

Quantum Genesis Priority Applications

Introduction

As part of the Quantum Genesis Mission, the Department of Energy (DOE) is leading the creation and deployment of *scientifically relevant* quantum computers (SRQCs). SRQCs refer to fault-tolerant quantum computers that move past hardware demonstrations and solve problems of interest to DOE’s scientific mission and its supported communities, where the relevance lies in the result itself, not the machine that produced it. These computers will represent a monumental leap beyond current capabilities and provide a powerful new tool for the next decade of scientific discovery.

This document identifies *Quantum Genesis Priority Applications* (QGPAs) to serve as beacons for the community, providing a concrete basis for judging the “scientific relevance” of quantum computers, coordinating the hardware, software, and domain science R&D needed to achieve the goal, and making meaningful domain science advances not otherwise possible today. Progress on these applications will require a clear understanding of resource estimation and optimization, integration into the scientific workflow, and performance benchmarking against the best-known classical alternatives.

This document draws heavily from roadmaps produced by the DOE Laboratory Quantum Supercomputing Blueprint Team¹ and by the leadership of the DOE National QIS Research Centers. Additionally, the structure of this effort draws on DOE’s prior publications of the Genesis Mission National Science and Technology Challenges.²

Application Structure

Four primary *domains* have been identified for short-to-medium-term (within five years) scientific relevance: chemistry, materials, subatomic physics, and applied mathematics. This should not be taken as a statement that other domains are not of interest either to DOE or to the scientific community, nor is it a judgment on the usefulness of quantum computers for other purposes. Additionally, the order of the domains does not imply any form of priority.

Within each domain, the QGPAs are identified corresponding to specific thematic barriers. Each application points toward a particular problem type where there is a strong scientific basis to believe that classical computers face fundamental scaling challenges that

¹ <https://doi.org/10.2172/3022533>

² <https://www.energy.gov/documents/genesis-mission-science-and-technology-challenges>

quantum computers can overcome. For instance, under “Materials” is included the application of “Dynamics of Materials Driven Out-of-Equilibrium and in Extreme Environments” – not a specific system to study but a class of problems with shared structure and common barriers.

Within each application, a short list of example targets is provided. These are individual uses or simulation campaigns that are appropriate for use by a quantum computer to demonstrate or benchmark that a quantum computer is responding to the QGPA. Example targets are intended to be early-stage exemplars from scalable families of problems that could form a deep basis for future work as quantum computing hardware and software becomes more capable. Rather than specific target numbers for problem sizes, applications attempt to identify problems where small demonstrations would be feasible on the first generation of scientifically relevant quantum computers. These example targets are not intended to be exhaustive, and as the Quantum Genesis Mission continues, participants and practitioners will discover other attractive target problems and figures of merit. At the end of this document is a description of some promising areas where the science of quantum computing applications is not yet mature enough to firmly spotlight.

Domain 1: Chemistry

A fundamental goal of chemistry is to predict and control chemical transformations across electronic, atomic, and molecular scales. Accomplishing this objective requires accurate treatment of electron correlation in quantum many-body systems, a task that exceeds the reach of classical computation as systems grow in size and complexity. For this reason, chemistry has long been viewed as a natural target for quantum computing, which promises a path beyond classical limits by directly representing quantum degrees of freedom.

Chemical transformations occur under structurally complex and dynamically evolving conditions. Reconciling this complexity with the need for accurate treatment of strongly correlated electronic structure remains a central challenge and one for which quantum computing could play a critical role. Within the chemistry domain, two thematic applications are identified that offer both near-term and long-term opportunities: **reaction mechanisms** and **reaction dynamics**.

Application 1.A: Reaction Mechanisms in Complex Chemical Systems

Application Description

Understanding how the surrounding environment influences reaction pathways and energetics establishes a basis for controlling chemical transformations. Approximate approaches such as density functional theory (DFT) have enabled major progress in

describing reaction mechanisms in realistic environments across a wide range of DOE-relevant applications. However, accurate treatment of systems with strong electron correlation has largely remained confined to idealized settings because of the steep computational cost. Quantum computing may offer a distinct advantage by extending systematically accurate quantum-state descriptions beyond isolated benchmarks and toward chemically realistic settings. One potential route is through hybrid quantum-classical approaches that combine tractable, conventional computational descriptions of the broader chemical environment with high-accuracy treatment of strongly correlated subspaces on quantum computers. These descriptions must be integrated within a consistent framework capable of accommodating structural changes and dynamical evolution.

