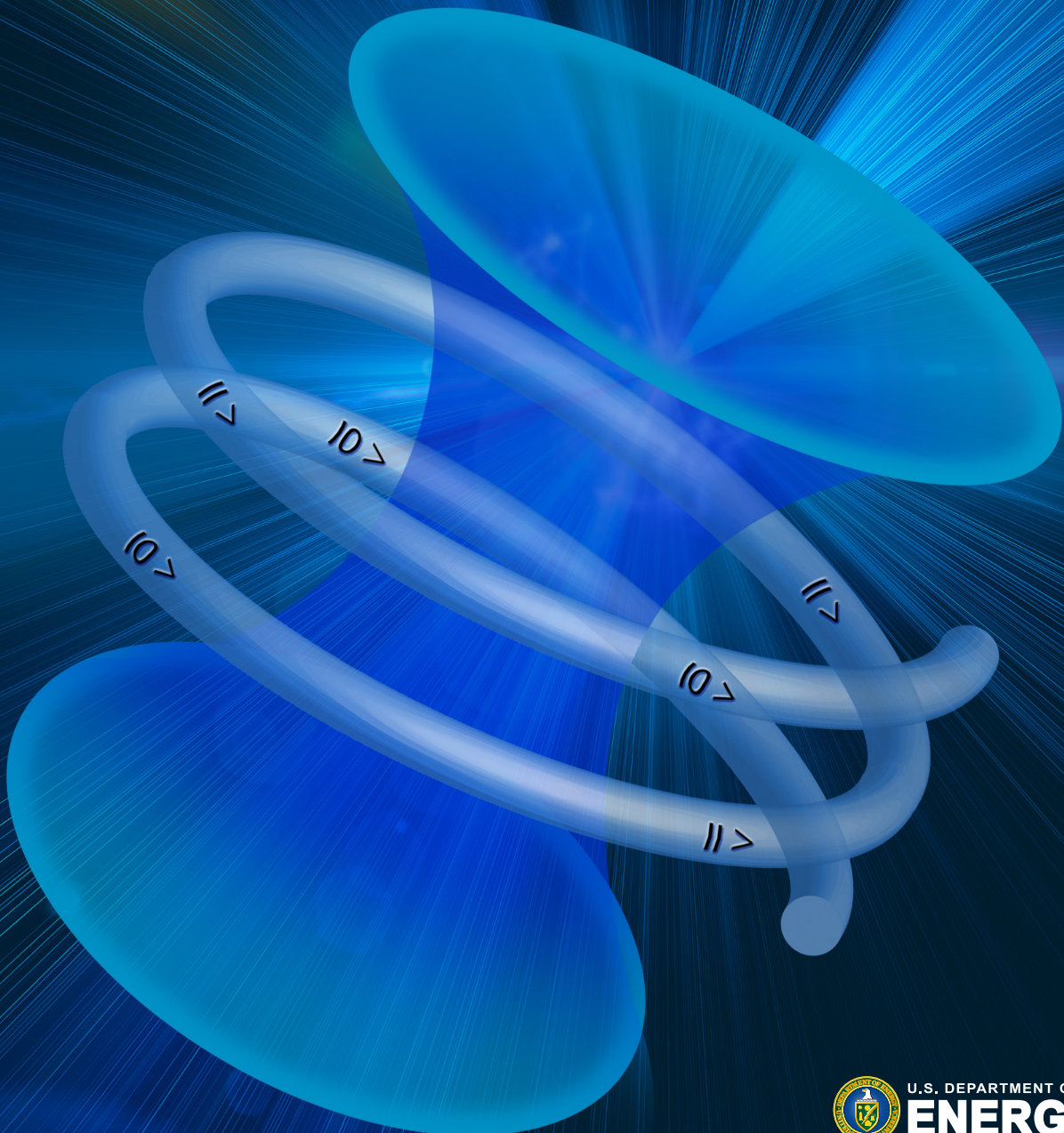


# Fusion Energy Sciences Roundtable on Quantum Information Science

May 01– 02, 2018



U.S. DEPARTMENT OF  
**ENERGY**

Office of Science



The cover shows an artistic interpretation of fusion and plasma themes and their connection to concepts of quantum information.

Image courtesy of Zosia Rostomian, Thomas Schenkel and Asmita Patel, LBNL.

## TABLE OF CONTENTS

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<b>EXECUTIVE SUMMARY .....</b>	<b>III</b>
<b>I. INTRODUCTION—FUSION FOR QUANTUM AND QUANTUM FOR FUSION.....</b>	<b>1</b>
FUSION FOR QUANTUM.....	1
QUANTUM FOR FUSION.....	2
<b>II. PRIORITY RESEARCH OPPORTUNITIES FOR QIS TO ADVANCE FES (QUANTUM FOR FUSION). 6</b>	<b>6</b>
<b>PRO 1: RECONCEPTUALIZING CLASSICAL PLASMA PHYSICS PROBLEMS FOR QUANTUM COMPUTATION.....</b>	<b>6</b>
<i>Scientific challenges for FES .....</i>	<i>6</i>
<i>Barriers to overcome.....</i>	<i>7</i>
MHD stability.....	7
Plasma heating .....	8
Matrix exponentials .....	8
Stellarator confinement .....	9
Nonlinear interactions.....	9
Transport coefficients .....	9
<i>Potential Impacts for FES .....</i>	<i>10</i>
<b>PRO 2: NEAR-TERM OPPORTUNITIES (QUANTUM SIMULATION FOR FUSION PROBLEMS) .....</b>	<b>11</b>
<i>Scientific challenges for FES .....</i>	<i>11</i>
<i>Barriers to overcome .....</i>	<i>12</i>
<i>Potential impact for FES.....</i>	<i>14</i>
<b>PRO 3: QUANTUM SENSING FOR PLASMA DIAGNOSTICS .....</b>	<b>15</b>
<i>Scientific challenge for FES.....</i>	<i>15</i>
<i>Barriers to overcome .....</i>	<i>15</i>
<i>Potential impact for FES.....</i>	<i>16</i>
<b>III. PRIORITY RESEARCH OPPORTUNITIES FOR FES TO ADVANCE QIS (FUSION FOR QUANTUM) ....</b>	<b>17</b>
<b>PRO 4: HIGH ENERGY DENSITY LABORATORY PLASMA SCIENCE FOR NOVEL QUANTUM MATERIALS .....</b>	<b>17</b>
<i>Scientific challenge for QIS.....</i>	<i>17</i>
<i>Barriers to overcome .....</i>	<i>17</i>
<i>Potential impact for QIS.....</i>	<i>20</i>
<b>PRO 5: RELATIVISTIC PLASMA SCIENCE FOR QUBIT CONTROL AND QUANTUM COMMUNICATION .....</b>	<b>23</b>
<i>Scientific challenge for QIS.....</i>	<i>23</i>
<i>Barriers to overcome .....</i>	<i>24</i>
<i>Potential Impact for QIS.....</i>	<i>25</i>
<b>PRO 6: PLASMA SCIENCE TOOLS FOR SIMULATION AND CONTROL OF QUANTUM SYSTEMS.....</b>	<b>26</b>
<i>Scientific challenge for QIS.....</i>	<i>26</i>
<i>Barriers to overcome .....</i>	<i>28</i>
<i>Potential Impact for QIS.....</i>	<i>29</i>
<b>APPENDIX A. AGENDA .....</b>	<b>30</b>
<b>APPENDIX B. PARTICIPANTS.....</b>	<b>31</b>

