Integrated Simulation of Cavity Design and Radiation Transport (*ACE3P + Geant4*)

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October 3, 2024

Outline

- Introduction
- Simulation workflow
  - ACE3P
  - Geant4
  - ACE3P and Geant4 integration
- Applications
- Summary

Introduction

- Dark current radiation affects the performance of accelerators
  - Field emission and its adverse consequences observed at CEBAF upgrade cryomodules
- Radiation simulation requires multiple separate calculations
  - Electromagnetic field
  - Particles tracking
  - Radiation
- A standalone software package integrates ACE3P and Geant4 for dark current radiation effects study
  - Provide a geometric tool to match the boundaries at the interface of different computational domains used in ACE3P and Geant4.
  - Develop a particle data transfer capability between ACE3P and Geant4 based on the standardized openPMD format.
  - Implement a Python script to control the integrated simulation workflow.
- Project is supported by US DOE HEP US-Japan Science and Technology Cooperation Program (2022-2025)

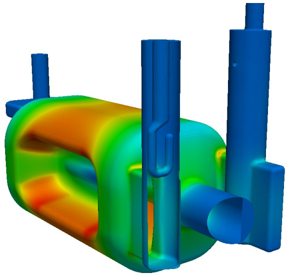
ACE3P for Multi-Physics Accelerator Modeling

- **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

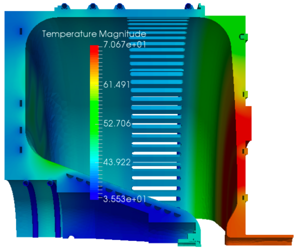
ACE3P (Advanced Computational Electromagnetics 3P)

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**

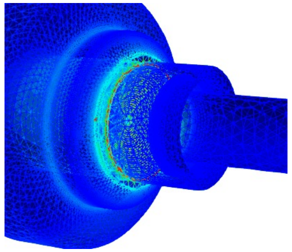
High-fidelity, high-accuracy simulation for virtual prototyping of accelerator components at large scale



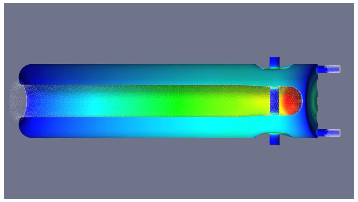
LHC-HL crab cavity
resonant mode



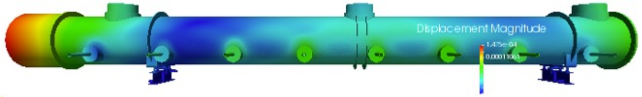
LCLS-II gun
temperature distribution



IOT gun
beam propagation



FRIB cavity
multipacting



LCLS-II cryomodule
deformation

High Performance Computing (HPC) for Solution Speedup

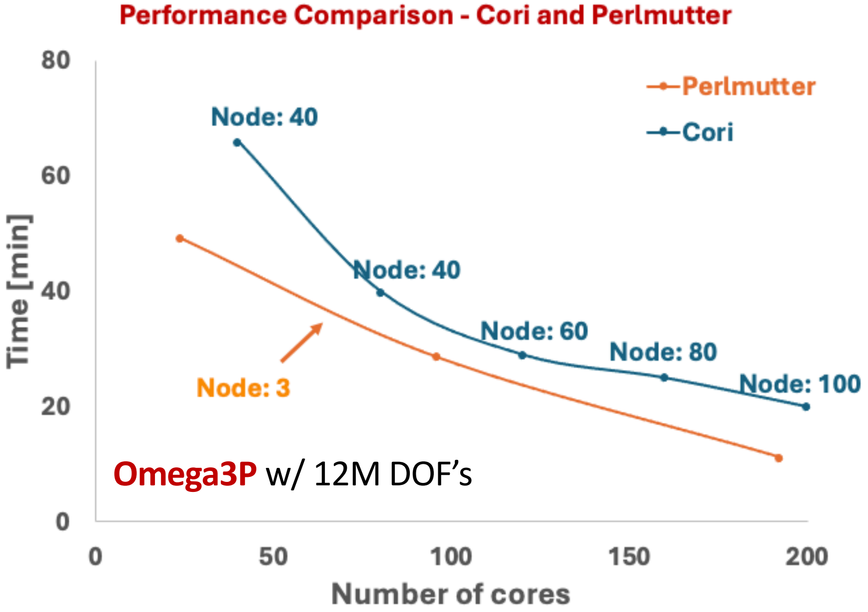
Cori: Cray XC40
- 632,672 compute cores
- 1 petabytes of memory
- peak performance of 27.9 petaflops/sec

Perlmutter: Cray EX
- 3072 CPU nodes
- 1536 GPU nodes
- 2.2 petabytes of memory
- peak performance: 3-4 times Cori