Solving this challenge will allow researchers to describe chemical reaction mechanisms that cannot be modeled with sufficient accuracy today, with potential applications in photochemistry, catalyst design, and biochemistry, among others.

Example Targets

- Calculate experimentally relevant properties of strongly correlated catalytic or redox centers embedded in complex chemical or biomolecular environments, such as transition-metal active sites in catalysts or metalloproteins.
- Predict competing reaction pathways, free-energy landscapes, and selectivity for chemical and biochemical processes involving strongly correlated electronic states.
- Characterize the interplay between correlated electronic states and local or long-range structural reorganization, including conformational gating and cooperative changes that influence reactive-site energetics and function.

Application 1.B: Reaction Dynamics in Complex Chemical Systems

Application Description

To understand how chemical transformations unfold in complex systems requires the ability to simulate and model the real-time dynamics of chemical reactions. Typical reaction dynamics simulations rest on two approximations: describing the electronic structure with approximate methods such as DFT and propagating the nuclei adiabatically on a single potential energy surface. Both approximations break down as nuclear motion couples closely spaced electronic states and strong electron correlation is important, a regime relevant across many photochemical, catalytic, electrochemical, and biochemical transformations. Quantum computing offers a promising path forward for treating coupled electronic and nuclear dynamics in strongly correlated systems, enabling nonadiabatic effects to be addressed within a unified framework. The applications here mirror those of the previous area, as dynamical propagation of the reactive regions must be integrated with

the broader system through reduced representations in a manner that remains valid throughout the dynamical evolution.

Solving this challenge would enable predictive simulation of chemical dynamics under realistic conditions, providing new capabilities to understand and ultimately control chemical transformations.

Example Targets

- Understand how coupled electronic and nuclear dynamics govern state-to-state transitions, passage through conical intersections, and branching among competing reaction pathways and products, as encountered in excited-state chemistry.
- Determine how strong electron correlation and nuclear motion jointly control charge transfer, proton-coupled electron transfer, and other nonadiabatic chemical processes in reactive transformations involving multiple electronic states.
- Characterize the dynamical response of strongly correlated systems to excitation, ionization, or redox perturbations, including changes in populations, electronic correlations, and relaxation pathways relevant to nonequilibrium molecular processes.

Domain 2: Materials

The study of materials is the study of how individual constituent atoms and molecules come together to form nanoscale to macroscopic structures and how they determine their properties. Common physical properties of interest are electronic, mechanical, thermal, structural, interfacial, and topological properties controlled by the electronic band structure. Often defects have large effects on these, except when topologically protected. Materials scientists must understand the motion and interaction of the nuclei, as well as the complicated interactions and emergent behavior of the lighter, more mobile electrons, to predict the nature of current materials and engineer the next generation of materials. At the frontier of quantum materials, many-body quantum interactions present significant challenges to classical computers for making progress in understanding these systems. In the materials domain, two challenges are identified for materials: **equilibrium and ground state of quantum materials** and **dynamics of materials driven out-of-equilibrium and in extreme environments**.

Application 2.A: Equilibrium and Ground State of Quantum Materials

Application Description

New phases of matter emerge at low and even at absolute zero temperature when many-body quantum interactions or long-range entanglement are strong between electrons. DFT

and other first-principles methods, using classical computers, are limited to either weak interactions, mean-field approximations, quantum embedding methods, or small system sizes. As a result, the nature of the equilibrium ground state solution may be unknown when many-body interactions and quantum effects are significant, as in high-temperature superconductors, Mott insulators, and quantum spin liquids, where effective weak-interaction and short-range entanglement descriptions break down. Quantum computing may allow complicated spatial structures of striped antiferromagnetic phases, superconductivity, or entanglement spin disorder to be simulated directly for large lattice sizes, with the possibility of accessing properties that may be difficult or impossible to examine with current computational and experimental techniques, by naturally representing the full Hilbert space of electron correlations.

Solving this challenge would enable researchers to enhance their understanding of complex quantum materials. This could allow scientists to better understand phenomena like high-temperature superconductivity and topological materials with potential applications in energy and computing technologies by using parameters that correspond to current or planned experiments.

