Toward 3D General-Purpose Computational Quantum Electromagnetics Modeling

PURDUE UNIVERSITY

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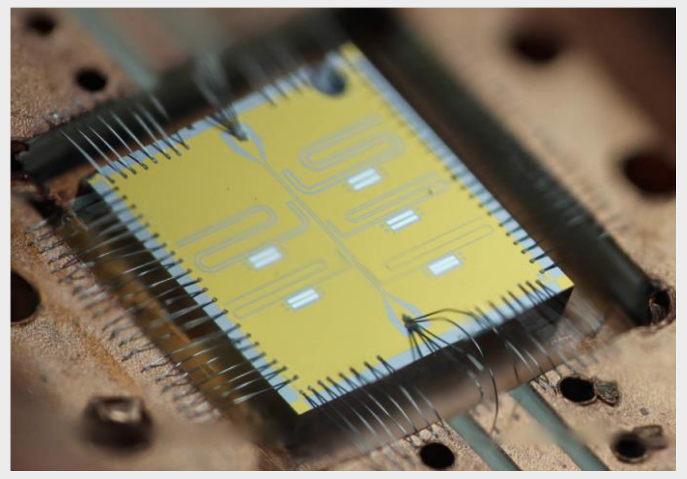
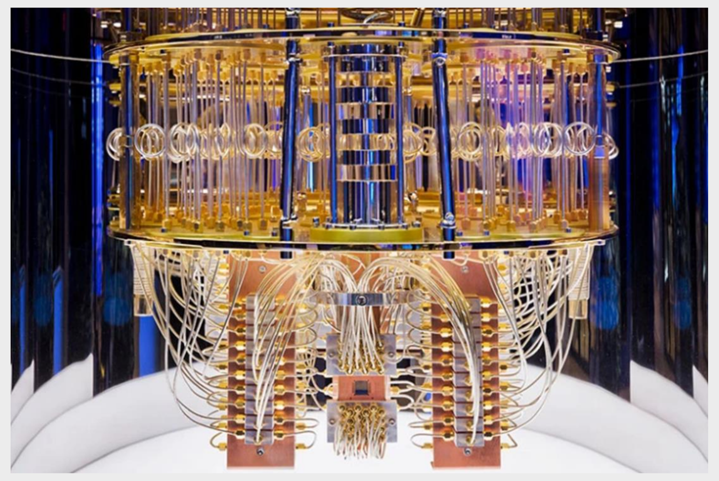
INTRODUCTION

- Developing accurate numerical methods for quantum electromagnetic (QEM) technologies is needed to successfully model their behavior



Lawrence Berkeley National Lab's multi-qubit chip



Credit: IBM

- We are developing a custom QEM simulation tool that incorporates these features:
  - **Finite element potential-based eigensolver** to characterize the 3D fields in a device [1]
  - Mesh refinement with h-adaptive and p-adaptive capability to achieve increasingly accurate solutions
  - Open quantum system dynamics via **quantum jump approach** [2]
- **Semester Goal:** build a suite of features to accurately model quantum processes, and combine them into one tool to be released as an open-source framework

FINITE ELEMENT METHOD BASICS

- The finite element method (FEM) is a flexible discretization technique that can analyze complex and arbitrary geometries with high accuracy
- For an arbitrary linear partial differential equation

Differential Operator → $\mathscr{L}\varphi = f$ ← Source Function

Unknown Solution

- The unknown solution is expanded using a set of basis functions, then the equation is integrated with a weighting function over the solution domain Ω

Basis Function

$$\int_\Omega w_i \mathscr{L}\left(\sum_{j=1}^{N} c_j v_j\right) d\Omega = \int_\Omega w_i f \, d\Omega$$

Expansion Coefficients — Unknown Solution — Weighting Function

- By making the basis and weighting function sets identical, the resulting formulation is called Galerkin's method

$$\sum_{j=1}^{N} S_{ij} c_j = b_i \qquad i = 1, 2, \ldots, N$$

- This leads to a square matrix system where the expansion coefficients can be solved for after applying the corresponding boundary conditions

