cell:	**Pic3P**	**– RF guns & space charge effects**
Multi-physics:	**TEM3P**	**– EM,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

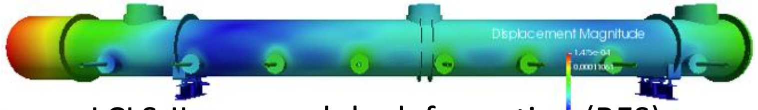

LHC-HL crab cavity (HEP)

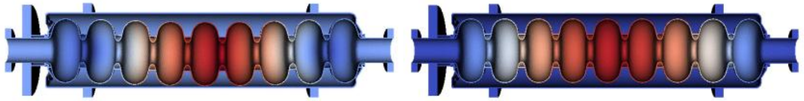

LCLS-II gun (BES)


EIC crab cavity (NP)


CLIC wakefield (HEP)


FRIB multipacting (NP)

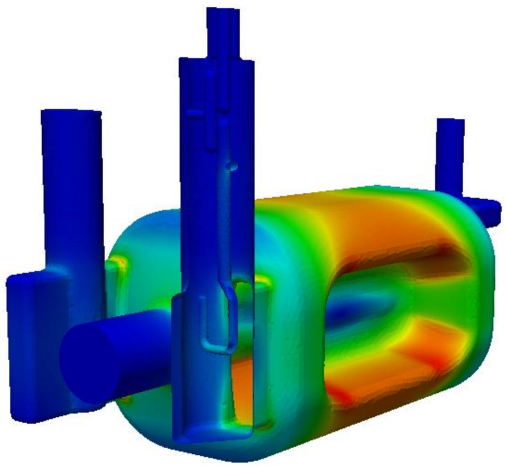

LCLS-II cryomodule deformation (BES)


LCLS-II cavity mechanical modes (BES)

“Design-to-Prototype" of Accelerator and RF Components

Prototyping crab cavity for LHC HiLumi Upgrade

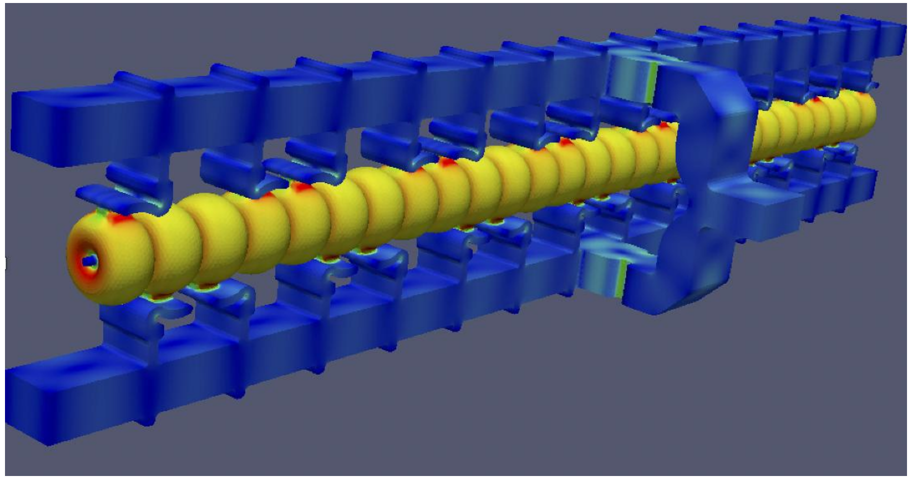
- Installation of rf crab cavities is a key for luminosity enhancement.
- **ACE3P** used to optimize cavity rf design, and keep/update final cavity geometry for engineering

