A Bayesian Optimization-Assisted, High-Performance Simulator for Modeling RF Accelerator Cavities

U.S. DEPARTMENT OF ENERGY

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Abstract

- High-quality radio-frequency (RF) cavities are key components for high energy particle accelerator research at DOE: SLAC, LBNL, Fermi
- Its multi-objective optimization-based design requires an efficient 3D full-wave eigen solver
- Integral equation (IE) method:
  - Linear eigen problem with smaller DoFs as compared to finite-element methods (FEM)
  - Fast solvers with high performance computing
  - ML algorithms to search for resonance modes
- We present an efficient ML algorithm by combining Gaussian Process with Downhill-simplex methods to find resonance frequencies
- Tested for single-cell cavity design to quickly and accurately locate all resonant modes

GPTune

- GPTune: an ECP product based on Gaussian Process for autotuning HPC and ML codes.
- Applied to multiple ECP application codes including SuperLU_DIST, ScaLAPACK, Hypre, STRUMPACK, MFEM, ButterflyPACK etc.
- Supports multi-task, multi-objective, multi-fidelity and distributed-memory parallelism
- Available via Github, Spack, E4S, xSDK

Optimization Task

- Search for the resonance frequency f such that

$$\mathbf{Z}[f]\boldsymbol{I} \approx \mathbf{0}$$

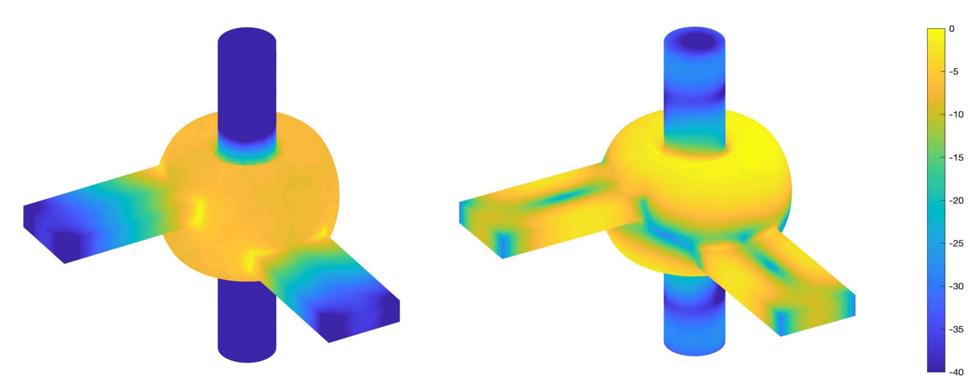
- $\boldsymbol{Z}$ is the discretized IE operator, $\boldsymbol{I}$ is the resonance mode vector
- Each trial sample f requires solving a linear eigen problem.

Methodology

- The objective function has multiple sharp minimums
- Global optimizer like Gaussian process (e.g., GPTune) has smoothing effects and cannot capture the sharp minimums
- Local optimizer like Downhill-simplex requires a good initial guess.
- Locating all minimums by first identifying regions of resonance using GPTune and then refining the search using Downhill-simplex

Single-Cell Cavity Modeling

- Single-cell cavity
  - 2 circular + 2 rectangular beam ports
  - Mesh used leading to a 25000 × 25000 system $\boldsymbol{Z}$ (much smaller than FEM)
  - Each eigen solver uses 16 NERSC Cori Haswell nodes (512 cores)
  - GPTune: 3.5 hours, GPTune+Simplex: 6.2 hours.