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



Performance Comparison - Cori and Perlmutter

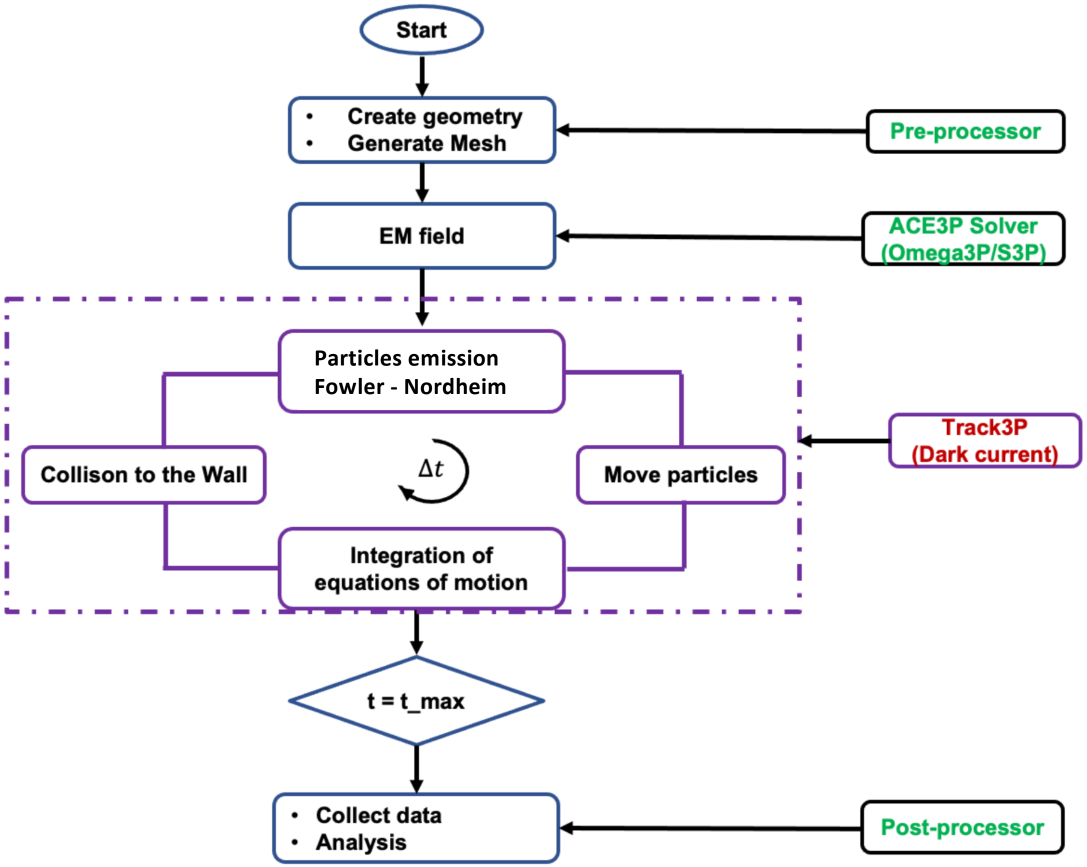
Omega3P w/ 12M DOF's

Migration from NERSC Cori to Perlmutter (2023)

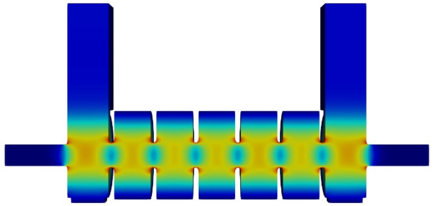
- Numerical libraries installed using spack for managing HPC packages
- Interfaced to PETSc GPU backend for linear/nonlinear solvers

Robust code infrastructure exploits compute power of emerging architecture.

ACE3P Dark Current Simulation Workflow



- Model built and mesh generated by Cubit
- EM field solved by Omega3p/S3P



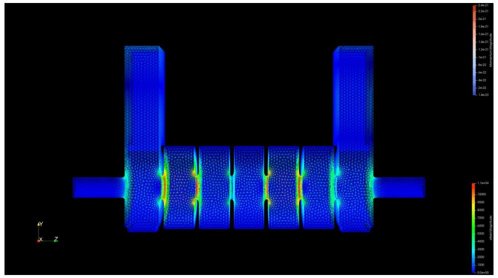
- Track particles in RF field by Track3P

Fowler-Nordheim formula for particles emission

$$J(r,t) = 1.54 \times 10^{\left(-6+\frac{4.52}{\sqrt{\phi}}\right)} \frac{(\beta E)^2}{\phi} e^{\left(\frac{-6.53\times10^9 \phi^{1.5}}{\beta E}\right)}$$

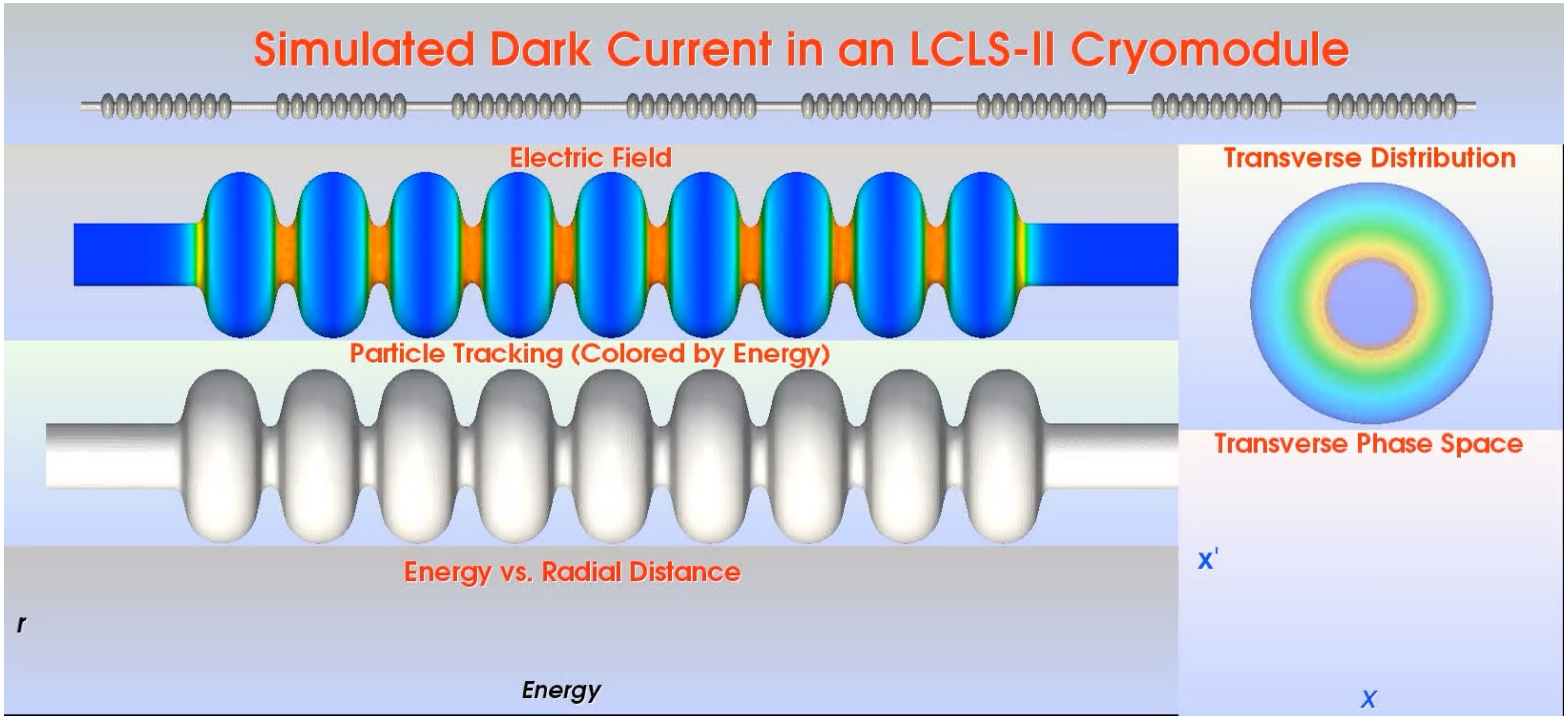
Lorentz force equation for particles motion