Formulation from [3]

FINITE ELEMENT METHOD FORMULATION

- We are implementing a 3D FEM potential-based eigensolver for analyzing the EM fields that can exist in arbitrary cavities
- The Helmholtz wave equation can be rewritten by substituting the electric field and scalar potential with:

$$\vec{E} = i\omega\vec{A} - \nabla\Phi$$

$$\frac{1}{\mu\epsilon^2}\nabla\cdot\vec{A} = i\omega\Phi$$

$$\nabla\times\frac{1}{\mu}\nabla\times A - \epsilon\nabla\frac{1}{\mu\epsilon^2}\nabla\cdot\epsilon A = \omega^2\epsilon A$$

- Applying FEM to this formulation of the Helmholtz equation yields:

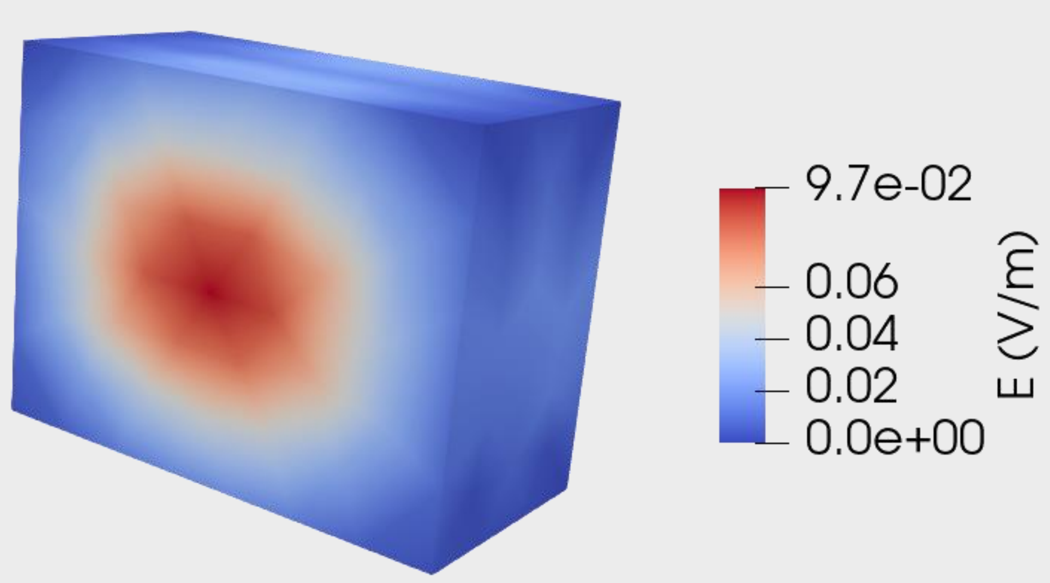
$$[K_1]\{A\} = \omega_c^2[K_2]\{A\}$$

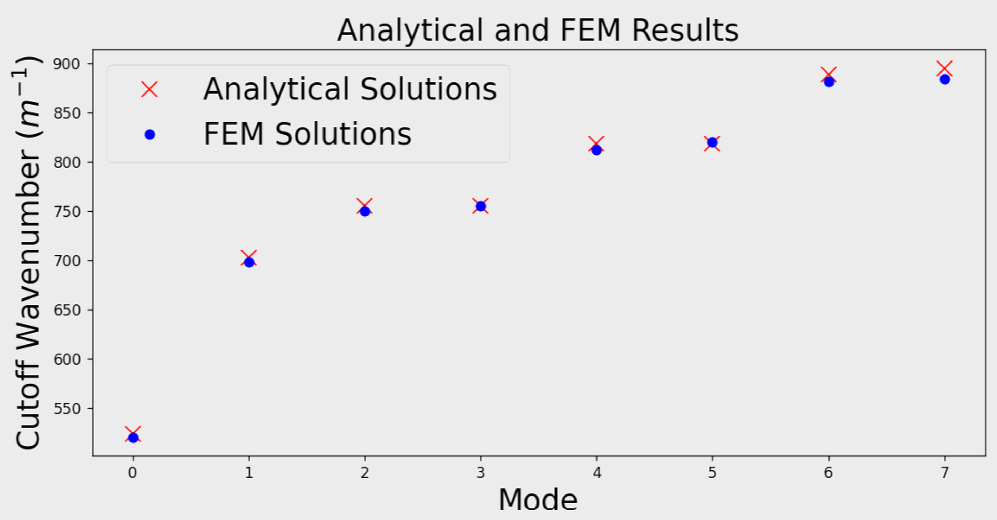
- Solving the eigenvalue problem yields the resonant frequency of a cavity mode and its corresponding spatial distribution