Example Targets

- Compute the ground state energy and energy gap of the doped Fermi-Hubbard model, including at half filling for multi-orbital interactions on lattice sizes beyond what is currently possible with classical computers.
- Simulate the Kitaev quantum spin liquid on a perturbed 2D honeycomb lattice (deformed lattice or Heisenberg interaction included) and show that long-range entanglement arises, consistent with topological order and the existence of Majorana fermions.

Application 2.B: Dynamics of Materials Driven Out-of-Equilibrium and in Extreme Environments

Application Description

Researchers can apply external fields and forces to drive materials out-of-equilibrium and manipulate their structural, topological, electronic, and magnetic symmetries. This opens unprecedented opportunities to discover and exploit nontrivial properties for fundamental research and future technologies. However, calculating dynamics in materials, particularly in quantum materials, is one of the most demanding problems in computational physics. In addition to the large number of interacting electrons, out-of-equilibrium states typically exhibit high degrees of entanglement, causing many classical computing platforms to hit

the so-called entanglement wall. Quantum computers can overcome these challenges by directly representing non-classical states in the quantum processor.

Solving this challenge with quantum computers will enable the exploration of distinct dynamical signatures in quantum materials. These include accessing and characterizing topological phases of matter, probing light-induced superconductivity, resolving excitonic and phononic dynamics, and performing Floquet engineering to tailor driven, non-equilibrium phases of matter. By directly representing highly entangled, non-classical states, quantum computers can reveal dynamical signatures that are inaccessible to classical simulation methods, thereby opening pathways for understanding and controlling quantum materials under strong external driving.

Understanding how matter behaves under extreme external driving through quantum computation is also of great interest. Insights from these studies can support the development and optimization of materials capable of functioning in extreme environments, such as those found in future fusion energy devices.

Example Targets

- Compute the chiral edge dynamics of Kitaev quantum spin liquids to test the conditions required for topological stability and observe distinct dynamical signatures of topological phases in matter.
- Simulate the behavior of light-induced superconducting states under driving in a Fermi-Hubbard model to study the microscopic pairing mechanism without classical approximations.
- Simulate the polaron formation and transport using the Holstein Hamiltonian to track real-time transitions of polarons.
- Simulate Floquet engineering on a disordered spin system and observe the stabilization of exotic quantum states.
- Compute the stopping power of a plasma-facing material under fusion-relevant conditions.

Domain 3: Subatomic Physics

At very small scales, such as those encountered in nuclear and particle physics, quantum effects become inescapable. Computing the structure and behavior of nuclei requires calculations to treat dozens of interacting particles, posing challenges to classical physics and opening opportunities for quantum computing. In addition to many-body quantum physics effects, proper treatment of physics in these domains often requires the use of quantum field theory. One such field theory of particular relevance to DOE applications is

quantum chromodynamics (QCD), the theory of the strong force that binds quarks and gluons into hadrons such as protons and neutrons and ultimately into nuclei. Physicists have developed the techniques of *lattice gauge theory* (LGT) to perform QCD calculations. As a result of computations like these, physicists have been able to determine hadron masses, decay constants, and quark masses. LGT calculations represent a significant fraction of supercomputing demand, approximately 19% of computational effort at NERSC, but there are barriers to what can be accomplished even with this expenditure of computing power. In this domain, three types of problems are identified that classical computers struggle with where quantum computers may allow for new breakthrough: **dynamics of strongly-interacting matter, physics at high density, and nuclear structure.**

Application 3.A: Dynamics and Thermalization of Strongly-Interacting Matter

Application Description

The success of conventional classical supercomputing in predicting the properties of matter relies on its use of Monte Carlo sampling techniques, but these sampling techniques are limited in their ability to represent dynamic processes. To avoid the path-integral formalism and associated sign problem that underlies classical techniques, the simulation must be done in a Hamiltonian simulation formation. Classical simulation of Hamiltonian time evolution is difficult in general but is native to the quantum computing framework and one of the best-studied quantum computing primitives. While classical-statistical lattice simulations have made progress, they are approximations. A quantum computer, by its nature, can directly simulate the unitary time evolution of the quantum state without such approximations.