$$\frac{d}{dt}\left(m\vec{V}\right) = q\left[\vec{E} + \vec{V} \times \vec{B}\right]$$



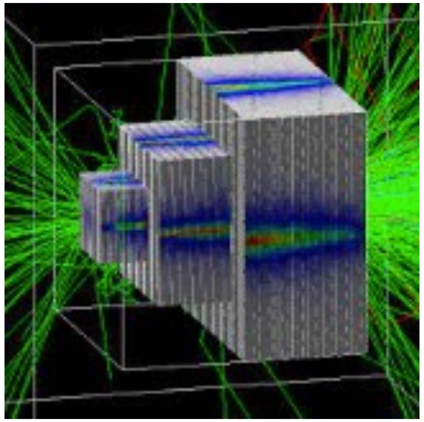
Large-Scale Dark Current Simulation by Track3P

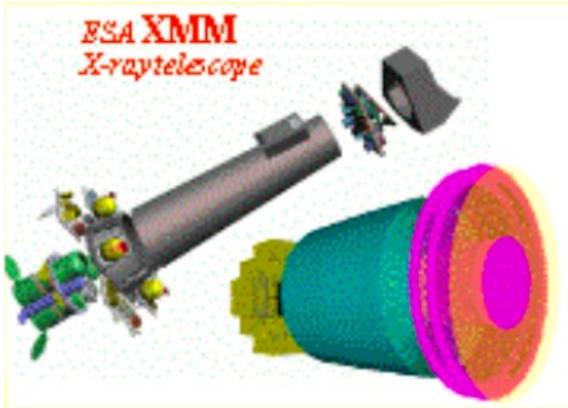
- Track3P run on NERSC Edison
  - 10 nodes
  - 240 cores
  - 7 minutes
  - 50 RF cycles

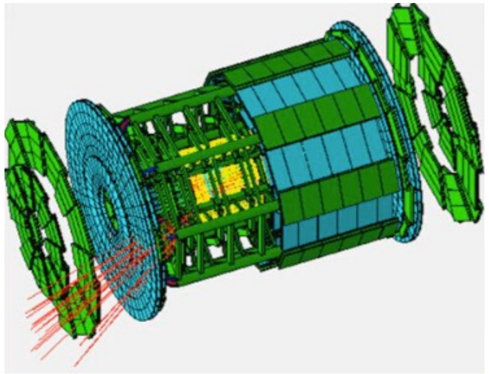


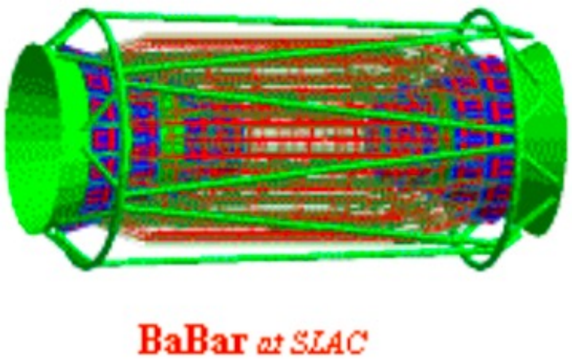
Geant4 for Radiation Transport Simulation

- A toolkit to create simulations of the passage of particles or radiation through matter
    - …
    - Radiation dose
    - Positron source
    - …
- Open source license
- Webpage: https://geant4.web.cern.ch
- Development for this project
    - Geometry model converter
    - Particles I/O