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# Report of the Fusion Energy Sciences Roundtable on Quantum Information Science

**May 01 – 02, 2018**

**Gaithersburg, Maryland**

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## EXECUTIVE SUMMARY

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Quantum Information Science (QIS) is poised to revolutionize information technology, with significant impacts in many areas of science and technology. QIS includes general-purpose quantum computation, quantum simulation, quantum sensing and quantum communications. A fifth element is quantum materials, which can enable quantum computing (through physical embodiment of qubits) and which are a frontier of fundamental science in themselves.

The Department of Energy is undertaking QIS initiatives across the Office of Science. Recently, the Office of Fusion Energy Sciences (FES) charged the fusion community to address the relationship of Fusion Energy Sciences and emerging QIS areas. A Roundtable was held in early May of 2018 to discuss Quantum Information Science in the FES context. Two main threads were developed:

- How QIS might have a transformative impact on FES mission areas, including fusion and discovery plasma science (Quantum for Fusion), and
- How fundamental science supported by FES might advance QIS (Fusion for Quantum).

The goal was to provide FES with a set of priority research opportunities (PROs) that can inform future research efforts in QIS and build a community of next-generation researchers in this area. **The findings of this roundtable meeting are summarized in this report and express the enthusiasm and excitement of the plasma and Fusion Energy Sciences community to deeply engage in QIS, both to advance plasma and fusion science and to support the development of QIS with techniques, concepts and tools from Fusion Energy Sciences.**

At the Roundtable, a panel of scientists from diverse backgrounds in plasma science and quantum computing (including theorists and experimentalists from each of those areas) convened and discussed ideas and potential PROs. Two sets of three PROs were identified;

### “Quantum for Fusion” Priority Research Opportunities

PRO 1: Reconceptualizing Classical Plasma Physics Problems for Quantum Computation

- Develop concepts and then algorithms to solve important problems in fusion and plasma physics with emerging quantum computers—in the long run with error correction

PRO 2: Near-Term Opportunities (Quantum Simulation for Fusion Problems)

- Identify and refine quantum simulation capabilities that can solve important fusion and plasma science problems in the near term, possibly complementing and reaching beyond classical simulation capabilities with 50 to 100 noisy qubits in the next 5 to 10 years

PRO 3: Quantum sensing for fusion energy sciences

- Identify quantum sensing approaches that enhance diagnostics capabilities for plasma science in general and to advance fusion plasma development for the burning plasma era

## “Fusion for Quantum” Priority Research Opportunities

PRO 4: High energy density laboratory plasmas science (HEDLP) for novel quantum materials

- Use HEDLP drivers and techniques to form novel quantum materials at ultra-high pressures and by isochoric heating and integrate these materials to advance QIS

PRO 5: Relativistic plasma science for qubit control and quantum communication

- Explore the adaptation of techniques from relativistic plasma science for quantum optics with formation and control of tailored plasma states and applications to ultra-fast photonic qubit control and communication

PRO 6: Plasma science tools for simulation and control of quantum systems

- Refine (semi)-classical techniques for simulation and control of plasmas and apply them to the simulation and control of quantum systems such as quantum computers based on trapped ions and electrons

In the near term, emerging quantum simulation tools with limited numbers of noisy qubits are highly promising take-off points to advance the mapping of fusion plasma problems onto quantum algorithms.<sup>1</sup> Methods from HEDLP now extend the parameter range of materials into new regimes of pressure and temperature with access to novel quantum materials. In this report we detail these and the four other PROs above that were identified by an enthusiastic panel, and by their colleagues who contributed to the discussions with viewgraphs and narratives.

The panel also addressed the critical question of why the FES community should be involved and what the relationship was to other QIS programs in the Office of Science. The answer was clear: FES has long been a driver of innovation and advancement in high performance computing, and it is essential for the mission of FES to be deeply engaged in and drive progress in QIS. In the long term, general-purpose, error-corrected quantum computers will be able to solve certain problems exponentially faster than classical computers, and a wider range of problems with polynomial speedups. Progress in fusion and plasma science might be substantially advanced by quantum simulations and quantum computing.

The general excitement surrounding QIS is based on solid, foundational progress, from experimentally-driven qubit design to more abstract work on algorithms and architectures, and there is much important work to be done. Many details about how a general-purpose quantum computer will actually work remain to be developed. FES can contribute by providing an application space and significant domain expertise to motivate algorithm research, and by supporting the development of QIS technologies. FES can also tap into and amplify the broad excitement for QIS, which will very likely attract a generation of highly talented scientists to the fusion energy sciences communities.

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<sup>1</sup> John Preskill, “Quantum Computing in the NISQ era and beyond,” *Quantum* 2 (31 July 2018), p. 79; <https://doi.org/10.22331/q-2018-08-06-79>

## I. INTRODUCTION—FUSION FOR QUANTUM AND QUANTUM FOR FUSION

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Quantum information science (QIS) is a broad frontier area of science and technology. In May, 2018, a roundtable discussion of how QIS might affect and be affected by research sponsored by the Department of Energy’s Office of Fusion Energy Sciences (FES) took place. Two themes emerged early and were treated in part through breakout discussions. These two themes were “FES for QIS” (how the research sponsored by FES could contribute to progress in QIS), and “QIS for FES” (how technologies such as quantum computers and quantum sensors could advance the research priorities of FES). A few topics do not fit neatly into only one of these bins, but because most generally do, we have organized our report correspondingly.