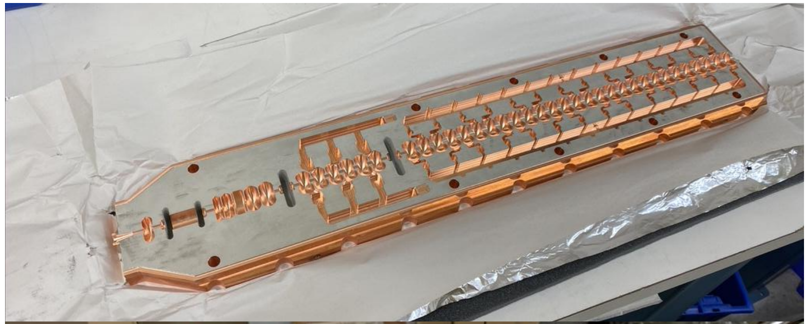


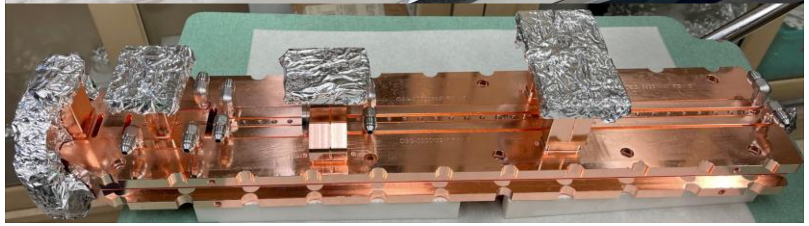
Cavity in production

Distributed coupling Linac RF modeling

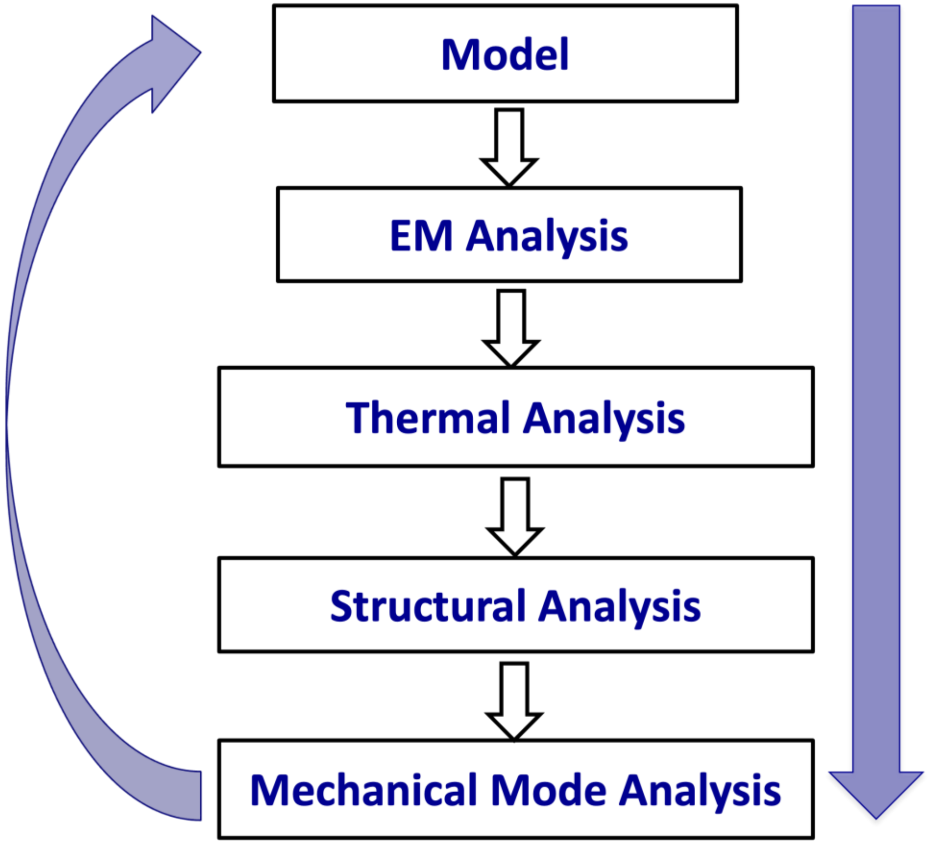
- RF coupling and power distribution waveguide optimization
- Full cavity system rf simulation





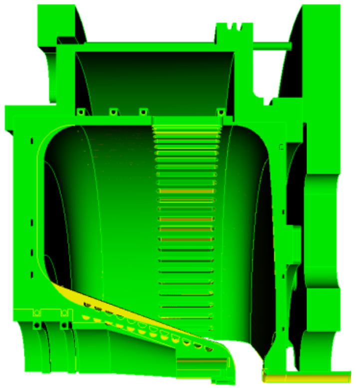


Virtual Prototyping through Multi-Physics Workflow



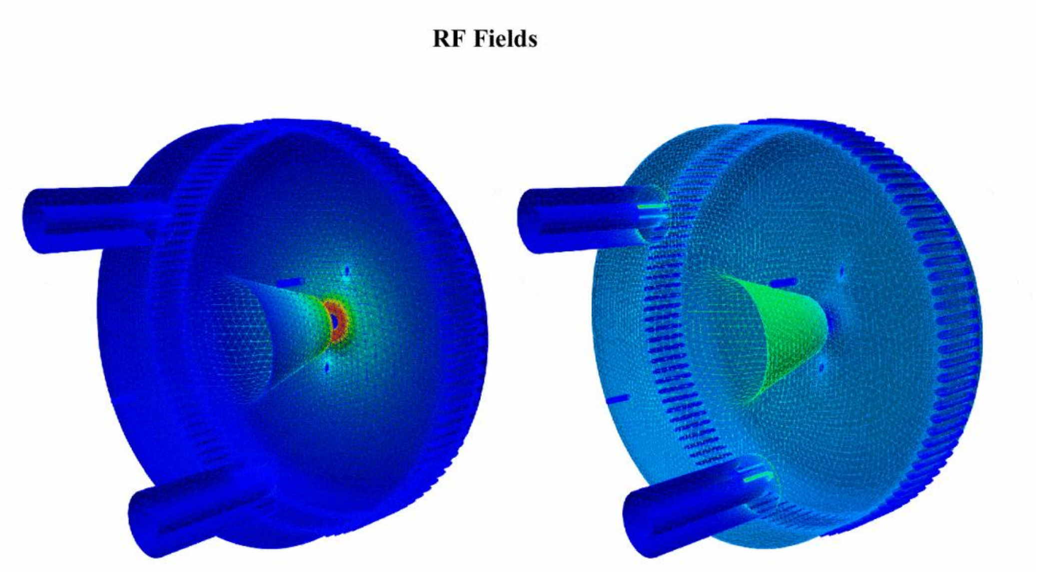
High-fidelity multi-physics calculations using ACE3P modules ensure reliable design.