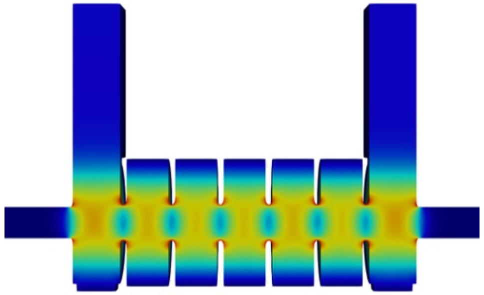


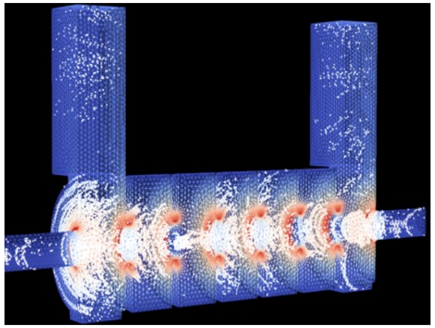


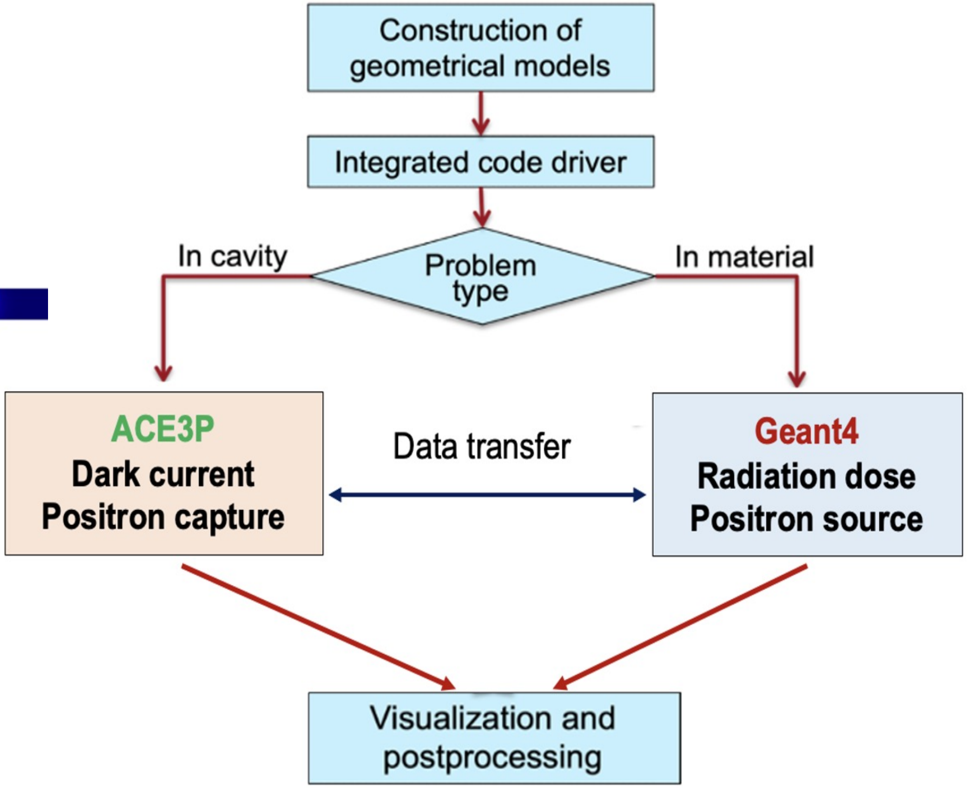




Workflow for Integrated ACE3P and Geant4 Simulation







Construction of geometrical models

Integrated code driver

Problem type

In cavity

In material

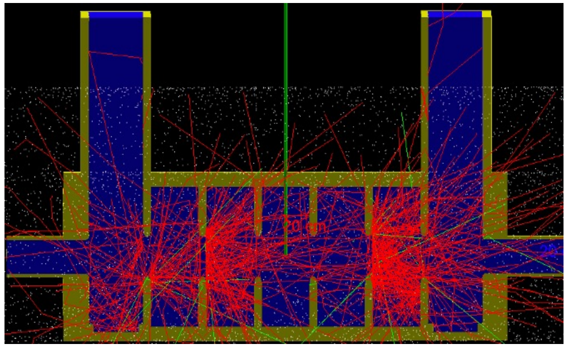
ACE3P
Dark current
Positron capture

Data transfer

Geant4
Radiation dose
Positron source

Visualization and postprocessing

- **Install and run on massively parallel computers**
- **Enable solutions of large-scale problems**

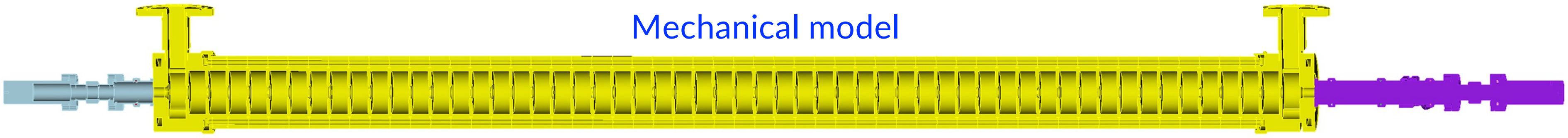


Import of CAD Geometry Model into Geant4

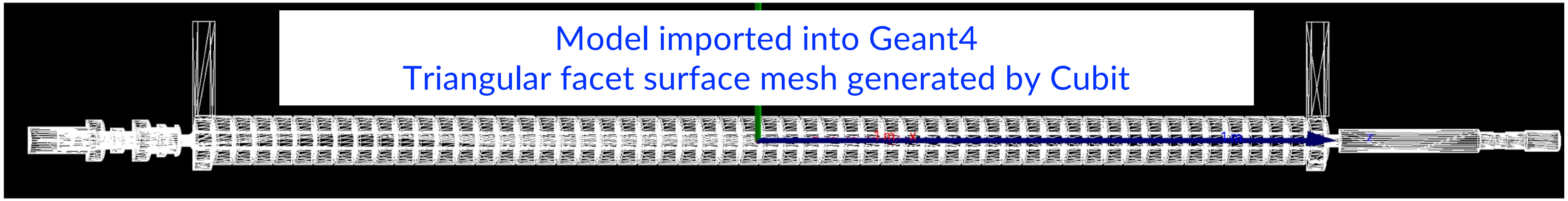
- Cubit: mesh generation tool
  - Generate triangular surface mesh
  - Export mesh file in stl format
- CADMesh: direct CAD model import interface for Geant4
  - Triangular facet surface mesh
  - https://github.com/christopherpoole/cadmesh

- Include the header #include "CADMesh.hh"
- Use built-in readers to load mesh

```
 #include "CADMesh.hh"
    ....
    auto mesh =
CADMesh::TessellatedMesh::FromSTL("mesh.stl");
    G4VSolid* solid = mesh->GetSolid();
```



Mechanical model



Model imported into Geant4
Triangular facet surface mesh generated by Cubit

Particle Data I/O

- Develop a particle data transfer capability between ACE3P and Geant4
- Based on the standardized openPMD format