Roundtable panel members and observers were invited by the Office of Fusion Energy Sciences. Recognizing that advances in QIS are currently being driven by groups in industry, at universities and at national laboratories (in the US and elsewhere), representatives and observers were invited from national laboratories who are active in fusion energy sciences and/or have established or emerging programs in QIS (LANL, LBNL, LLNL, ORNL, PPPL and SNL), from industry (Google Research and General Atomics) and from universities (Auburn, Colorado, Maryland, MIT, Princeton, Rochester, and William and Mary).

Not all aspects of quantum technology specifically or QIS generally were represented or discussed by the roundtable participants. We did not spend significant time discussing any issues directly related to cryptography or quantum networks. We did discuss quantum computing and special materials that may be useful for quantum computing. While “quantum computing” is a subset of QIS, it is a vast subset. We divided the discussions between near-term quantum computing technologies, which might be characterized as “noisy”, as “simulations”, as quantum circuits with limited depth, as systems with approximately 50 qubits, or in other ways; and longer-term, by which we generally meant future fault-tolerant, error-corrected, general-purpose quantum computers.

We did not attempt to forecast which of the many proposed quantum systems might first be in the latter class, but we had representatives of a few prominent research efforts participating in the discussions, in part to manage our expectations. We also discussed how fundamentally new materials might contribute to quantum computing in the long term, with a specific focus on what properties of quantum materials might be most relevant, and how research facilities and expertise within the FES portfolio could contribute to the production of these materials.

### **FUSION FOR QUANTUM**

The main elements of the “FES for QIS” discussions were centered on this latter possibility. Tools and methods that are being developed as part of FES (such as high energy density science and HEDLP) are expanding our knowledge of and our ability to produce novel phases of matter, particularly under extreme conditions. For example, the very high pressures uniquely attainable in laser-driven shock experiments lead to the formation of novel phases in materials such as carbon and may induce new forms of high temperature superconductivity in some materials.



When such novel phases can be stabilized for *ex situ* studies, it becomes possible to think about advancing QIS. One early example is the formation of color center qubits under conditions near warm dense matter (0.5 eV) in diamond.<sup>2</sup> Special materials such as these are the focus of FES-sponsored research. While there is no agreement now on which of many candidate physical systems will end up being most useful for quantum computing, it is clear that systems based on the existence of entangled quantum states that can be manipulated at high speed without dissipative losses are highly relevant. Color center qubits, for example, could perhaps be tailored to enable efficient spin-photon entanglement using near-infrared photons. Also, capabilities from the high-energy-density physics with laboratory plasmas (HEDLP) research program, such as ultrafast, laser-driven plasma manipulation, have the potential to inform or perhaps even drive ultrafast optical control schemes that could be impactful for quantum computing, quantum memory, and quantum networks.

In addition to the possibilities for long-term impacts on the broad QIS enterprise, the roundtable discussion included ways that FES research will likely have short-term impacts on QIS. Because fusion systems are extraordinarily complex physical systems with highly nonlinear interactions, involving a huge range of space and time scales, there is a strong tradition of custom-built, high-quality, high performance computing throughout the FES portfolio. The plasma physics community has a history of producing first-principles simulation tools and of using them to interpret and design complex experiments on a regular basis. The panel noted how this tradition and reputation have already led to the development of simulation tools to support some quantum systems (such as ion traps). Classical and semi-classical simulation tools that exist in the FES portfolio or that could be developed on the basis of the traditions, experience and expertise of the FES community could advance QIS research in the short term.

## QUANTUM FOR FUSION

How will near- and long-term advances in quantum information science likely affect FES research? This is the “QIS for FES” part of the discussion. Two broad topics were discussed within this framework: FES problems from quantum mechanics, and FES problems from classical physics. The former category includes problems related to plasma-material interfaces generally, and to cross-sections, equations of state, opacities, material properties, conductivities, etc. A wider range of exact solutions of the many-body Schroedinger equation may be accessible *via* quantum computation than otherwise, and these quantum problems could benefit enormously. Advances in quantum simulations might also connect scientific communities that are presently disconnected. If, for example, digital quantum simulation of the uniform electron gas “jellium” were possible, it would be of real interest to both the plasma physics and condensed matter communities, particularly if such computations resolved long-standing questions about jellium’s

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<sup>2</sup> J. Schwartz et al., “Local formation of nitrogen-vacancy centers in diamond by swift heavy ions,” *Journal of Applied Physics* **116**, 214107 (2014), 214107; <https://doi.org/10.1063/1.4903075>

zero temperature phase diagram at low density. The related properties of a warm, dense uniform electron gas are a current hot topic in plasma science.<sup>3,4</sup>

We now turn to problems from classical physics, which are the bread and butter of plasma physics research. The equations and problems of classical plasma physics are challenging. They range from first-principles calculations of dynamics and thermodynamics of non-equilibrium systems to optimization problems that relate physics goals and engineering constraints. The features that make these problems challenging generally also make them hard targets for quantum computation: they are typically *nonlinear, multiscale, open (driven and dissipative)* systems, with an enormous number of degrees of freedom. On the other hand, plasma problems are often well-characterized as maps from a (modest) list of inputs to a (very modest) list of outputs. For example, energy confinement calculations for tokamaks take a small number of inputs (describing the geometry and similarly macroscopic quantities) and produce a very small number of essential outputs (such as the energy confinement time, or perhaps a turbulence-averaged diffusion coefficient as a function of one spatial dimension). The calculations required to get from inputs to outputs tend to stress available computational resources and involve terabyte representations of the turbulent fluctuations, but only a few integrals over these tremendous datasets finally matter. In this aspect, they are well suited to potential quantum algorithms. Another helpful example is related to plasma heating with electromagnetic waves. This system can be treated as a Hamiltonian problem with a handful of global outputs, and is therefore more naturally expressed in the language of quantum mechanics. Still, the most pressing questions in plasma heating typically involve dissipation and nonlinearity, so important work must be done to re-express even wave problems for quantum computations.

