– Quantum Computing – Promise of a New Future for Computational Mechanics

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Over the past several decades, computational mechanics heavily relied on advances in semiconductor-based computing technology to solve increasingly complex mechanics and multi-physics problems. As transistors approach their physical limits, the advancement in "classical" computing technology no longer follows the celebrated "Moore's Law" – hence the expected speed-up and scaling in mechanics computations due to hardware improvements have stagnated (*Figure 1a*).

This stagnation underscores the necessity for alternative computing paradigms that are being currently developed such as in-memory computing [Sun et al. (2023)], neuromorphic computing [Kudithipudi et al. (2025)], biological computing [Grozinger et al. (2019)] among several others. Quantum computing (QC) emerges as a viable solution, leveraging the principles of quantum mechanics to perform computations that would be infeasible on classical systems.

While measurable impact on everyday mechanics computing is still some time away, QC is a very rapidly developing field. Qubit and gate scalability, and circuit depth are increasing at an impressive rate [IBM (2024)]. Moreover, developments in quantum error mitigation and correction algorithms are progressively enhancing the reliability of quantum computations. These rapid hardware improvements are bringing practical applications of QC in engineering fields closer to reality.

Unlike classical binary systems that utilize bits as the smallest unit of data, QC relies on quantum bits or qubits. Qubits exhibit unique properties such as superposition (existing in multiple states simultaneously) and entanglement (inherent link between the states of multiple qubits regardless of physical distance between them) that do not exist in classical devices. These characteristics enable quantum systems to store, process and analyze large datasets exponentially faster than classical systems.

These advancements not only promise increased computational power but also a new class of computational algorithms needed to evaluate mechanics problems at scale. Establishing high fidelity digital twins, predictive multiscale computations, and reliable machine learning models require both the computational power

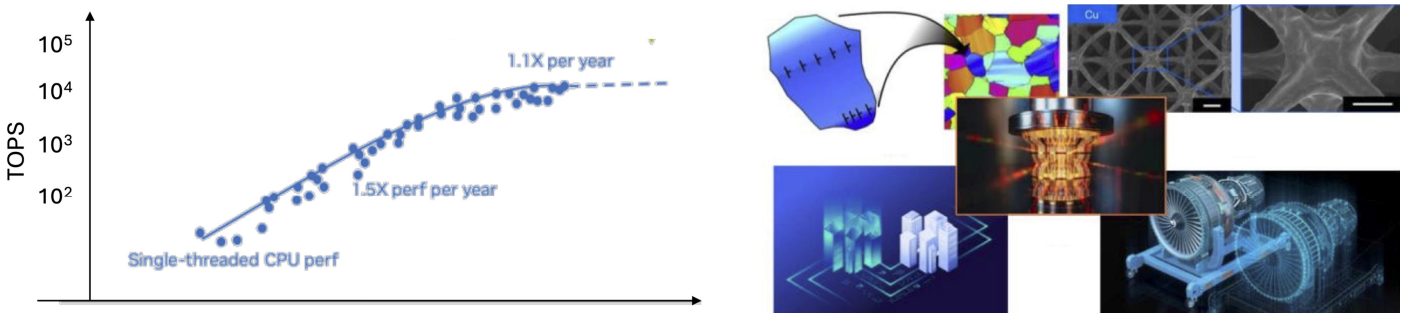

Figure 1:
(a) Moore's law no more – loss of scalability in transistor and hence speed-up since 2010s. TOPS: Terra operations per second.
(b) technology pull for quantum computing in computational mechanics – multiscale modeling; digital twins.
Figure sources: (a) NVIDIA; (b) top left: Montagnat et al. (2014); bottom left: AZoBuild; center: Live Science; top right: Saccone et al. (2022); bottom right: Pvplive.

and the algorithmic scale up promised by QC (*Figure 1b*). Optimization problems prevalent in structural mechanics, materials science, and fluid dynamics are also prime candidates for quantum algorithms, which could outperform their classical counterparts. A shift away from classical architectures heralds a new era where complex simulations can occur in real-time, responsive to live data, and under various constraints.