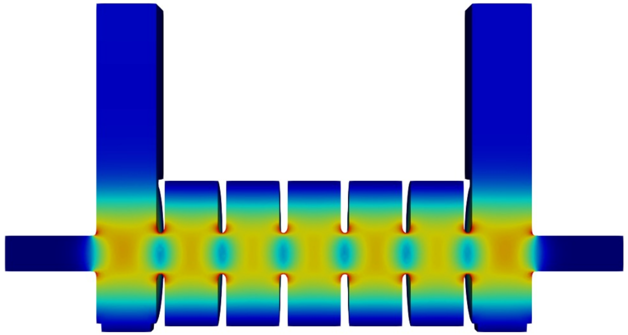
X	Y	Z	Time (RF Cycle)	Energy	Num. Electrons	Mom_X	Mom_Y	Mom_Z	Boundary ID
3.98453e-02	1.11643e-02	4.46050e-02	1.08810e+00	1.64804e+05	6.49938e+03	9.61114e-01	2.69174e-01	-6.16865e-02	6
8.35555e-03	-1.18983e-02	-8.51440e-02	1.12348e+00	3.35163e+05	6.22911e+03	3.68485e-01	-5.23249e-01	-7.68394e-01	6
5.92626e-03	1.39628e-02	5.49185e-02	1.47410e+00	3.42393e+05	6.73727e+03	2.46472e-01	5.81169e-01	-7.75560e-01	6
1.01297e-02	-1.31314e-02	5.49850e-02	1.49753e+00	3.60403e+05	6.52320e+03	3.70080e-01	-4.80048e-01	-7.95358e-01	6
3.63805e-03	1.19656e-02	-8.89980e-02	1.54512e+00	1.81794e+05	1.08322e+04	9.82131e-02	1.62213e-01	9.81856e-01	6
6.02885e-03	-4.09382e-02	4.17373e-02	2.06998e+00	1.61448e+05	6.36634e+03	1.45044e-01	-9.86273e-01	-7.89183e-02	6
2.38938e-03	-2.22900e-02	5.49851e-02	2.38574e+00	4.73590e+05	7.75671e+03	2.90391e-02	-1.01166e-01	-9.94446e-01	6

OpenPMD

- Open standard for particle-mesh data files
- Standard for metadata and naming schemes
- Suits for any kind of hierarchical, self-describing data format
- Improve code portability and performance

ACE3P+Geant4 Integrated Tool Test - 7-Cell Structure

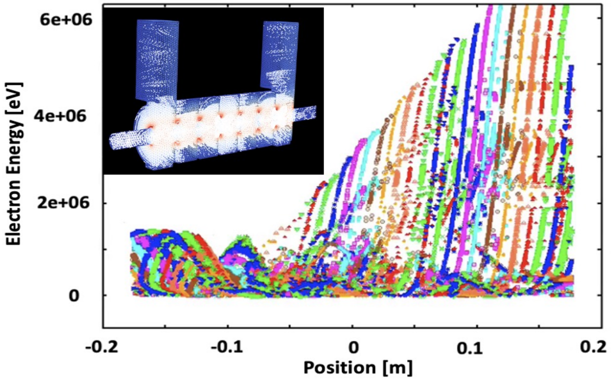
E field (complex) magnitude



Electromagnetic RF field (S3P)

- Mesh : 750k tetrahedral elements
- Frequency: 2.856 GHz
- On NERSC Cori: 10 nodes, 320 cores, < 1 minute

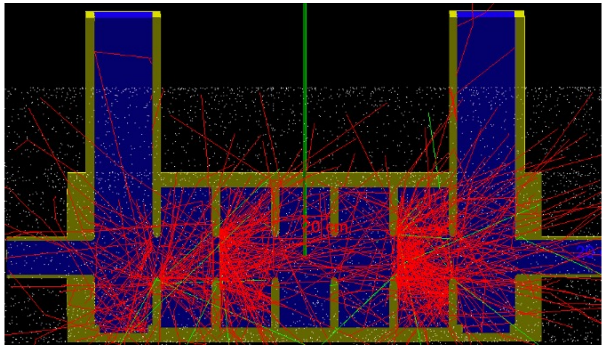
Electron energy in the structure



Dark current simulation (Track3P)

- Particles emitted for 6 RF cycles
- Total emitted particles: 2.6 million
- Run 12 RF cycles
- On Cori: 2 nodes, 30 minutes

Particles trajectories

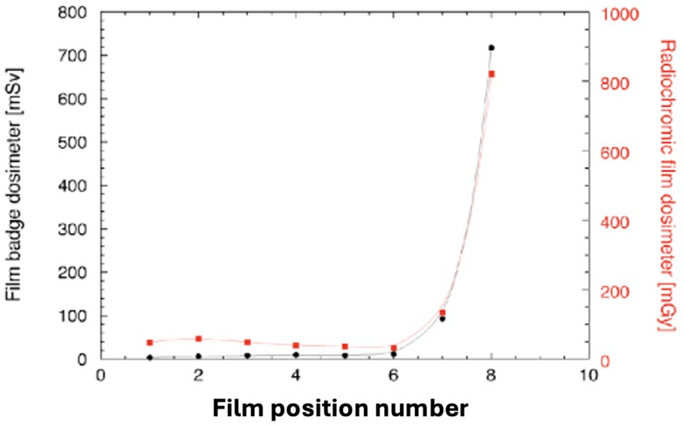


Radiation simulation (Geant4)

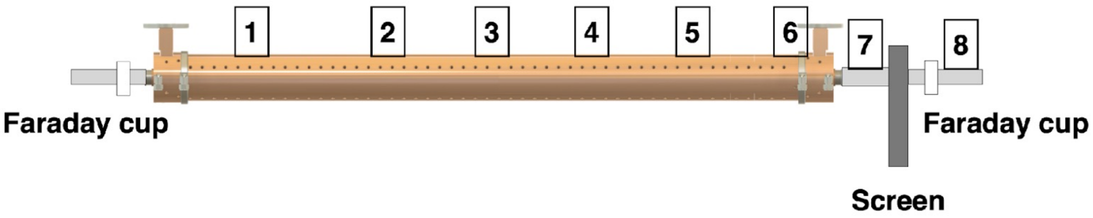
- Load particles information from Track3P to Geant4
- Define structure from CAD model
- Radiation simulation

Radiation Dose Measurements for KEK 56-Cell Structure

Radiation doses along the structure measured by using two kinds of dosimeter



Film position



Performed at KEK

ACE3P Field Calculation for 56-Cell Structure

EM field calculated by S3P

Model & mesh

- S-band structure provided by KEK
- Simulation model built by Cubit
- 3.4M curved tetrahedral mesh generated by Cubit