A program to identify long-term QIS applications to classical plasma physics problems will benefit from long-term advances in quantum computing. Long-term progress will also depend upon efforts within FES to reconceptualize the most interesting FES problems to fit within a quantum simulation framework, and then to identify, study, and resolve algorithmic bottlenecks. Such efforts can begin now, and were categorized as “near-term” tasks, manifestly in service of long-term opportunities.

A handful of key near-term tasks could also lead to near-term opportunities for quantum computation of classical FES problems. The most important key step is to develop the formalism to describe some interesting nonlinear (or multiscale, or optimization) plasma problems in the quantum gate model (i.e., for a fault-tolerant, error-corrected, general-purpose quantum computer with a nonspecific physical representation). With a general formalism in hand, the search for near-term FES targets for demonstrations of quantum supremacy would be more credible and easier to manage.

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3 R. Babush et al., “Low-Depth Quantum Simulation of Materials,” *Phys. Rev. X* **8**, 011044 (2018), <https://doi.org/10.1103/PhysRevX.8.011044>

4 T. Dornheim, S. Groth, and M. Bonitz, “The uniform electron gas at warm dense matter conditions,” *Physics Reports* **744** (30 May 2018), pp. 1-86; <https://doi.org/10.1016/j.physrep.2018.04.001>

Two other key steps related to quantum computations of classical physics were identified. First, it has already been shown that one can identify superior algorithms for some classical problems on classical computers using ideas and insights from QIS.<sup>5</sup> In particular, extensions of Hamiltonian descriptions of plasma dynamics may help ideas from QIS “tunnel” over to classical plasma problems on conventional, non-quantum hardware. Second, there are already quantum algorithms that run on quantum hardware (such as HHL; see below) to solve demanding problems from linear algebra with quantum speedups. There will likely continue to be progress in this area, as it will be driven very broadly by both science and commerce. The multiscale nature of typical plasma problems means the linear algebra problems they generate are hard to solve (e.g., because matrices to be inverted have inherently large condition numbers). It is hard to identify short-term opportunities for quantum supremacy for plasma problems using these approaches, but there is every reason to look more carefully at this question.

Quantum supremacy refers broadly to the demonstration of a computation or simulation that cannot be matched by a classical computer.<sup>6</sup> Precisely how quantum supremacy (in any context) will emerge is unclear. There are several developing physical models of quantum computation, each supporting and supported by a variety of qubit technologies. To reiterate, the panel agreed that an apparent precondition for using quantum hardware to advance FES science in the short run is the development of a better formal understanding of some plasma problems in the context of the generic model of general-purpose quantum computing. However, there were also productive discussions around the different models of quantum computing that are available now or within a few years. Our understanding of these platforms can be summarized as follows.

- **The Circuit Model.** Several qubit technologies for circuit model computation are under intense development, with superconducting charge qubits based on Josephson junctions and qubits encoded in the electronic states of ions trapped in an electrostatic potential presently in the lead. Semiconductor manufacturing techniques support qubit models based on few-electron quantum dots and on nuclear spin of impurity atoms in silicon. Other technologies that would implement circuit models of quantum computation include qubits encoded in the spin states of color centers and the hyperfine states of neutral atoms trapped in optical lattices. It remains unclear as to which of these technologies will ultimately be best suited to realizing a large-scale gate model system. Moreover, even within this paradigm, there is tremendous variation with respect to the most natural algorithms for each.
- **Quantum annealing.** The model of quantum computation for this hardware might be thought of as a cousin of homotopy (or continuation) methods. There remain open questions for the ultimate computational power of this general approach, but commercial systems exist, and have been installed e. g. at LANL and several other sites.

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<sup>5</sup> George Vahala, Jeffrey Yezpez, and Linda Vahala, “Quantum lattice gas representation of some classical solitons,” *Physics Letters A* **310**, 2-3 (14 April 2003), pp. 187-196; [https://doi.org/10.1016/S0375-9601\(03\)00334-7](https://doi.org/10.1016/S0375-9601(03)00334-7)

<sup>6</sup> Aram W. Harrow and Ashley Montanaro, “Quantum computational supremacy,” *Nature* **549**, pp. 203–209 (14 September 2017), <https://doi.org/10.1038/nature23458>.



- **Analog quantum simulation.** This approach is novel, and perhaps well-matched to plasma problems. An example from this class consists of a driven, superconducting circuit of qubits (as in the first class), but set up to allow certain interactions with the environment, so that one is not restricted to the study of standard quantum Hamiltonians. With such hardware, one can model systems described by the Lindblad equation. Whether this approach might open doors for the plasma community was discussed at length.
- **Everything else.** Many other approaches (such as topological quantum computation, qubits represented by neutral atoms in optical lattices, etc.) are under intense development, but were not the focus of this roundtable discussions.

To summarize the discussion of QIS for FES, the panel agreed that near-term efforts focused on identifying representative plasma problems (either classical or quantum) that would benefit from adaptation to algorithms for a general-purpose quantum computer could pay off in both the near and the long term. Such efforts would naturally and efficiently drive near-term implementations, including using existing quantum algorithms for important problems now. In the long-term, the science program of FES is very likely to remain strongly dependent upon advances in high performance computing (HPC), including general-purpose quantum computing. Even before the availability of error-corrected, general quantum computers, there may be opportunities to advance FES science with tools and techniques from QIS. These range from straightforward attacks on existing problems using existing and emerging quantum algorithms of modest circuit depth, to more exotic (and so far unidentified) opportunities to demonstrate quantum supremacy (probably with quantum simulation techniques instead of with general gate models of computation), to exciting cross-fertilization opportunities, such as the stimulation by ideas and concepts from QIS of new classical algorithms for old plasma problems.

In addition to the core area of quantum computing and simulations, quantum sensing was also discussed as a rapidly evolving QIS area with high impact potential to advance diagnostics capabilities in general plasma science and key fusion applications.

Finally, the panel agreed that a workshop or series of workshops to facilitate these developments would likely jumpstart healthy, national capabilities in QIS for FES (and FES for QIS), particularly if such activities were designed specifically to include the strong or even dominant participation of young scientists (including graduate students).