Solving this challenge will allow the understanding of how isolated quantum systems, far from equilibrium, evolve and eventually thermalize, such as during the formation of quark-gluon plasmas or the early universe. Researchers would be able to calculate thermalization times, transport coefficients (like shear viscosity), and the evolution of entanglement from first principles, with possible applications in studying fundamental fusion reactions.

Example Targets

- Observe the production of light quark-antiquark pairs through string breaking in a 2+1D SU(3) lattice.
- Compute the energy-energy correlations of a pure SU(3) lattice gauge theory in 1+1D.
- Track the growth in entanglement entropy as a simplified gauge theory (e.g., 1+1D SU(2) or QED) thermalizes from a far-from-equilibrium initial state.

- Compute a key transport coefficient, such as the shear viscosity to entropy density ratio, for a strongly coupled system by simulating its response to a perturbation.

Application 3.B: Physics at High Density

Application Description

Lattice gauge theory has been instrumental in exploring the behavior of QCD at extreme temperatures and densities. These calculations have established that the transition from a gas of hadrons to a deconfined quark-gluon plasma—a state of matter that existed in the early universe—is a smooth crossover rather than a sharp phase transition at near-zero baryon density. However, in addition to being troubled by the move to real-time dynamics, many quantum Monte Carlo techniques experience substantial challenges when considering a system with high particle density. The addition of the chemical potential term that arises in this case leads again to sign problems that are difficult to address classically. By avoiding sign problems, quantum computers can address the challenge of simulating how matter behaves in these extreme environments.

Solving this challenge will provide crucial theoretical support in interpreting the results of experimental programs at facilities like the Relativistic Heavy Ion Collider (RHIC) and the Large Hadron Collider (LHC). This will help DOE researchers understand how matter behaves in conditions that are typical in stars, in heavy-ion colliders, and in the early universe.

Example Targets

- Simulate the QCD phase diagram at a range of temperatures and densities, extracting the chiral condensate at each point, in one dimension, identifying potential critical points or novel phases.
- Simulate the collective flavor oscillations of neutrinos at an astrophysically relevant point in parameter space, computing the time evolution of entanglement in the flavor degrees of freedom.

Application 3.C: Nuclear Structure and Interactions

Application Description

A detailed, first-principles understanding of nuclear structure and interactions is fundamental to a wide range of discovery science. Classical computational methods for modeling atomic nuclei are severely limited, due to the number of single-particle states required for the calculation. This "curse of dimensionality" means that only the properties of small or medium-sized nuclei can be calculated with high precision. In contrast, the computational cost for certain quantum algorithms grows more gently with the number of states included. By unlocking simulation of larger nuclei, early fault-tolerant quantum

computers could perform scientifically relevant calculations that are intractable today, offering a clear path to quantum advantage.

Solving this challenge will enable the search for new physics beyond the Standard Model, such as CKM non-unitarity, CP violation in radioactive molecules, and lepton number violation in neutrinoless double beta decay. It is also critical for reducing uncertainties in neutrino studies that depend on neutrino-nucleus interactions, such as the Deep Underground Neutrino Experiment (DUNE).

Example Targets

- Implement a realistic nuclear shell-model calculation for a medium-mass nucleus, calculating nuclear properties such as low-lying excited state energies or magnetic moments.
- Calculate nuclear matrix elements for neutrinoless double beta decay, using parameters that correspond to current or planned experiments.
- Simulate neutrino-nucleon scattering, calculating an experimentally relevant observable such as the ratio of protons to neutrons produced.

Domain 4: Applied Mathematics

In addition to simulation-based approaches to specific scientific problems outlined elsewhere, DOE's mission space includes significant activities in the general problems of applied mathematics. Research into scalable algorithms, machine learning, and mathematical libraries underpin a wide range of scientific work and are key to obtaining maximum performance from both classical and quantum computers. Understanding the potential uses and applications, including where quantum computers exhibit advantages and the scale of those advantages, is key to the general application of quantum computers and to DOE mission areas. However, while some algorithms promise significant advantages in fundamental scientific problems, rigorous demonstrations of these advantages remains difficult on near-term devices. As the sole near-term Application under this domain, **linear equations and PDEs** are identified as a priority topic area.