Quantum algorithms for mechanics –

A key development that prompted interest from computational community is the availability of quantum solver algorithms for linear systems of equations that exhibit exponential scaling compared to existing classical algorithms. Harrow-Hassidim-Lloyd (HHL) [Harrow et al. (2009)] is considered the foundational quantum algorithm for linear systems, which has polylogarithmic complexity in terms of system size, compared to polynomial complexity of classical iterative solvers.

Subsequent research has led to the development of other algorithms and improvements that extend their applicability and efficiency. More recent quantum linear system solvers exhibit polynomial complexity with sparsity, condition number, and polylogarithmic complexity with inverse of error tolerance, and with system size dependence only through block encoding [Morales et al. (2025)]. The general framework for use of such linear systems in the context of finite element (or other) methodologies lie in efficient encoding of the system properties (i.e., the stiffness matrix and the force vector) such that the exponential scaling of the solvers could be leveraged.

The quantum linear system solvers mentioned above are designed to operate on error-corrected (i.e., fault tolerant) quantum computers. Existing systems remain to be noisy (hence the terminology "noisy intermediate scale quantum" or NISQ era). The variational quantum linear solver (VQLS) algorithm relies on hybrid computers and more amenable to computations using available NISQ devices [Bravo-Prieto et al. (2020)].

In VQLS, the solution of the linear system is posed as an optimization problem, where a cost function is minimized using classical optimization algorithms (in a classical computer). The function, and if needed, Jacobian and Hessian are computed in a quantum computer. This approach has recently been deployed to solve a limited number of solid and structural mechanics problems [Liu et al. (2024), Lu et al. (2023), Trahan et al. (2023)].

In addition to quantum algorithms that rely on linear system solvers, alternative approaches are also being investigated including iterative solvers [Raisuddin and De (2024)], quantum Fourier transform [Liu et al. (2024)], Hamiltonian simulations [Sato et al. (2024)], quantum annealing [Raisuddin and De (2022)] among several others.

There is also a growing literature on quantum algorithms for evaluating nonlinear partial differential equations (PDEs). In view of the fundamentally linear nature of quantum systems, many of the proposed algorithms rely on linearization of the underlying nonlinear PDE system. One approach is direct mapping of the nonlinear PDE to a linear PDE by using the level set method [Jin and Liu (2024)].

The second and more common approach relies on semi-discretization (i.e., spatial) of the underlying PDE to obtain a discrete nonlinear ordinary differential equation (ODE) system, linearization of the ODE system, and evaluation of the linearized ODEs with an established quantum ODE solver (e.g., Lloyd et al. (2020), Costa et al. (2023)). Spatial discretizations have so far (almost exclusively) relied on strong form finite difference method, which naturally places restrictions on domain morphology and the grid structure. Two approaches to ODE linearization are the Carleman method (e.g., Gnanasekaran et al. (2024), Krovi (2023)), which replaces a nonlinear term that is a polynomial of the cardinal variable with an infinite linear series; and the Koopman-Von Neumann approach (e.g., Jin et al. (2023),Tanaka and Fujii (2025)) which maps the nonlinear ODE to Hamiltonian dynamics via observables (i.e., functions) of the cardinal variable.

An early finite element implementation

We recently began exploring a quantum computing implementation of the finite element method named the Quantum Finite Element Method (Q-FEM) [Arora et al. (2025)]. QFEM is a methodology for implementing finite element analysis on noisy intermediate-scale quantum (NISQ) computers based on the variational quantum linear solver (VQLS) algorithm.

We developed a framework that leverages classical FEM procedures to decompose stiffness matrices into unitary operations and design explicit quantum circuits that maintain the structure of traditional FEM discretization, allowing for element and material coefficient variability.