## II. PRIORITY RESEARCH OPPORTUNITIES FOR QIS TO ADVANCE FES (QUANTUM FOR FUSION)

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### PRO 1: RECONCEPTUALIZING CLASSICAL PLASMA PHYSICS PROBLEMS FOR QUANTUM COMPUTATION

#### Scientific challenges for Fusion Energy Sciences

Fusion energy devices are expensive to build and operate. We know the fundamental equations that describe their operation – Newton, Maxwell, and Boltzmann themselves built the essential foundations – but the solutions we need are notoriously difficult to calculate, for many reasons. Fusion plasmas are unstable and turbulent. They are heated with waves that propagate through inhomogeneous, active media. Plasma interactions with material surfaces strongly influence reactor performance. In magnetic confinement systems, the shape of the magnetic field is critical to performance and is determined partly by external magnets and partly by self-consistent plasma dynamics. Critical reactor time scales range from days and weeks all the way to nanoseconds. A reactor that runs for weeks at a time slowly erodes the material surfaces facing the fusing plasma, and accumulates unprecedented radiation damage in large, important structures. Electric currents require tens of seconds to diffuse through the system. The thermonuclear energy must typically be confined for seconds to maintain the nuclear burn. The topology of the magnetic field evolves over tens of milliseconds. Turbulent eddies turn over in microseconds. Waves used to heat the plasma have periods of nanoseconds. Each of these processes interacts with the rest in significant ways, and in nearly every case nonlinearly. Inertial confinement systems are similarly challenged by nonlinear dynamical interactions encompassing an astonishing range of timescales. The range of interacting spatial scales is equally daunting for all fusion devices.

It is not possible simply to engineer solutions to these challenges. The development cycle has been accelerated by a strong program of theory and simulation, extending back decades. As a result, the science of plasma physics is solidly grounded and computationally mature. Plasma simulations typically use equations that are well-matched for specific sub-problems, and that have been derived with sophisticated asymptotic and/or field-theoretic approaches. They use state-of-the-art numerical algorithms running on the most powerful computers. To date, the development cycle still includes constructing and testing increasingly expensive devices, because we cannot yet produce reliable predictions of performance from theory and computations alone. However, even after the first fusion device produces net power, there will be substantial opportunities to compute improved designs and more advanced operational scenarios, and perhaps even to use simulations within real-time feedback loops in the reactor control room. Fusion power will not come to be without extensive machine-based computation.

Will *quantum* computers accelerate the quest for fusion power? Perhaps. Fusion power and quantum computing are both audacious ideas. There have been exciting and surprising

breakthroughs in each, but neither will become fully mature soon. There is a more interesting question to consider: Will quantum information science deepen our understanding of plasma physics? The answer is again, “perhaps,” but one can develop a specific plan to answer this question today by reconceptualizing problems from (classical) plasma physics in a language well-matched to algorithms for an idealized, fault-tolerant, general-purpose quantum computer of the future.

### Barriers to overcome

It is already clear that certain tasks (such as period-finding)<sup>7</sup> could be radically accelerated with access to a quantum computer, but the general mapping of problems to quantum resources is certainly not yet clear. Problems from classical physics in particular cannot yet be generically mapped to quantum algorithms. Efforts should be made to find such maps for problems from plasma physics (and from fusion energy science generally). Only then can one understand (even in principle) how to marry quantum computing and fusion research. Plasma physics problems are generically multiscale, nonlinear, and open (driven and damped), and are therefore not obviously good candidates for quantum algorithms. It would be interesting to understand this terrain – to understand the barriers standing in the way of using future quantum computers for plasma physics. A few examples can be given to illuminate the opportunity and the barriers to be overcome.

#### *MHD stability*

The equations of ideal magneto-hydrodynamics (MHD) describe the macroscopic stability in typical magnetic confinement devices. From Bernstein et al.’s early statement of the MHD energy principle<sup>8</sup> to analyses based on the non-canonical Hamiltonian structure of the theory such as that of Morrison and Greene,<sup>9</sup> to more recent formulations such as that of Brizard,<sup>10</sup> numerous authors have found the Hamiltonian structure of ideal MHD to be very helpful in designing algorithms to determine macroscopic stability. Extensions to Hamiltonian descriptions of kinetic systems abound. Can the generic problem of determining ideal MHD stability be restated in the language of generic quantum gates? If so, under what conditions could such problems be accelerated if given access to an idealized quantum computer? Are there quantum algorithms (*cf.* the classical Newcomb algorithm) which can return “stable” or “unstable” efficiently, without directly calculating details of mode structure or growth rates? Can the data

<sup>7</sup> Peter W. Shor, “Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer,” *SIAM Review* **41**, 2 (4 August 2006), pp. 303-332; <https://doi.org/10.1137/S0036144598347011>

<sup>8</sup> I.B. Bernstein, E.A. Frieman, M.D. Kruskal, R.M. Kulsrud, “An energy principle for hydromagnetic stability problems,” *Proc. Royal Society London A* **244**, pp. 17-40 (25 Feb. 1958), <http://dx.doi.org/10.1098/rspa.1958.0023>

<sup>9</sup> Philip J. Morrison and John M. Greene, “Noncanonical Hamiltonian Density Formulation of Hydrodynamics and Ideal Magnetohydrodynamics,” *Physical Review Letters* **45**, 790 (8 September 1980), <https://doi.org/10.1103/PhysRevLett.45.790>

<sup>10</sup> Alain Brizard, “Hermitian structure for linearized ideal MHD equations with equilibrium flows,” *Physics Letters A* **168**, 5-6 (7 September 1992), pp. 357-362, [https://doi.org/10.1016/0375-9601\(92\)90518-Q](https://doi.org/10.1016/0375-9601(92)90518-Q)



required to describe an MHD equilibrium be loaded into quantum memory efficiently? If the answers to these questions are encouraging, can one determine which quantum resources potentially provide direct advantage? Answers to these (and similar) questions are needed for the long-term development of quantum MHD stability algorithms, but could perhaps also drive near-term efforts to demonstrate quantum supremacy with quantum simulators, or with other available quantum hardware. Without a systematic effort to identify a “standard” quantum formulation of the basic problem, it is unlikely that any near-term effort along similar lines could gain traction.