Analysis from [1]

FINITE ELEMENT METHOD RESULTS

- We calculated the eigenmodes for transverse magnetic (TM) and transverse electric (TE) waves





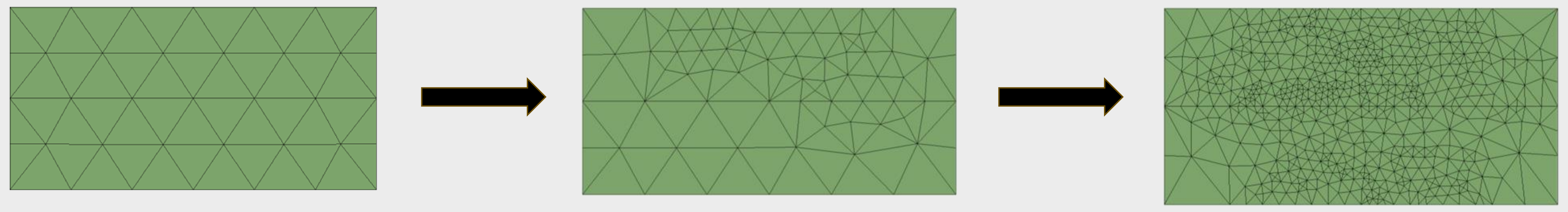
- Resulting resonant frequency reveal excellent accuracy compared to analytical solutions

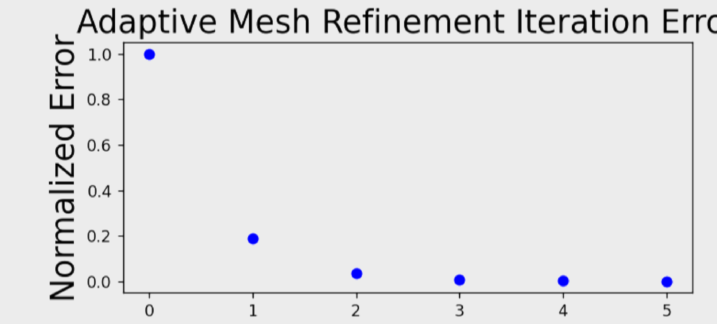
ADAPTIVE MESH REFINEMENT

- FEM can be used to calculate $\vec{E}$ and $\vec{H}$ independently to find error within each element:

$$\delta = \frac{1}{\omega W}\int\left(\vec{E}\cdot\vec{J} - \vec{H}\cdot\vec{M}\right)d\Omega,\ W = \frac{1}{2}\int\left(\epsilon\left|\vec{E}\right|^2 + \mu\left|\vec{H}\right|^2\right)d\Omega$$

- Elements with error above $\frac{1}{2}\delta_{max}$ are subdivided to minimize global error