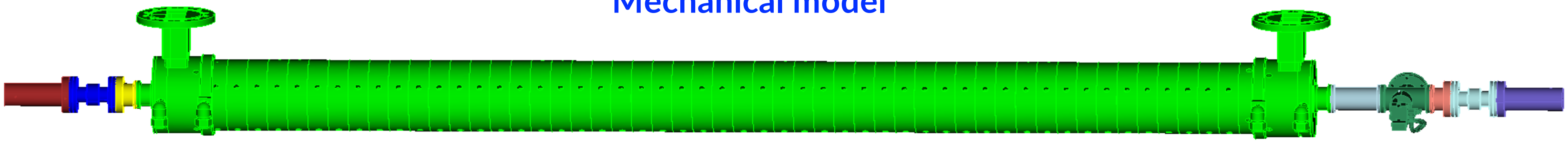
S3P calculation

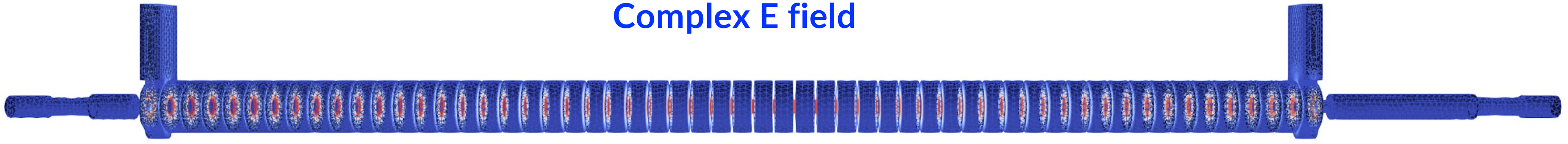
- Frequency: 2.856 GHz
- S-parameter calculation

S(0,0)	S(0,1)	S(1,0)	S(1,1)
2.1e-02	6.9e-01	6.9e-01	3.73e-02

Computational resource

- NERSC supercomputer
- 4 CPU nodes, 64 cores/node
- Several minutes to solve one mode


Mechanical model

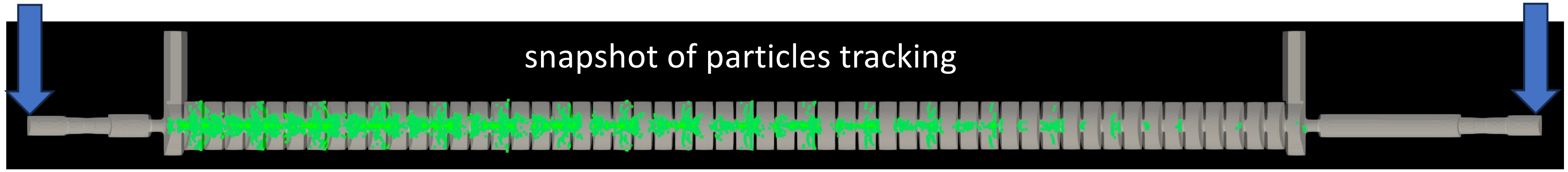

Complex E field

ACE3P Particle Tracking Calculation for 56-Cell Structure

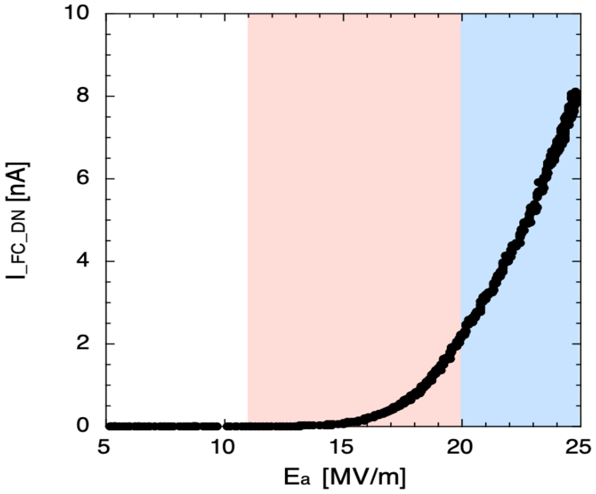
Dark current calculated by Track3P

Faraday cup upstream

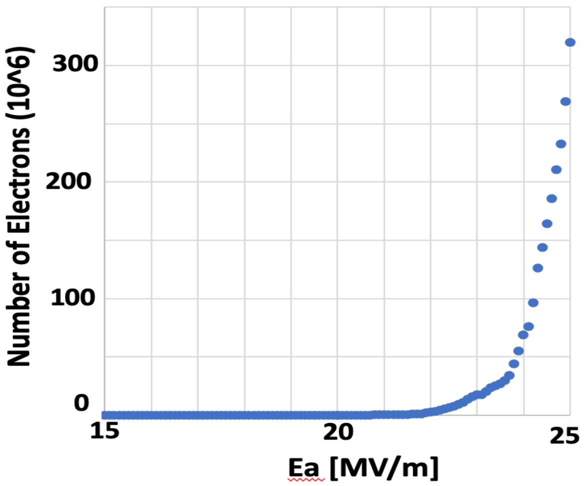
Faraday cup downstream



Dark current measured by KEK



Dark current calculated by Track3P



Summary

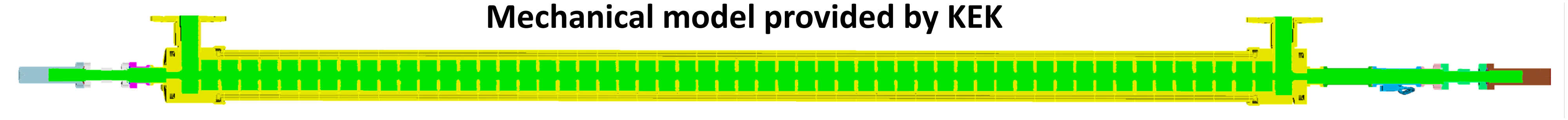
- Total run: 30 RF cycles
- Particles emission: Fowler - Nordheim formula

$$J(r,t) = 1.54 \times 10^{\left(-6+\frac{4.52}{\sqrt{\phi}}\right)} \frac{(\beta E)^2}{\phi} e^{\left(\frac{-6.53\times10^9 \phi^{1.5}}{\beta E}\right)}$$