### *Plasma heating*

Full-wave modeling of radio-frequency (RF) heating in magnetic confinement fusion devices is tractable today, but expensive. The problem might be well-matched to known quantum algorithms. For stationary backgrounds, the system consists of linear, monochromatic waves traveling through an inhomogeneous medium. The discretized problem can be cast as a standard linear algebra problem, such as solving for  $\mathbf{x}$  in the equation  $\mathbf{A} \mathbf{x} = \mathbf{b}$ . The matrix  $\mathbf{A}$  is sparse. Can instances of this problem be efficiently “solved” with the Harrow-Hassidim-Lloyd (HHL) algorithm,<sup>11</sup> or variants thereof? More specifically, are there quantities of interest (related to integrals or weighted sums over the elements of  $\mathbf{x}$ ) that the HHL algorithm can determine efficiently? Are typical fusion problems well-conditioned enough for HHL as it is available today? If not, what is the roadmap for development, and roughly when might a quantum full-wave heating calculation become advantageous? Under what conditions can the entries of  $\mathbf{A}$  be calculated and loaded into memory efficiently enough to permit speedups over classical computation?

### *Matrix exponentials*

For non-stationary backgrounds, some RF heating problems can be recast<sup>12</sup> in manifestly quantum form. Key information can be obtained from evaluation of a matrix exponential. Can problems like this, which can be directly stated in standard quantum mechanical terms, be efficiently “solved” with a generic quantum computer? As above, what does it mean to have a physical “solution”? Can the required information be extracted efficiently at the end of the execution of the algorithm? What constraints exist on what can be learned efficiently? Problems like this are closely related to mode conversion problems, which are in turn closely related to many familiar problems from the condensed matter community. Can meaningful, solid analogues be established, and if so, what can they teach us?

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<sup>11</sup> Aram W. Harrow, Avinatan Hassidim, and Seth Lloyd, “Quantum Algorithm for Linear Systems of Equations,” *Physical Review Letters* **103**, 15 (7 October 2009), 150502; <https://doi.org/10.1103/PhysRevLett.103.150502>

<sup>12</sup> Daniel E. Ruiz and Ilya Y. Dodin, “Ponderomotive dynamics of waves in quasiperiodically modulated media,” *Physical Review A* **95**, 3 (14 March 2017), 032114; <https://doi.org/10.1103/PhysRevA.95.032114>

### *Stellarator confinement*

Stellarator magnetic fields are three-dimensional and non-axisymmetric. The quality of particle confinement can be related to Kolmogorov–Arnold–Moser (KAM) surfaces, whose existence can be related to a particular quantity called Greene’s residue.<sup>13</sup> (This is a general result from nonlinear dynamics, so its study may be of broader interest.) Greene’s residue, which can be estimated using information gleaned from long-period orbits, plays a key role in stellarator optimization. Can the well-known period-finding attributes associated with quantum algorithms (such as in Shor’s factoring algorithm) be brought to bear for stellarator optimization? If so, are there related problems from nonlinear dynamics that could be attacked with quantum algorithms? Are the details of what is needed for and from Greene’s residue efficiently accessible for some specific (general gate model) quantum algorithm?

### *Nonlinear interactions*

Zonal flows and their nonlinear interactions with turbulence are thought to be very important elements of plasma turbulence in tokamaks and stellarators. Mathematically, they are one of the simplest nonlinear plasma systems. Several models of these interactions have appeared in the literature, based variously on severe Galerkin truncations, *ab initio* simulations, general theoretical principles, wave-kinetic equations, etc. Can interesting properties of this prototypical system from turbulent gyrokinetic dynamics be discovered with a quantum computer? If so, which of the many formulations from the literature are most directly mapped to a generic quantum framework? What are the limitations associated with the nonlinear nature of the problem? If the nonlinearity does not preclude meaningful quantum-based calculations, how might one extend such a study to a more complicated nonlinear problem from plasma physics?

### *Transport coefficients*

Fusion devices run on fuel that is out of thermodynamic equilibrium. Strong gradients are inherently present. Calculations of the collisional and laminar, nearly collisionless and laminar, and turbulent fluxes of particles, momentum and energy that arise as a consequence of these gradients are important to the fusion program. The dynamics may be Hamiltonian in some descriptions, but not in all. The fluxes obey Onsager symmetries in some cases, but not in all. The dynamics can be nonlinear in some cases. In nearly all cases, one needs to extract only a handful of integral quantities, even when the integration is over a very large number of degrees of freedom. Typical simulations today use billions of degrees of freedom, and sometimes many more. Under what conditions might a quantum computer return useful information from quantum simulations of such systems? Which of the several formulations of the problem(s) are best adapted for quantum algorithms? What are the features of a particular formulation that make it more or less amenable to such adaptation? Given the potentially low-noise nature of integral estimates from a quantum system, how many qubits would be required for any particular calculation, compared to the number of degrees of freedom required for a current,

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<sup>13</sup> John M. Greene, “A method for determining a stochastic transition,” *Journal of Mathematical Physics* **20**, 6 (6 June 1979), pp. 1183-1201; <https://doi.org/10.1063/1.524170>

classical algorithm? How should one think about dissipation in such systems, and how does one's model of dissipation (which is physically relevant in the original, classical system) map to the quantum algorithm domain? Within the class of particle-based classical algorithms, which are more amenable to translation to quantum contexts: particle-in-cell (PIC) codes, N-body, or something else?

### **Potential Impacts for FES**

In the foregoing, we have focused on a handful of fusion-specific problems as examples. There are many more examples, of course. More importantly, there are many problems from plasma physics that are not central to the quest for fusion itself. For decades, insights from the fusion program have been important in other areas of plasma science (such as for magnetospheric, heliospheric, weapons, and astrophysical applications). This cross-fertilization, in turn, reinforces confidence in the vitality of (and the prospects for) the fundamental FES mission. One imagines that in addition to accelerating the quest for fusion power, advances from QIS for FES would also lead to advances in plasma science generally.

## PRO 2: NEAR-TERM OPPORTUNITIES (QUANTUM SIMULATION FOR FUSION PROBLEMS)

### Scientific challenges for FES

The FES portfolio includes research in areas that are fundamentally quantum mechanical in nature. These research areas will benefit significantly from any advances in realizing quantum simulation technologies that efficiently and exactly solve the many-body Schroedinger equation. Classical approaches to solving this equation either incur an exponential cost while remaining exact (e.g., unbiased quantum Monte Carlo (QMC)) or achieve a polynomial cost while incurring a difficult to quantify systematic error (e.g., density functional theory (DFT) or biased QMC). Thus there is a very clear advantage to pursuing quantum simulation technologies for these research areas. We have previously described a particular application related to computing the properties of jellium with digital quantum simulation.<sup>2</sup> In fact, the properties of jellium are used as input to DFT calculations, and could thus impact this broad area of research. More generally, however, quantum simulation techniques can leapfrog the need for DFT altogether and promise to enable efficient exact solutions of the many-body Schroedinger equation for a number of research problems within FES.