The key contributions of the new implementation include a novel methodology for unitary decomposition of the global stiffness matrix leveraging the classical FEM construction procedure; a systematic approach to generate quantum circuits corresponding to the unitaries for linear and quadratic elements; a framework that allows for variable element lengths, material coefficients, and different boundary conditions; and introduction of the concept of "identical non-interacting elements" that reduces the number of required unitaries. Reduction of the unitary matrices do come with a price, the circuit depths and circuit complexity increases, albeit linearly with respect to the number of identical non-interacting elements.

VQLS for FEM

The overall methodology of the QFEM approach using the VQLS algorithm is summarized in *Figure 2*.

The methodology consists of three steps:
(1) preparation of quantum circuits needed in the cost function evaluations,
(2) execution of the VQLS optimization in a hybrid computer, and
(3) extraction of the solution following successful completion of the algorithm.

In the first step, the stiffness matrix is represented using a linear combination of unitary matrices, the quantum circuit associated with each unitary matrix is constructed. The force vector, typically an arbitrary vector is prepared using a state preparation algorithm. We note that efficiency of force vector preparation typically relies on knowledge of the structure (e.g., sparsity) of the force vector, since state preparation is a computationally complex operation. In this step, the circuit that represents the chosen variational ansatz is also prepared.

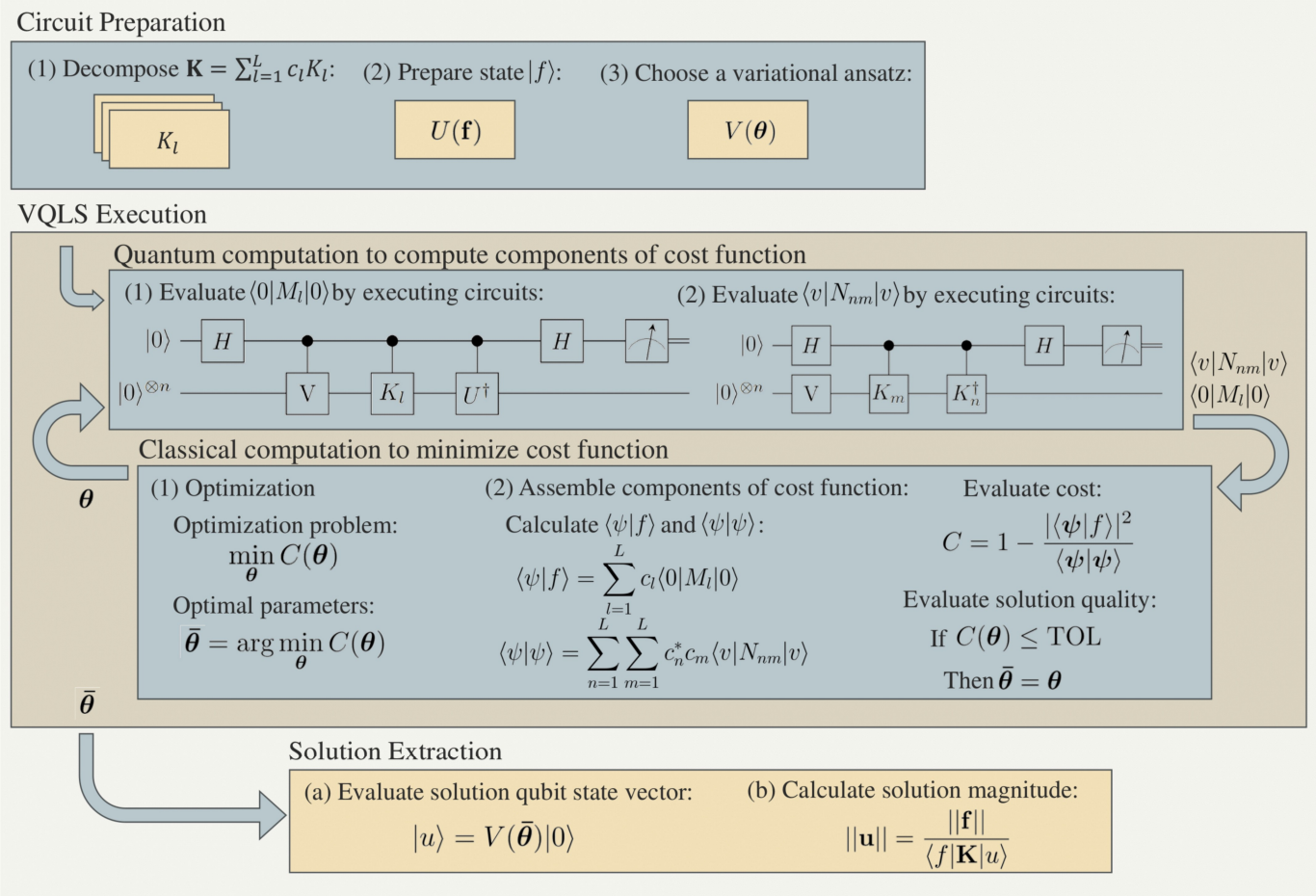

Figure 2:
The overall methodology for the variational quantum linear solver applied to a finite element problem. Figure reproduced from Arora et al. (2025).

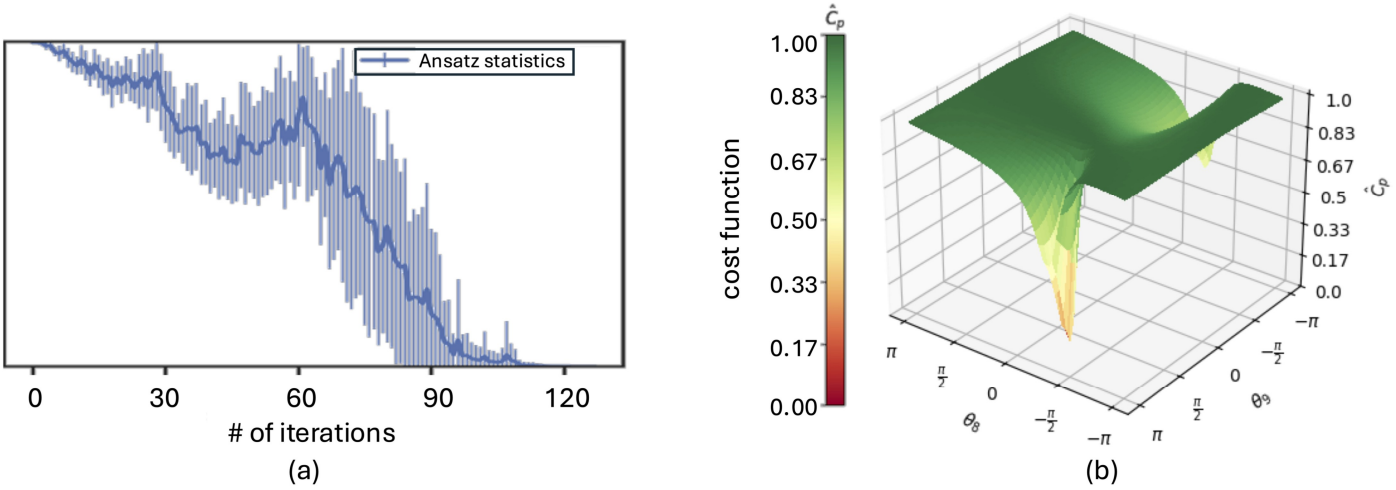

Figure 3:
(a) statistics of cost function evaluation with number of iterations;
(b) cost function topology that demonstrate deep gorges and plateau regions.
Figures reproduced from Arora et al. (2025).

In the second step, a classical optimization is performed using a hybrid (quantum–classical) computer to minimize the cost function. The variational ansatz parameterizes the space within which the cost function is minimized. The selection of the form of variational ansatz and the associated parameterization is important as this selection defines the topology of the cost function space.