Application 4.A: Linear Systems and Partial Differential Equations

Application Description

Systems of equations, such as linear systems and systems of differential equations, are ubiquitous across science. Classical algorithms for these settings are well-developed and mature, but face challenges confronting scenarios (such as turbulence) where the large

disparity in relevant time and length scales requires impractically dense meshes and small time steps for feasible computation. Quantum algorithms for tackling these problems have been an area of focus for years, starting with the Harrow–Hassidim–Lloyd (HHL) algorithm for linear systems and continuing with the development of algorithms such as quantum singular value transform and quantum signal processing. Many of these methods can also be applied to differential equations, for example, through Schrödingerization. Although quantum computers are naturally suited to the simulation of linear equations (due to the linear nature of quantum mechanics), methods have also been developed to enable quantum computers to attack nonlinear differential equations, including with dissipation.

Solving this challenge would unlock a wide variety of possible applications, for example, in fluid dynamics, meteorology, and plasma physics, by enabling the solution of a generic class of problems that currently require significant high-performance computing resources.

Example Targets

- Demonstrate sampling from the solution of a linear problem with access to the problem matrix implemented efficiently as a quantum oracle.
- Use a quantum computer to simulate a turbulent classical fluid flow.

Emerging Application Areas

These applications balance the very wide range of areas where curious researchers are pushing the boundaries of quantum applications and the narrow range of areas that have been explored in detail so far, where advantage is expected and can be sought on first-generation SRQCs. To guide immediate efforts such as the Quantum Genesis, the named and numbered applications and example targets in this document have favored better-studied examples where algorithms, resource estimates, and early implementations already exist. Beyond these examples, many other transformative applications of quantum computers have been proposed but require different types of effort to bring them to maturity. Examples of knowledge gaps that need to be closed include: moving beyond conceptual identification of systems of interest into concrete algorithm design, moving beyond algorithm design into concrete resource estimates, moving beyond estimates into implementation onto specific and realistic quantum architectures, and moving beyond quantum implementation to full integration of a computational workflow with a clear understanding of how quantum processors will enhance existing scientific discovery pathways. In other cases, an application may have been studied, but the current estimates of required quantum resources may place it out of reach for the first generation of SRQCs.

Such assessments are necessarily short-term. Focused research on applications can close these gaps and future documents like this one will likely identify different targets, including ones not yet on the horizon. DOE's Office of Science will continue to guide and encourage its scientific communities to further expand the suite of quantum algorithms, understand the requirements of current and future DOE-relevant applications, and implement for impact on future quantum computers.

Below, there is a short, non-exhaustive, list of interesting problems with brief descriptions that could be valuable targets for future quantum applications research with alignment to key DOE mission areas. Full-fledged, fault-tolerant quantum computing applications for these subjects are likely to require a longer time horizon than those identified in the main Domains, but in the meantime focused research can begin to bring these closer to practical relevance on emerging SRQCs.

- **Biological modeling.** Exploration of quantum computing for analysis of diverse and complex biological data is an ongoing endeavor. Quantum computing has the potential to enable modeling of entire biological systems that currently is beyond reach using conventional computational biology. Example target areas include biomolecular/protein and cell modeling which are crucial for advancing biotechnology, biomanufacturing, and biomedicine (drug discovery).
- **Fusion and plasma science.** Early SRQCs could serve as specialized accelerators within larger classical fusion workflows, initially addressing reduced, verifiable calculations that produce useful inputs for existing models. Promising targets include atomic collision and radiation data for fusion-relevant elements such as neon, argon, and tungsten; quantum processes in plasma-facing materials, including secondary electron emission and defect behavior; and opacity, transport, and response properties of warm-dense matter. Quantum algorithms may also address plasma equations, beginning with linear electromagnetic-wave, kinetic, and transport problems. Nonlinear turbulence and full plasma simulations remain important longer-term goals as algorithms and hardware mature.
- **Data analysis.** The large Hilbert space native to quantum computing may enable the representation of high-dimensional data sets with potential implications for DOE's user facilities. Other possibilities may arise in multi-omics or precision medicine. Quantum methods may also allow for new methodologies such as topological data analysis to be efficiently implemented.
- **Optimization.** Optimization is a key generic subroutine in a range of applications. Quantum computers may be able to improve optimization by navigating complex landscapes through annealing or annealing-like algorithms, with applications in scientific modeling, industrial settings, and super intelligence training.