One such area is understanding the static and dynamic properties of warm dense matter (WDM). While recent experimental advances have made it possible to probe properties such as equations of state, conductivities, stopping powers, and opacities in the WDM regime, the financial, temporal, and cost per experiment is relatively high. Because the MHD models used to explore fusion concepts depend on models of these properties over a wide range of thermodynamic conditions, frequently computational models of materials properties computed using density functional theory (DFT) or quantum Monte Carlo (QMC) are used to supplement experimental data. A better understanding of this range of problems could also advance progress towards ignition in inertial fusion experiments by improving experimental designs and improving our ability to interpret available diagnostic information.

WDM is not the only area of FES materials research with quantum mechanical problems that must be resolved. Plasma-facing materials have or develop important heterogeneities at the atomic scale (boundaries, lattice impurities, dislocations, helium bubbles, hydrogen loading, etc.) and cannot yet be fully characterized in the laboratory. First-principle simulations of critical aspects of these structures start from Schroedinger's equation and need to be solved in Hilbert spaces that are too big for current classical computers.

Within the plasma itself, some aspects of the fusion cross sections are not fully known. A detailed evaluation of spin-polarization as a way to boost reactivity (of DD, DT, and perhaps D-<sup>3</sup>He reactions) would illuminate the ultimate opportunity there. The cross-sections underlying muon catalyzed fusion have not been calculated in full detail. While it is not easy to see how a deeper understanding of these cross sections would profoundly affect the FES mission, it is easy to see that one would like to understand the problems fully, to be certain.

At very high densities, fusion reaction rates may be affected by many-body quantum effects. The original derivation from Gamow described free particles tunneling through the Coulomb barrier. Because the tunneling rate depends exponentially on the average energy of the fusing particles and the height of the barrier, small changes in either can be significant. In addition to classical Salpeter screening, in very dense plasmas there are (in principle) further quantum mechanical corrections.<sup>14</sup> Our understanding of high-density fusion cross-sections is central to and constrained by our understanding of stellar processes. It would be exciting to resolve the full story theoretically.

### Barriers to overcome

Among the earliest proposed applications of quantum computers is quantum simulation, the efficient calculation of the properties of physical systems governed by the Schrodinger equation, first suggested by Richard Feynman in the early 1980s. Algorithmic primitives including the quantum Fourier transform<sup>15</sup> and quantum phase estimation<sup>16</sup> led to the first concrete proposals for quantum simulation.<sup>17,18</sup> Subsequently significant progress has been made toward experimentally realizing analog and digital quantum simulation.<sup>19,20,21,22</sup> Quantum problems in the FES portfolio are likely just as appropriate for demonstrating quantum supremacy as any other quantum simulation target, but there is work to be done to remove the word “likely” from this sentence. What is needed is a program aimed at defining and prioritizing FES problems that may be appropriate for near-term quantum simulation and then matching these problems to appropriate simulation technologies.

Some candidate directions are outlined in this section. These directions pair naturally with ongoing DOE ASCR-supported programs. One of the key “subroutines” necessary to realize quantum simulation is state preparation. In the context of analog simulation, this amounts to ensuring that the quantum simulator is in contact with a bath that thermalizes it to a desired temperature, or otherwise leaves it in some state the properties of which we would like to evaluate with the simulator. For digital simulation, the goal is the same but complicated by the

<sup>14</sup> V.M. Galitski and V.V. Yakimets, “Particle Relaxation in a Maxwell Gas,” ZhETF, Journal of Experimental and Theoretical Physics (U.S.S.R.) **51** (September 1966), pp. 957-964; [http://www.jetp.ac.ru/cgi-bin/dn/e\\_024\\_03\\_0637.pdf](http://www.jetp.ac.ru/cgi-bin/dn/e_024_03_0637.pdf)

<sup>15</sup> Peter W. Shor, “Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer,” SIAM Review **41**, 2 (23 April 1999), pp. 303-332; <https://doi.org/10.1137/S0036144598347011>

<sup>16</sup> Alexy Yu. Kitaev, “Quantum measurements and the Abelian Stabilizer Problem,” arXiv:quant-ph/9511026 (20 November 1995).

<sup>17</sup> Daniel S. Abrams and Seth Lloyd, “Simulation of Many-Body Fermi Systems on a Universal Quantum Computer,” Physical Review Letters **79**, 13 (29 September 1997), pp. 2586-9; <https://doi.org/10.1103/PhysRevLett.79.2586>

<sup>18</sup> Daniel S. Abrams and Seth Lloyd, “Quantum Algorithm Providing Exponential Speed Increase for Finding Eigenvalues and Eigenvectors,” Physical Review Letters **83**, 24 (13 December 1999), pp. 5162-5; <https://doi.org/10.1016/j.physrep.2018.04.001>

<sup>19</sup> P.J.J. O'Malley *et al.*, “Scalable Quantum Simulation of Molecular Energies,” Physical Review X **6**, 3 (18 July 2016), pp. 031007-1 to-13; <https://doi.org/10.1103/PhysRevX.6.031007>

<sup>20</sup> H. Bernien *et al.*, “Probing many-body dynamics on a 51-atom quantum simulator,” Nature **551** (30 November 2017), pp. 579–584; <https://doi.org/10.1038/nature24622>

<sup>21</sup> Abhinav Kandala *et al.*, “Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets,” Nature **549** (14 September 2017), pp. 242-6; <https://doi.org/10.1038/nature23879>

<sup>22</sup> James I. Colless *et al.*, “Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm,” Physical Review X **8** (12 February 2018), 011021 (2018); <https://doi.org/10.1103/PhysRevX.8.011021>



fact that the physical degrees of freedom of the system being simulated are encoded in a quantum register comprised of qubits. This is reminiscent of the representation of a quantum state on a classical computer as a binary string encoding the complex amplitudes of some quantum state in a particular basis.