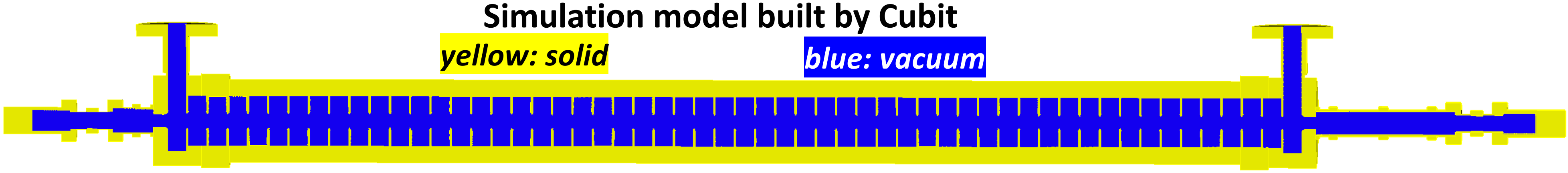
- Difference due to
  - Simulation β = 50
  - Unknown measured β

Geant4 Radiation Transport Calculation for 56-Cell Structure

Geometrical model for Geant4



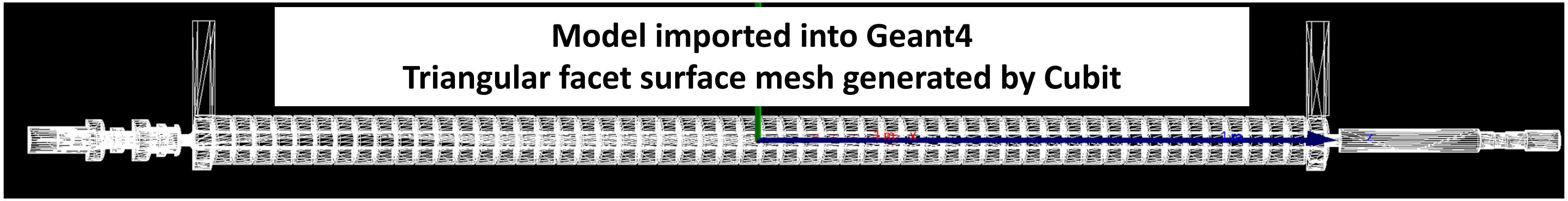
Mechanical model provided by KEK



Simulation model built by Cubit

yellow: solid

blue: vacuum

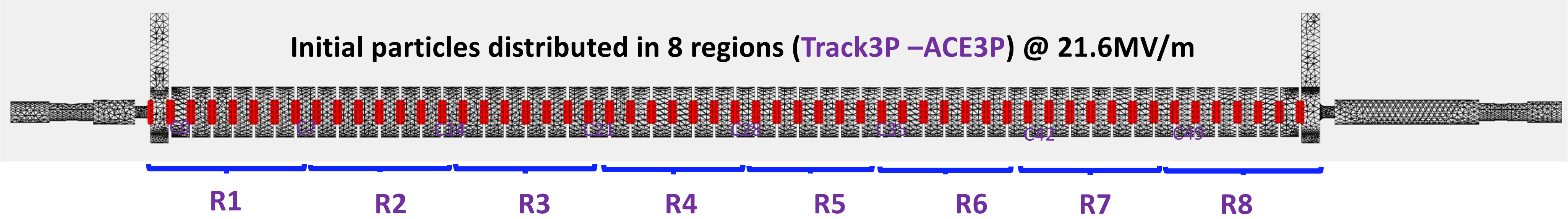


Model imported into Geant4

Triangular facet surface mesh generated by Cubit

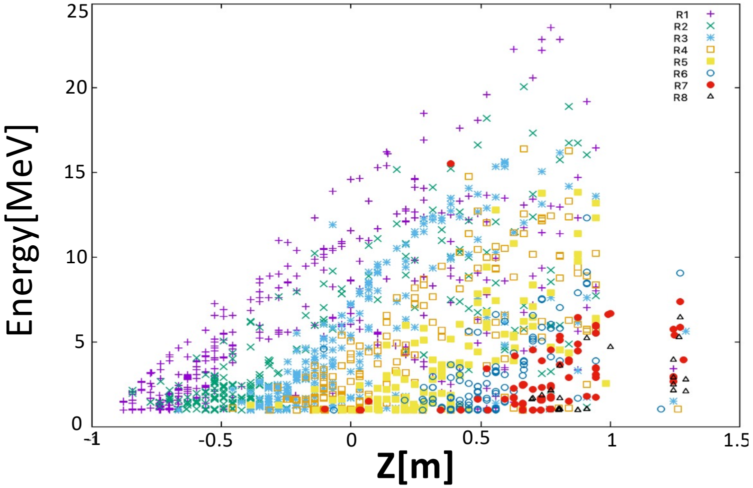
Geant4 Radiation Transport Calculation for 56-Cell Structure (Cont’d)