EM, thermal and mechanical analysis for rf gun



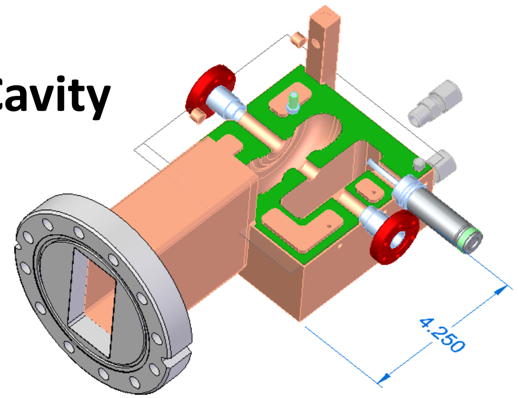
Spare gun design by modifying geometry to reduce dark current emission from cavity

Multiphysics analysis using **Omega3P**, **TEM3P** and **Track3P**



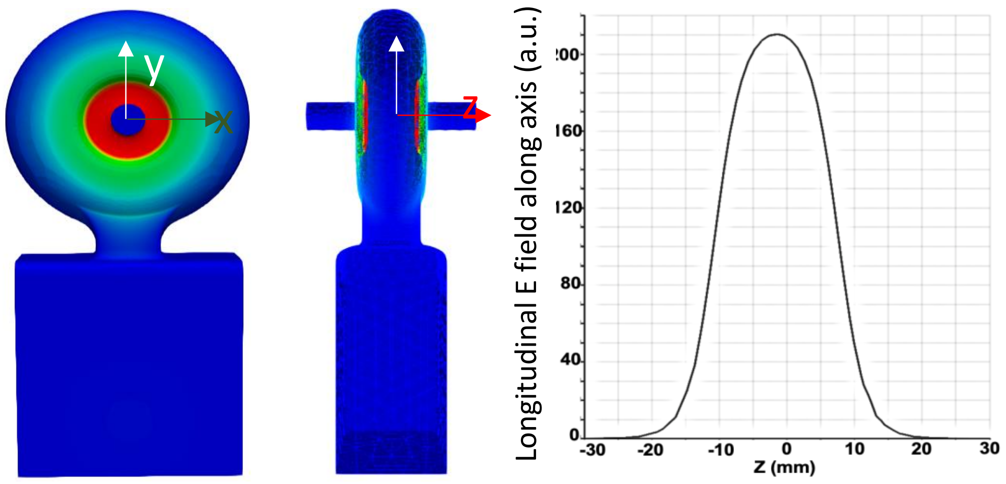
Muon S-Band Cavity Multipacting Study

S-Band Cavity

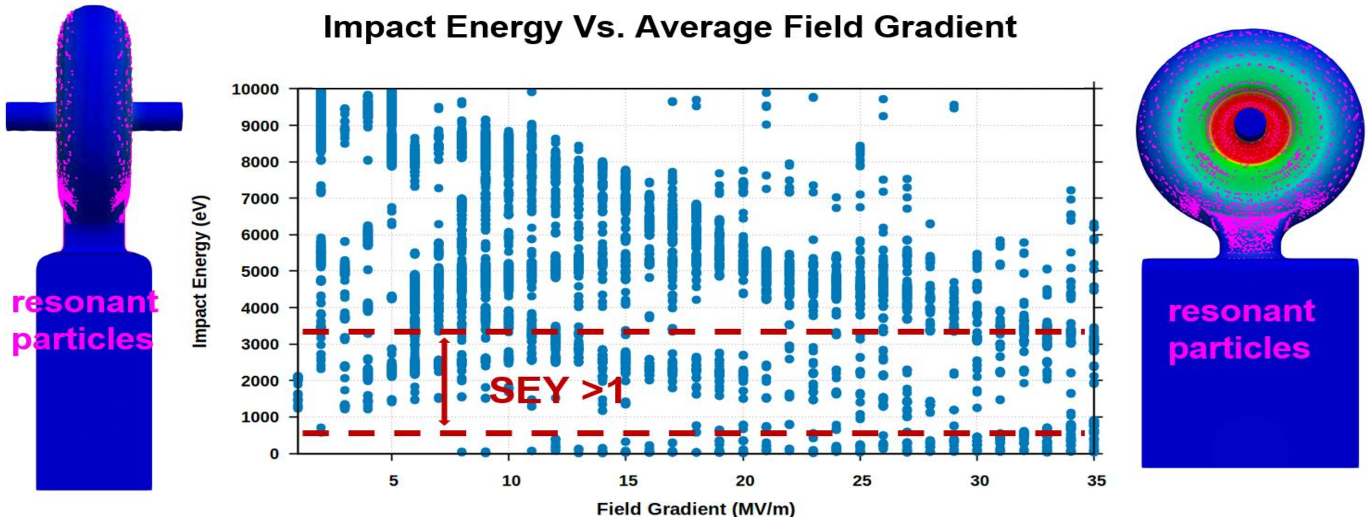


- **3D EM fields (ACE3P, f = 2.856 GHz)** loaded into Track3P for multipacting analysis
- **External magnetic field** (uniform, longitudinal): **0T, 1T, 2T,3T**
- **Accelerating gradient: 1- 35MV/m** (1MV/m increments)
- Construct **resonant particles maps**: location, impact energy, phase

EM field calculated by ACE3P, f = 2.856 GHz



Resonant Particles Map with 2T Magnetic Field



Magnetic field significantly alters multipacting resonance behavior and spatial distribution