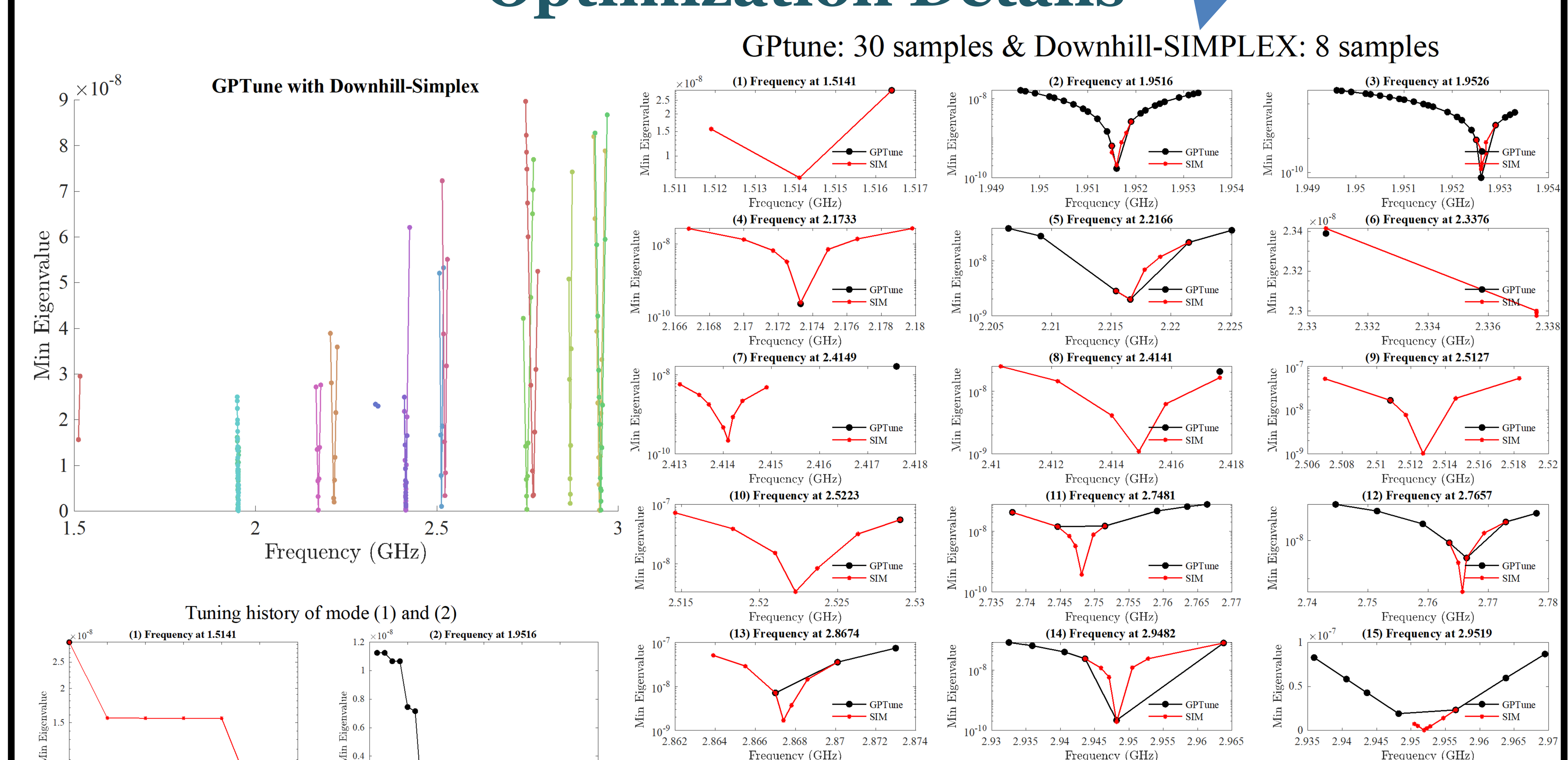
Mode vector $\boldsymbol{I}$ at f = **1.5149 GHz** (left) and f = **2.3329 GHz** (right)

Detected Frequencies			
#	GPTune	GPTune + Simplex	Omege3P
1	1.5164	1.5141	1.51
2	1.9516	1.9516	1.953
3	1.9526	1.9526	1.954
4	2.1733	2.1733	2.172
5	2.2166	2.2166	2.216
6	2.3306	2.3376	2.329
7	2.4176	2.4149	2.413
8	2.4176	2.4141	2.414
9	2.5108	2.5127	2.512
10	2.529	2.5223	2.522
11	2.7446	2.7481	2.747
12	2.7664	2.7657	2.764
13	2.867	2.8674	2.868
14	2.9482	2.9482	2.945
15	2.9482	2.9519	2.948

Above table: First 15 resonance frequencies found by GPTune, GPTune + Simplex, and the reference data from a FEM code developed by SLAC called ACE3P

The objective function plots

Optimization Details



Up Left Fig: 15 resonance modes found by GPTune+Downhill-SIMPLEX. Each color: the objective function associated with one resonance mode. **Down left Fig:** Historical best of first two resonance modes. **Above Fig:** Zoomed views.

Conclusions

- High-order modes in RF cavities need to be identified and suppressed in the design
- IE-based RF cavity modeling requires searching for resonance frequencies
- ML algorithm combining global feature of GPTune (Gaussian Process) and local feature of Downhill SIMPLEX are well-suited to locate all resonance modes with a small number of function evaluations.

Future Work

- Try finer mesh, higher order basis, more compute nodes for more accurate/expensive modeling tasks
- Combine the inner-loop eigen solver with the outer-loop multi-objective optimizer as an integrated design tool

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