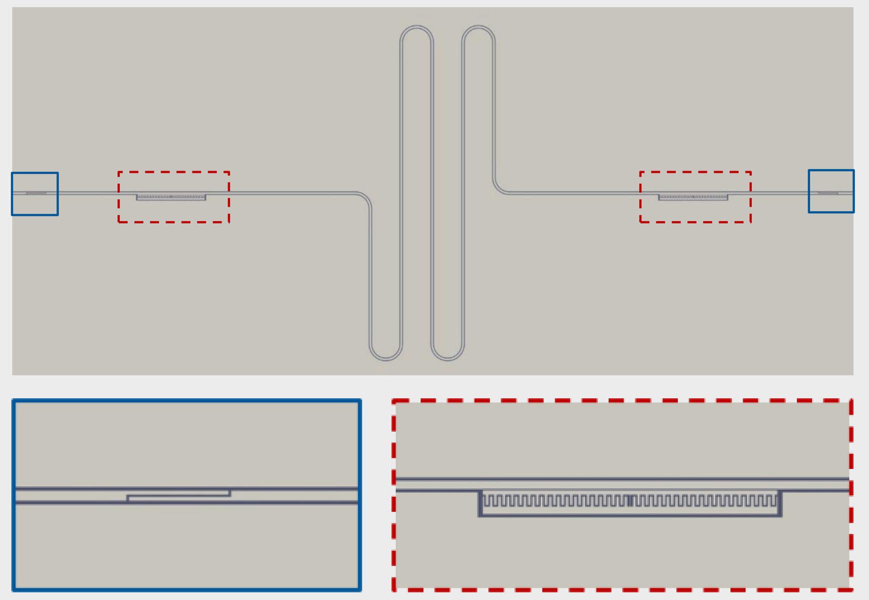


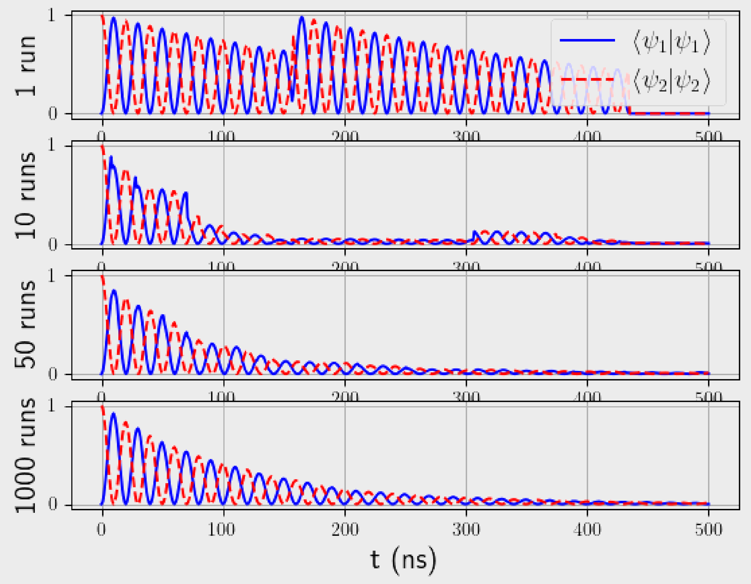


Analysis from [4]

OPEN QUANTUM SYSTEM DYNAMICS

- Open quantum system dynamics are computed by averaging quantum trajectories under the influence of stochastic quantum jumps due to noise
- Quantum trajectories are average for the two-qubit system to calculate expectation values





Analysis from [2]

CONCLUSIONS & FUTURE DEVELOPMENT

- Developed general purpose implementation of 3D FEM validated against analytical solutions
- Demonstrated efficacy of adaptive meshing
- Under development:
  - Potential-based FEM is in final stages of implementation
  - Efficiency of quantum jump approach simulation is being improved
  - A custom eigensolver will be implemented

REFERENCES

[1] Y. -L. Li, S. Sun, Q. I. Dai and W. C. Chew, "Finite Element Implementation of the Generalized-Lorenz Gauged A- Φ Formulation for Low-Frequency Circuit Modeling," IEEE Transactions on Antennas and Propagation, 2016.

[2] J.R. Johansson, P.D. Nation, Franco Nori, QuTiP: An open-source Python framework for the dynamics of open quantum systems, Computer Physics Communications, pp. 1764-1765, 2012.

[3] J.-M. Jin, *Theory and Computation of Electromagnetic Fields,* John Wiley & Sons, 2010.

[4] J. Lee, D. . Sun and Z. Cendes, "Full-wave analysis of dielectric waveguides using tangential vector finite elements," IEEE Transactions on Microwave Theory and Techniques, pp. 1267, 1991.