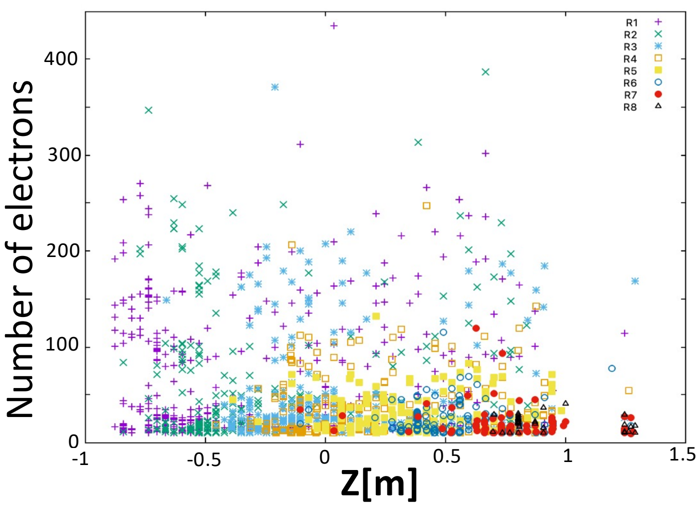
Radiation calculation by Geant4



Initial particles distributed in 8 regions (Track3P –ACE3P) @ 21.6MV/m

Particles used for Geant4 simulation: energy > 1 MeV

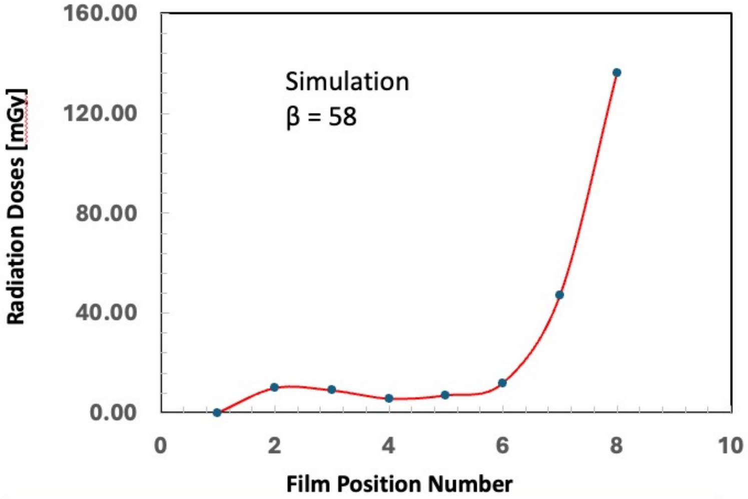




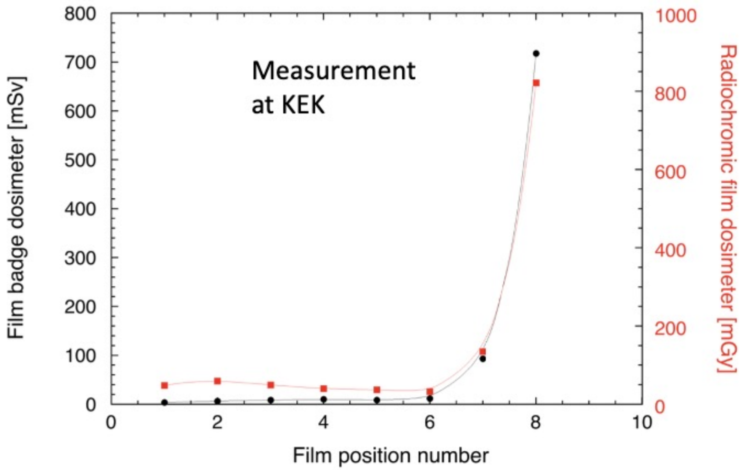
Radiation Dose along 56-cell Structure

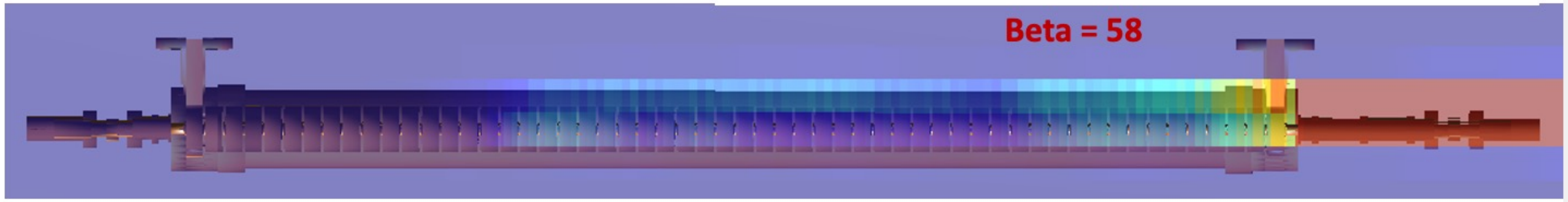
Radiation dose calculation by Geant4

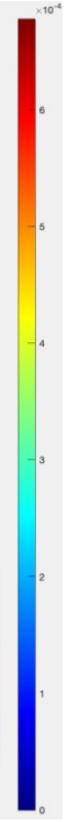
Radiation doses along the structure simulated by Geant4



Radiation doses along the structure measured by using two kinds of dosimeter





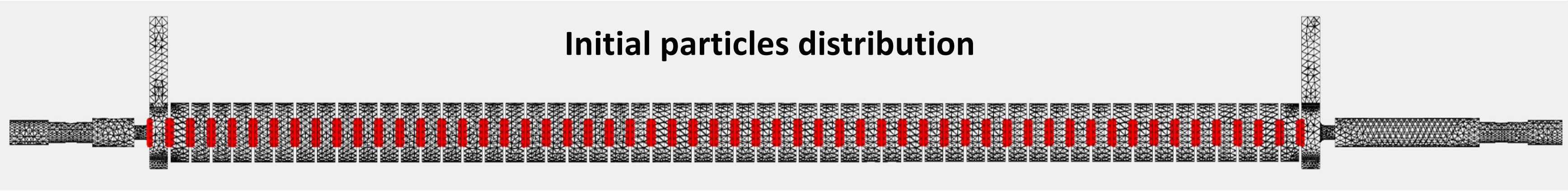


Inverse Approach for Dark Current Analysis – Future Work

Incorporation of machine learning (ML) tools based on multi-fidelity Bayesian optimization

- Using dark current and radiation measured data, Track3P/Geant4 simulation used to train ML model with objectives to
    - Identify locations contributing to dark current
    - Determine enhancement factor, β, distribution for field emission

- Identification of emission origins will provide insights on how to mitigate dark current effects through cavity processing and on establishing a better field emission model.
- Refer Auralee Edelen’s talk “Machine learning models for particle accelerator optimization.”



Conclusion

- An integrated simulation workflow for cavity design and radiation transport (ACE3P + Geant4) has been developed.
- The integrated tool has been used for large-scale dark current and radiation effects study of KEK 56-cell S-band accelerating structure and benchmarked well with measurement data.
- Positron source and its capture simulation capabilities will be added to the integrated tool.
- *Machine learning* tools are in the process of integrating into the tool from an inverse approach using measured data.

Acknowledgements

SLAC Collaborators

Zenghai Li, Cho-Kuen Ng, Liling Xiao

KEK Collaborator

Hiroyasu Ego, Yoshinori Enomoto, Hiroshi Iwase, Yu Morikawa, Takashi Yoshimoto

This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

Thank You!