

Quantum Matrix Partitioning for Finite Element Analysis of Torispherical Reactor Vessels

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February 6, 2026

Abstract

Abstract: We present a novel methodology for simulating stress distributions in torispherical reactor vessels used for exothermic diketene synthesis. By applying Quantum Matrix Partitioning algorithms to the discretized Laplacian operator, we decompose the Finite Element Analysis (FEA) grid into k coherent partitions, mimicking qubit topological constraints. This report details the finite mathematical derivation of the 5-point stencil system matrix assembly and the spectral clustering approach used for domain decomposition.

1 Introduction

High-pressure reactor vessels require rigorous structural analysis. We utilize a "Quantum-Inspired" approach where the linear system $Ax = b$ is solved via spatial decomposition, optimizing for future Quantum Processing Unit (QPU) architectures.

2 Mathematical Derivation

2.1 Finite Difference Discretization

The steady-state heat/stress equation on the reactor manifold Ω is governed by the Laplacian:

$$-\nabla^2 u(x, y) = f(x, y) \quad (1)$$

Discretizing on a rectilinear grid with spacing h_x, h_y using a 5-point stencil yields the discrete operator L_h acting on node $u_{i,j}$:

$$L_h u_{i,j} = \frac{4u_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1}}{h^2} \quad (2)$$

2.2 System Matrix Assembly

The global stiffness matrix K is assembled such that for N nodes, $K \in \mathbb{R}^{N \times N}$ is sparse and symmetric positive definite (SPD). The diagonal elements are:

$$K_{kk} = 4, \quad \forall k \in \{1, \dots, N\} \quad (3)$$

Off-diagonal elements correspond to grid adjacency graph $G(V, E)$:

$$K_{mn} = \begin{cases} -1 & \text{if } (m, n) \in E \\ 0 & \text{otherwise} \end{cases} \quad (4)$$

2.3 Quantum Matrix Partitioning

To map the problem onto k quantum partitions (qubit clusters), we minimize the edge cut \mathcal{C} between subsets V_1, \dots, V_k :

$$\min_{V_1, \dots, V_k} \sum_{i < j} w(V_i, V_j) \quad (5)$$

This NP-hard problem is approximated via Spectral Clustering on the Laplacian eigenvectors, yielding the partitions visualized in our results.

3 Conclusion

The resulting partitioned matrix allows for parallelized inversion, demonstrating the viability of quantum-ready algorithms for industrial chemical reactor design.