Toward General-Purpose Computational Quantum Electromagnetics Modeling

PURDUE UNIVERSITY

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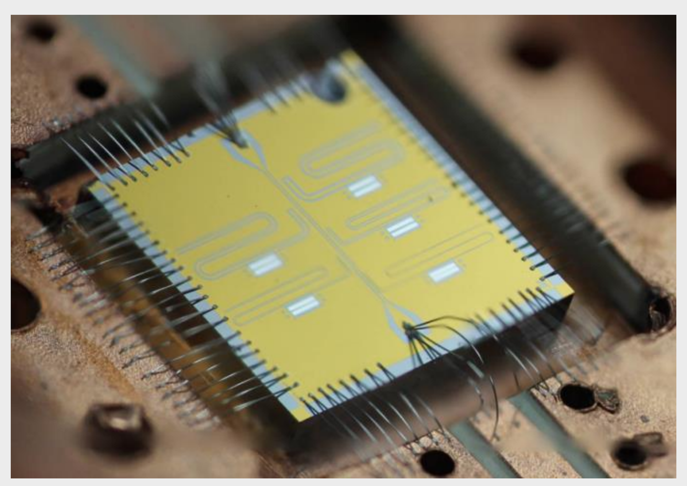
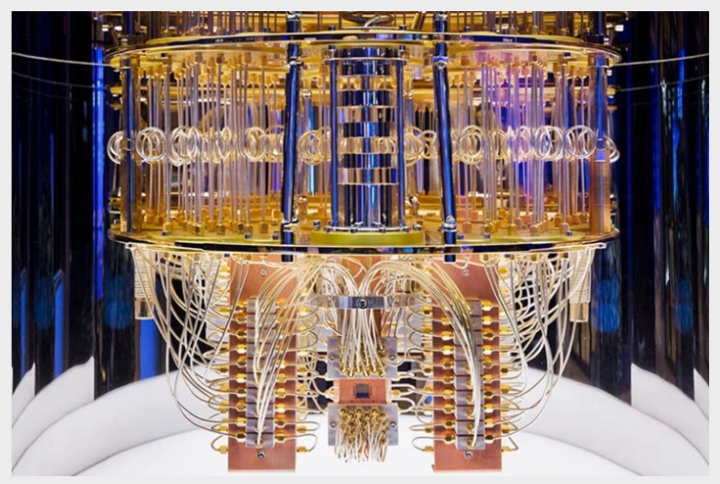
INTRODUCTION

- Developing efficient numerical methods for quantum electromagnetic (QEM) technologies is needed to successfully scale them to useful sizes [1]



Lawrence Berkeley National Lab's multi-qubit chip



Credit: IBM

- We are developing a custom QEM simulation tool that incorporates these steps:
  - **Finite element electromagnetic (EM) eigensolver** to characterize the 3D fields in a device
  - Data from the EM eigensolver is then used to **discretize a Hamiltonian** that describes the quantum interactions between EM fields and transmon quantum bits (qubits) [2]
  - A suite of **ordinary differential equation (ODE) solvers** can then time evolve the quantum states to calculate the quantum dynamics
- **Semester Goal:** build an initial capability for each step in parallel before merging into a single tool

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

$$\underbrace{\mathscr{L}}_{\text{Differential Operator}}\underbrace{\varphi}_{\text{Unknown Solution}} = \underbrace{f}_{\text{Source Function}}$$

- 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

$$\int_\Omega \underbrace{w_i}_{\text{Weighting Function}} \mathscr{L}\left(\sum_{j=1}^{N} \underbrace{c_j}_{\text{Expansion Coefficients}} \underbrace{v_j}_{\text{Basis Function}}\right) d\Omega = \int_\Omega w_i f \, d\Omega$$

Unknown Solution

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

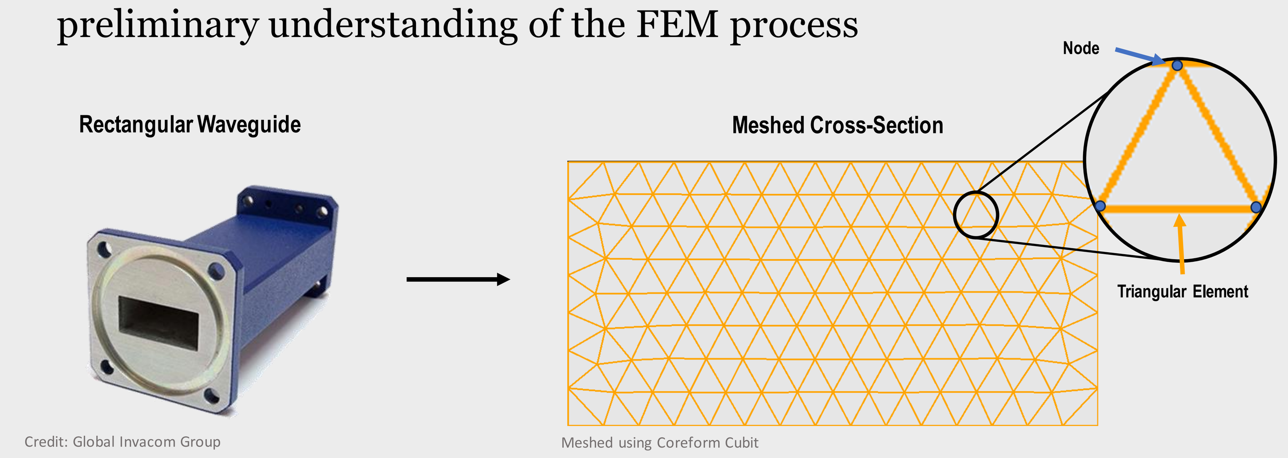
$$\sum_{j=1}^{N} S_{ij} c_j = b_i \qquad i = 1, 2, \ldots, N$$