Naturally, the ability of the selected classical optimization algorithm to find the cost function minimum (and the rate at which it finds it) is directly related to the cost function topology. Components of the cost function as well as the gradients of the cost function are performed in the quantum computer using the Hadamard test or other Hamiltonian expectation estimation techniques. The cost function is then assembled in the classical computer, where the search direction is computed by the optimization algorithm. Upon convergence, the optimized variational ansatz parameter set is used to obtain the solution vector (third step).

It is important to note that the aforementioned process only computes the direction of the solution vector as the state vector of the main qubit register. The magnitude of the solution vector is also computed in the post processing step.

Efficient Unitary/Circuit Construction

While there are several ways of generating unitary representation of the stiffness matrix such as block encoding or Pauli decomposition, in the absence of knowledge of the specific sparsity structure, they are computationally expensive. In the most general case, complexity of Pauli decomposition of a matrix with unknown sparsity structure is exponential. Such an approach cannot compete with classical finite element algorithms. In this study, we presented an approach to leverage the well-known finite element construction procedure in efficiently constructing the unitary decomposition of the stiffness matrix.

The proposed approach relies on two concepts. The first is the use of direct stiffness assembly: the stiffness matrix is expressed as a simple sum of “global” versions of the element stiffness matrices, where the local-global mapping is applied on element stiffness matrices. These are very sparse matrices which can be trivially represented by a unitary decomposition.

The second concept is the automated generation of the circuit representations of the unitaries. This is achieved through the concept of generator functions, which map the unitaries associated with each element to quantum circuit generators.

“ … the ability of the selected classical optimization algorithm to find the cost function minimum (and the rate at which it finds it) is directly related to the cost function topology. ”

In order to further reduce number of unitaries in the stiffness matrix decomposition, we introduce the concept of identical non-interacting elements. Two elements that are identical non-interacting have the same element stiffness matrix, but do not interact with each other (i.e., they are physically not neighboring elements). This allows concatenation of the corresponding circuits. We note that the circuit depth increases linearly with the number of non-interacting elements.

This approach could significantly simplify the unitary decomposition especially in meshes that are structured in parts of the problem domain.

Some Results and Discussion

We have assessed the capabilities of the Q-FEM approach in the context of a steady state heat equation discretized using linear and quadratic elements, in the presence of Dirichlet and Neumann boundary conditions, and with homogeneous and heterogeneous material constants. Q-FEM successfully converges to correct solutions for various problems and model discretizations, and the approach works effectively with variable element lengths, coefficients, and boundary conditions.

Figure 3a shows the statistical (i.e., the evolution of mean and the standard deviation) evolution of the cost function of a suite of simulations. The difference between simulations in the suite is the random initial ansatz parameter state. For any individual simulation, we observe a highly oscillatory convergence pattern, which points to the complexity of the cost function topology. The mean of the simulation ensemble demonstrates a relatively monotonic convergence behavior. A field plot of a cost function subspace near the optimal point when two of the ansatz parameters are varied indicates some of the features of the cost function topology. We observe that the topology is rather flat generally with hidden valleys and narrow gorges within which the optimal point is located *(Figure 3b)*. As the size of the problem is increased, the cost function topology further flattens over large swaths of the parameter hyperspace leading to what is commonly known as the "barren plateau" problem [Cerezo et al. (2021)].

These features of the cost function topology point to the importance of appropriate ansatz and optimizer selection in quickly achieving the optimal solution.

The Path Ahead –

QC is a very fast-moving field that promises to potentially make a step change in the state of computing. Computational mechanics is set to gain significantly from QC, and there is a tremendous opportunity to introduce a completely new way of thinking to algorithm development in computational mechanics.

However, quite a lot is yet to be done before tangible impact is observed in academic and industry applications both from the hardware and software perspectives. QC software stack is not yet available to perform high level computations that are hardware blind and that rely on existence of tools that are typically taken for granted (e.g., general purpose linear solvers, matrix-vector operations, etc.). The existing hardware computes with significant noise and bias that limit demonstration of algorithm efficacy on real devices.

Despite these and many other challenges, this is the right time for the computational mechanics community to become part of the quantum computing revolution.

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