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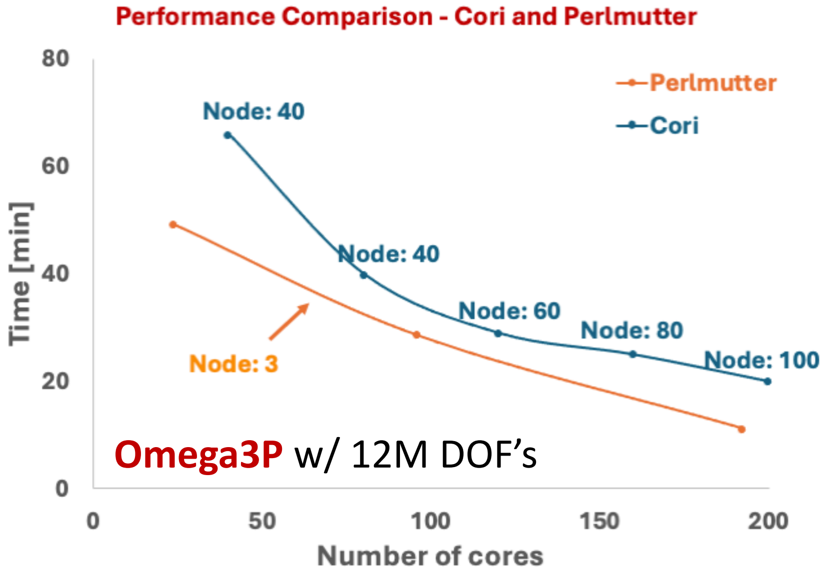
High Performance Computing (HPC) for High Fidelities