- 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 have implemented a 2D FEM eigensolver for analyzing the EM fields that can propagate in a homogeneous waveguide, allowing for preliminary understanding of the FEM process



- Applying FEM to the Helmholtz equation of the transverse component of the electric field results in an eigenvalue problem

$$\nabla_t^2 E_z + k_c^2 E_z = 0$$

FEM

$$[A]\{E_z\} = k_c^2 [B]\{E_z\} \qquad E_z = 0 \text{ On Conducting Walls}$$

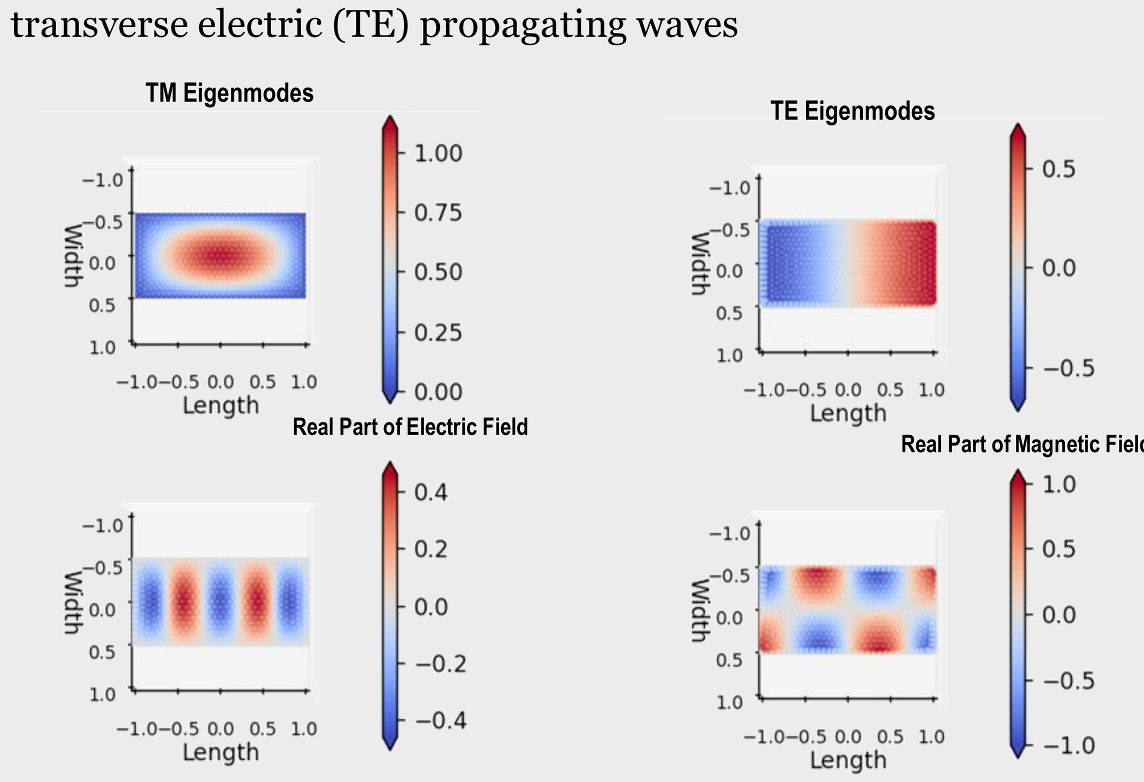
Nearby Node Interactions

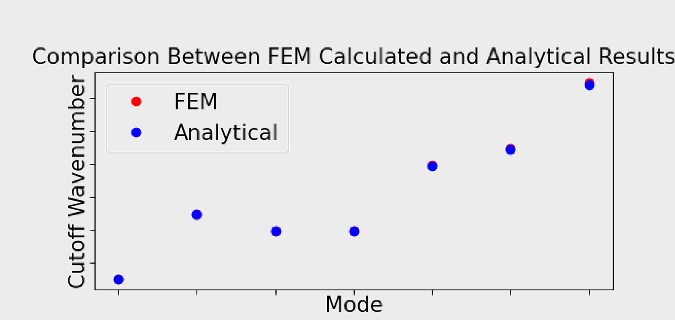
- Solving the eigenvalue problem yields the cutoff wavenumber and the corresponding field distribution for the transverse magnetic eigenmode
- The same process applies for the transverse electric eigenmodes by applying the Neumann boundary condition on the conducting walls

Analysis from [3]

FINITE ELEMENT METHOD RESULTS

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





- FEM exhibits excellent accuracy when compared to analytical solutions

HAMILTONIAN MATRIX GENERATION

- Hamiltonian operator characterizes the way that QEM fields can interact with the transmon qubits

$$\hat{H} = \underbrace{\sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k}_{\text{Electromagnetic Field}} + \underbrace{\sum_j \hbar\omega_j |j\rangle\langle j|}_{\text{Transmon Qubit}} + \underbrace{\sum_{k,j}\left(\hbar g_{k,j}\hat{a}_k^\dagger |j\rangle\langle j+1| + \hbar g_{k,j}^* \hat{a}_k |j+1\rangle\langle j|\right)}_{\text{Transmon Qubit and Electromagnetic Field Interactions}}$$ [2]

- Parameters in the Hamiltonian operator can be found from various FEM eigensolvers
  - EM field eigenvalue ω_k from EM eigensolver
  - Transmon energy eigenvalue ω_j from qubit eigensolver
  - Interaction rate $g_{k,j}$ depends on eigenvectors from EM and qubit eigensolvers
- The Hamiltonian matrix form is evaluated using the operator and initial and final basis states

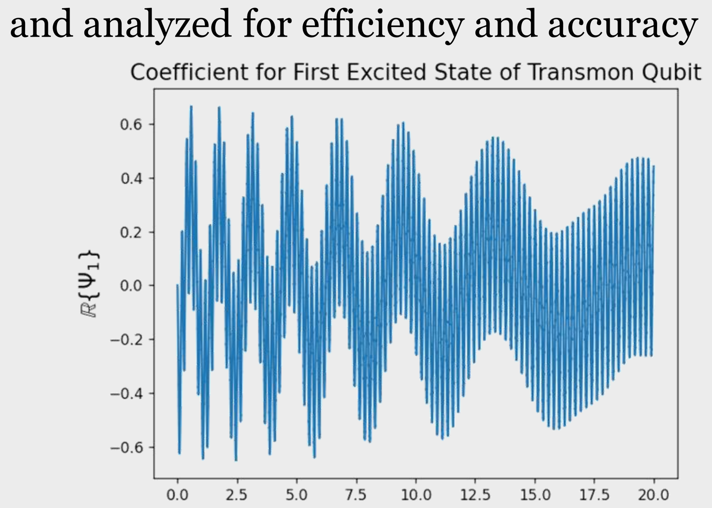
$$\begin{bmatrix} \langle f_0|\hat{H}|i_0\rangle & \cdots & \langle f_0|\hat{H}|i_j\rangle \\ \vdots & \ddots & \vdots \\ \langle f_j|\hat{H}|i_0\rangle & \cdots & \langle f_j|\hat{H}|i_j\rangle \end{bmatrix} \qquad \begin{aligned} |i\rangle &= |q_0 k_0 k_1 \cdots k_n\rangle \longleftarrow \text{initial states} \\ \langle f| &= \langle q_0' k_0' k_1' \cdots k_n'| \longleftarrow \text{final states} \end{aligned}$$

ORDINARY DIFFERENTIAL EQUATIONS SOLVERS

- Once the Hamiltonian is known, the quantum dynamics of the system can be analyzed by solving the Schrödinger equation numerically

$$\hat{H}\psi = i\hbar\partial_t\psi$$

- Various numerical solvers are being implemented and analyzed for efficiency and accuracy
  - Finite difference method
  - Runge-Kutta
    - Fixed time-step
    - Adaptive time-step
  - Bulirsch-Stoer
- Methods are being tested for their tradeoffs between accuracy and efficiency for both stiff and non stiff problems



CONCLUSIONS & FUTURE DEVELOPMENT

- Developed effective implementation of FEM for 2D waveguide demonstrating its versatility
- Initial Hamiltonian matrix generation code is functioning
- Under development:
  - Efforts are aimed towards producing 3D FEM that will be used to analyze complex QEM devices
  - Document comparison of numerical ordinary differential equation solvers
  - A custom eigensolver will be implemented
  - Finished FEM will include adaptive mesh refinement to obtain more accurate solutions

REFERENCES

[1] Z. K. Minev, Z. Leghtas, S. O. Mundhada, *et al.*, "Energy-participation quantization of Josephson circuits," *npj Quantum Information* 7, 131, 2021.

[2] T. E. Roth and W. C. Chew, "Macroscopic circuit quantum electrodynamics: A new look toward developing full-wave numerical models," *IEEE Journal on Multiscale and Multiphysics Computational Techniques*, vol. 6, pp. 109–124, 2021.

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