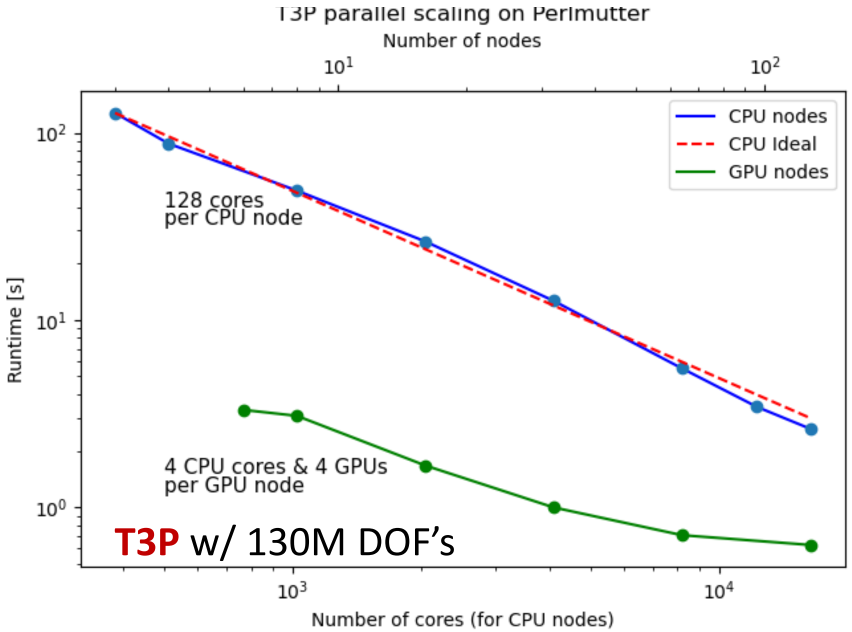
NERSC **Perlmutter:** Cray EX

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



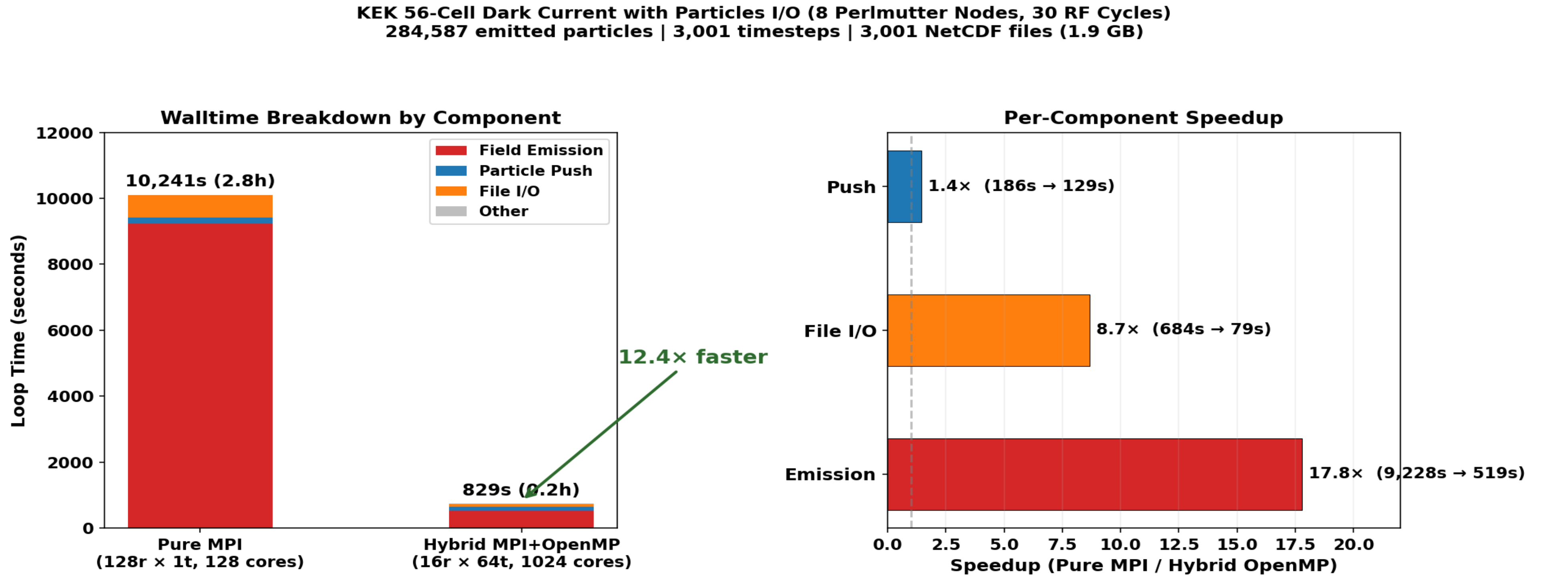
Numerical libraries used in ACE3P

- 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 solvers
- OpenMP adopted for CPU threads and GPU offload



Hybrid MPI+OpenMP Parallelization of ACE3P Track3P

- **Track3P:** Particle tracking for **multipacting** and **dark current** simulations
- **Pure MPI parallelism:** Each rank holds a complete mesh and field data -> leads to **idle cores** on modern HPC nodes
- **Hybrid MPI+OpenMP:** Enhance scalability and node-level efficiency by leveraging **OpenMP** threading



Hybrid MPI+OpenMP significantly improves node-level efficiency and overall performance

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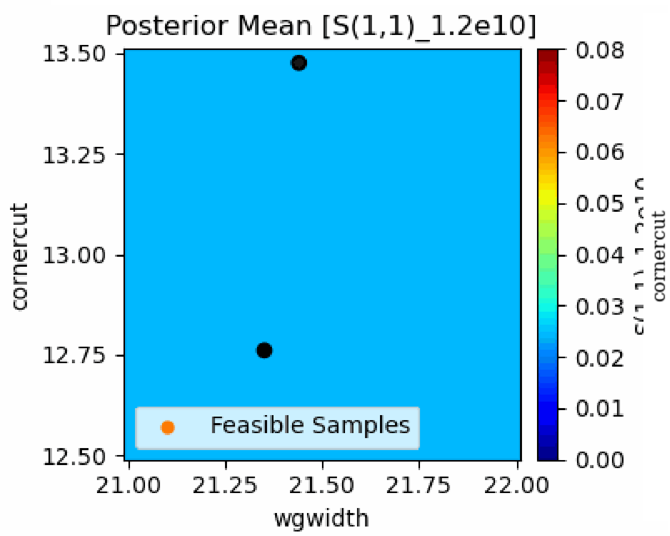
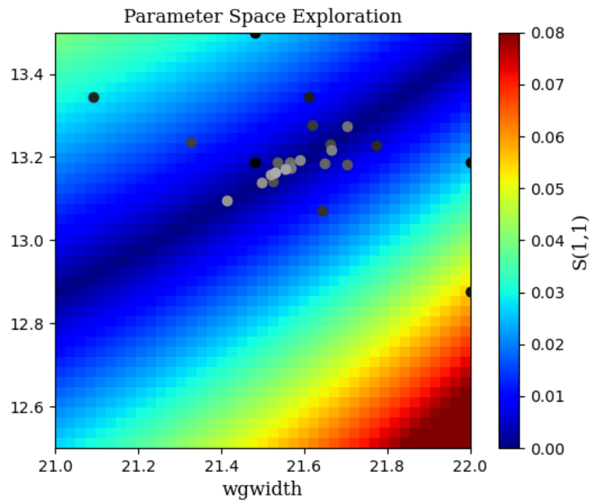
ML Bayesian Gaussian Process (GP) for RF Optimization

Bayesian Optimization with LUME-ACE3P-Xopt

- Add fidelity parameter “s” (controls mesh resolution)
- Train BO model of parameter space
- Use low fidelity (fast) and high fidelity (slow)
- Utilize Bayesian exploration to determine pareto fronts

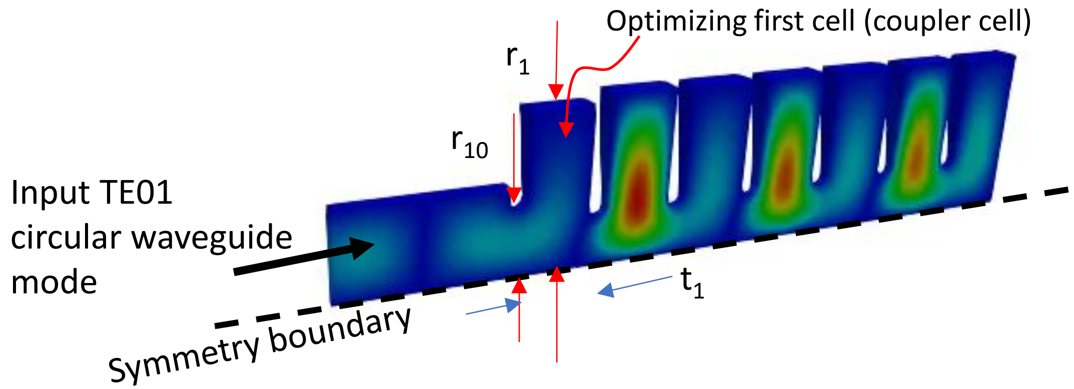
EM optimization of a waveguide bend with 2 design parameters



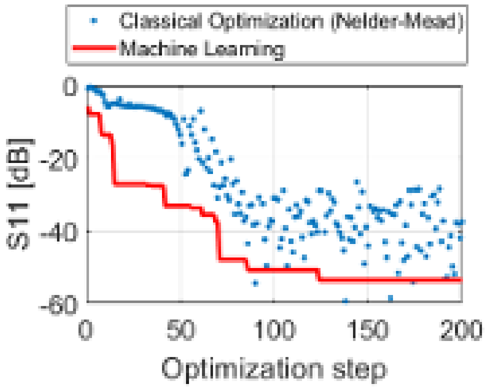


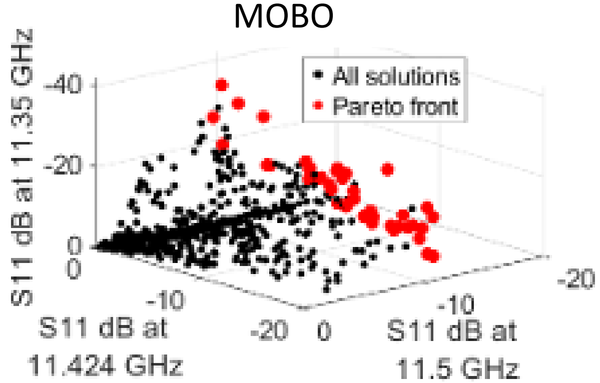
MF-BO converged with ~ 40 iterations (black and white dots for low- and high- fidelity, respectively)

”Brute-force” high fidelity scan with 1000 iterations



Single and multi-objective optimization with GP models

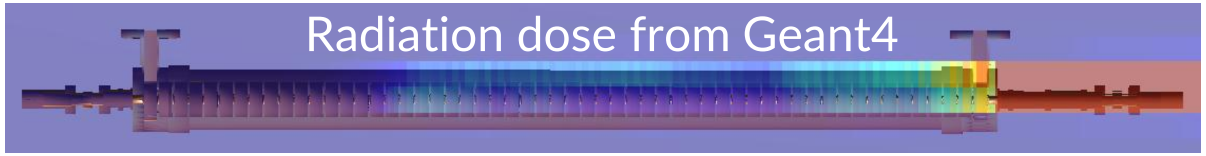


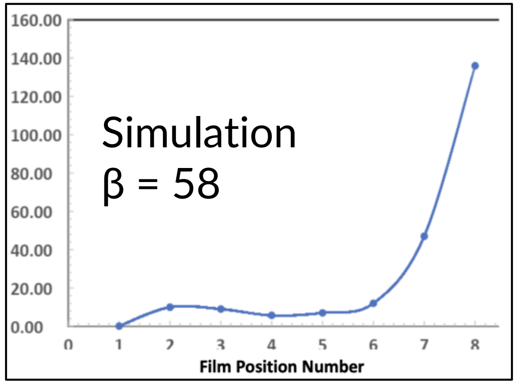


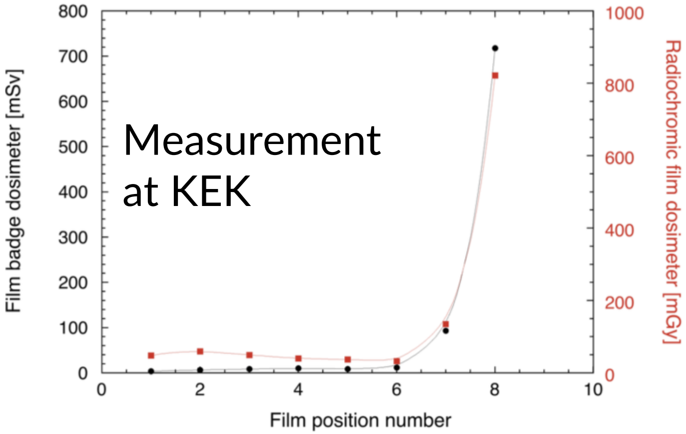
Faster optimal fronts via Machine Learning Exploration

Substantially reducing design cycles for RF cavities and components on HPC platforms

Integration of RF and Radiation Simulation – ACE3P + Geant4

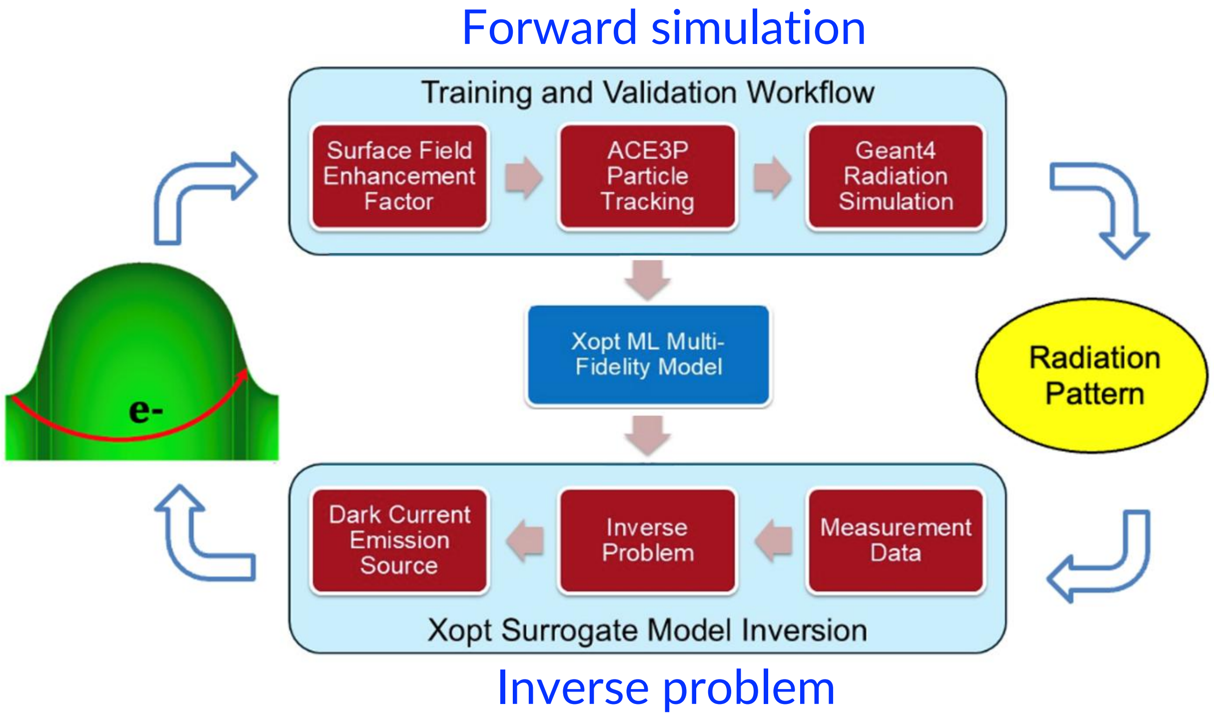






Radiation dose distribution

Matching of radiation pattern by varying *local enhancement factor* β for field emission by trial-and-error simulations – *AI/ML inverse approach bypasses this daunting process to identify emission origins.*



Bench test of S-band structure at KEK

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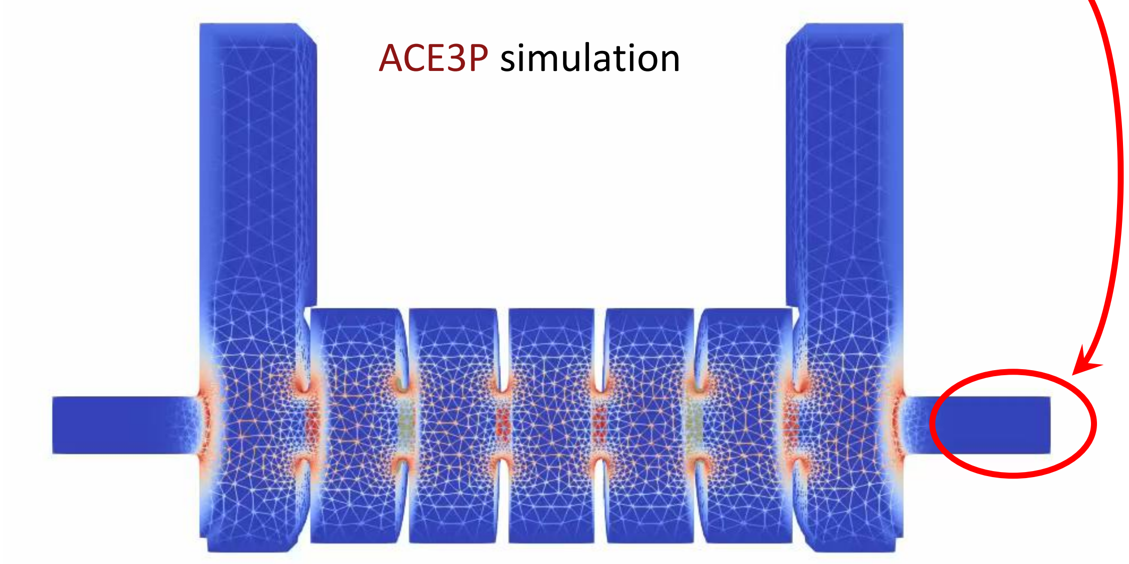
Surrogate Models for Inverse Problems – Field Emission Origin

KEK 7-cell structure example for dark current study

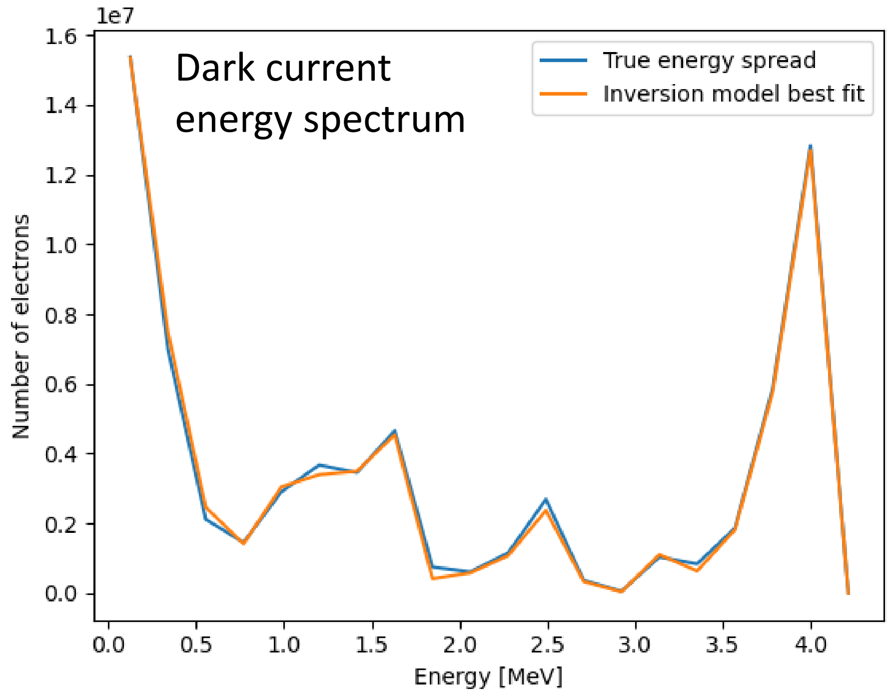
- Particles emitted from 8 irises (high field regions)
  - Each with unknown field emission factor β_1 to β_8
- Fowler-Nordheim law used to estimate emission
- Tracking and impacts monitored with Track3P
- Particle data collected at downstream beampipe



Dark current simulation will be extended to include radiation using Geant4.

Bayesian Gaussian process (GP) model built from synthetic data using forward simulations

- Energy spectrum plotted at downstream
- GP model inverted using validation data



(true calculation) validation β = [55, 45, 55, 55, 45, 45, 45, 55]
GP model inversion β = [55, 47, 54, 54, 49, 40, 42, 54]

Agentic Workflow to Automate Multi-Physics Simulation

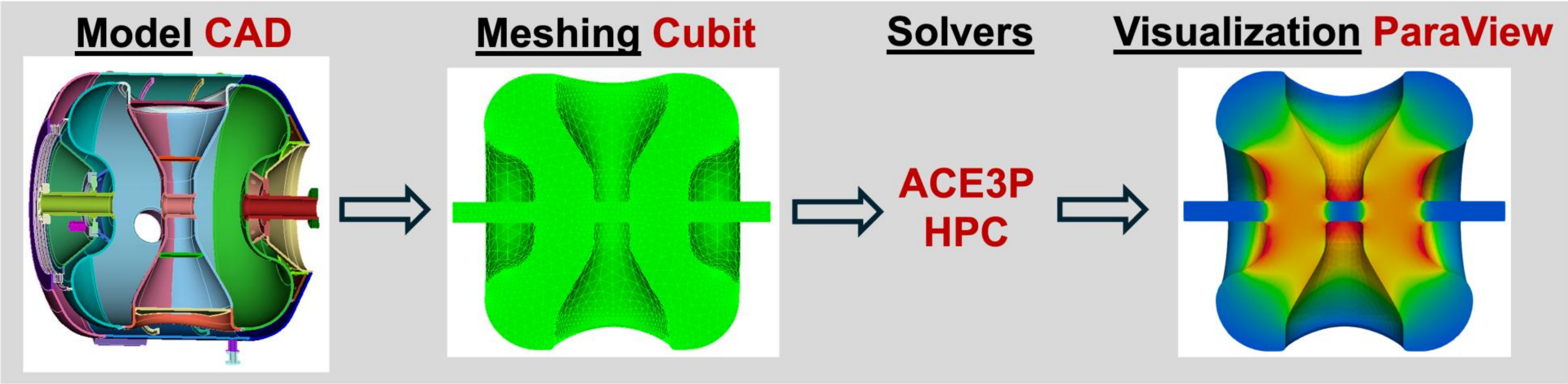
- CADSAT (CAD to Simulation Agentic Toolkit) project under DOE NNSA-funded Genesis/AI4NS lighthouse initiative – LLNL & SNL
- Approach applicable to ACE3P for accelerator modeling
  - Cubit group at SNL for CAD-to-mesh pipeline
  - MADA (Multi-Agent Design Assistant) group at LLNL for forward and inverse pipelines in MARBL inertial confinement fusion simulations

AI agents
- Preprocessor – Cubit
- Problem setup
- Design optimization
- Inverse problem
- Job submission
- Postprocessing

HPC system

lume-ace3p simulation workflow

Xopt backend



Summary

ACE3P Simulation Suite

- Parallel finite-element multi-physics codes (EM, thermal, mechanical) for high-fidelity accelerator and RF modeling on HPC platforms
- Hybrid MPI+OpenMP parallelization boosts node-level efficiency and performance

Design-to-Prototype Workflows

- Virtual prototyping via integrated modules (Omega3P, TEM3P, Track3P) for crab cavities, RF guns, and muon S-band multipacting studies

Machine Learning Integration

- Bayesian Optimization (LUME-ACE3P-Xopt) – faster optimization than parameter sweeping
- ML inverse approach identifies dark current field emission origins via surrogate models

Future Directions

- RF + radiation simulation (ACE3P + Geant4) and agentic workflows (CADSAT) to automate multi-physics pipelines