While there is existing research on state preparation, ranging from adiabatic to Metropolis-style algorithms, continuing to work out details particular to the extreme conditions realized in FES systems is an open research problem. To the extent that an analog simulator is a physical system at the desired temperature (the desired temperature normalized to the internal energy scale of the simulator) we might be concerned with the physical stability of the simulator relative to the time scale over which it can be measured. For digital simulation, stability is not a concern—rather, the concerns are working out the details of how to efficiently prepare states from thermal ensembles at high temperatures or assessing whether there are more efficient encodings that can exploit the effective classicality of high temperature tails. Both of these issues warrant further research.

Aside from preparing and simulating thermal states, non-local thermodynamic equilibrium (LTE) conditions are ubiquitous in the space of FES problems. These include plasma-material boundaries and systems that are strongly perturbed by mechanically- or laser-driven shocks and intense ultrafast excitation from X-ray free electron lasers. Algorithms for preparing these states on analog or digital quantum simulators, and subsequently extracting physically relevant observables must be developed.

At present, analog and digital quantum simulation technologies have focused on extracting different physical observables. Analog technologies have primarily been applied to measurements of quantum dynamics, and the measurement of correlation functions, whereas digital technologies have primarily been applied to calculations of total energies. In the context of being used to parametrize wide-range materials models for experimental design, we would ultimately like for quantum simulators to be used to compute both static properties (e.g., equation of state) and transport properties (e.g., conductivities, viscosity, stopping power, and opacity). A program to develop best practices for computing these quantities on analog and digital platforms will also be essential to making use of quantum simulation technologies for FES problems.

While quantum simulation might be the most obvious connection between quantum algorithms research and FES materials problems, there may still be other algorithms that find use in this space. One possibility might be whether HHL-inspired algorithms can find application to non-LTE (local thermodynamic equilibrium) kinetic modeling, where the dimensionality of systems of rate equations governing the populations of different atomic configurations in a plasma grow exponentially with ionic charge. Naively, the sparsity and stiffness of these linear systems are not amenable to HHL-like exponential speedups. Whether there may be a way to achieve a quantum speedup for this problem is unknown. Other examples include fitting surrogate models to large quantities of quantum simulation data, as is done with data from DFT or quantum chemical methods in generating many-body potentials for classical molecular dynamics. Such many-body potentials are presently used to enable high-accuracy atomistic

modeling for system sizes and time scales beyond the reach of density functional theory with exemplary applications towards defect kinetics that impact FES-relevant materials.

The goal of this PRO is to develop a community of users in the FES space interested in becoming familiar with the use of quantum simulation algorithms on existing, publicly available quantum devices. Chemical and nuclear sciences have already applied quantum simulation algorithms on such hardware to study simple instances of problems in their respective spaces (e.g., small molecules and the deuteron).<sup>23,24</sup> Developing a hands-on familiarity with existing quantum hardware might inspire some of the algorithmic research proposed above. In the long term, it is not difficult to imagine that this community of users will eventually be using fault-tolerant general-purpose quantum computers in much the same way that large DOE HPC resources are presently being used.

### Potential impact for FES

Ultimately, we may better understand materials problems facing fusion reactors and discover new solutions to accelerate and optimize experiments. More fundamentally, we will gain new insights into questions in planetary and space science, astrophysics, and fundamental plasma physics.

As one illustration of this rapidly evolving area, we show in Figure 1 a schematic representation of a quantum algorithm developed to solve sets of linear partial differential equations that has been applied to solving Poisson's equation in electrostatics.

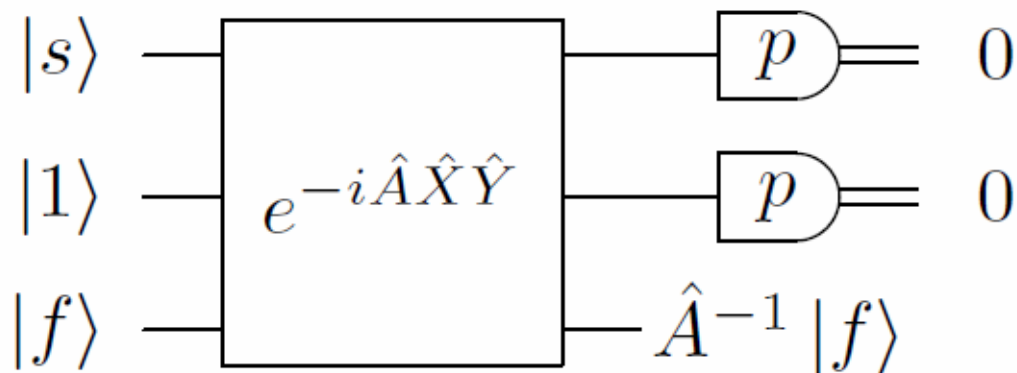


Figure 1. Schematic representation of a quantum algorithm for non-homogeneous linear partial differential equations that can be applied, e.g., to Poisson's equation in electrostatics. From J.M. Arrazola, T. Kalajdziewski and S. Lloyd, <https://arxiv.org/abs/1809.02622>.

<sup>23</sup> J.I. Colless et al., "Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm," *Physical Review X* **8**, 1 (12 February 2018), 011021; <https://www.doi.org/10.1103/PhysRevX.8.011021>

<sup>24</sup> E.F. Dumitrescu et al., "Cloud Quantum Computing of an Atomic Nucleus," *Physical Review Letters* **120**, 21 (23 May 2018), 210501; <https://doi.org/10.1103/PhysRevLett.120.210501>

## PRO 3: QUANTUM SENSING FOR PLASMA DIAGNOSTICS

### Scientific challenge for FES

Diagnostics are central to all experimental efforts in FES. Innovations in our ability to discern signal from noise could lower the cost of running expensive facilities and accelerate their research programs. The challenge here is to determine whether/how continuing breakthroughs in quantum sensing can be usefully ported to FES facilities.

### Barriers to overcome

In recent years, quantum optics has undergone a renaissance. Two major ingredients of quantum optics, entanglement and quantum noise reduction,<sup>25,26</sup> have found their way into sensors and can now outperform state of the art classical sensors. The ability to couple entanglement into nanoscale devices<sup>27,28</sup> and the demonstration of new techniques that take advantage of entanglement even in the presence of large losses<sup>29,30</sup> have moved quantum sensing into a realm where the classical optical power no longer needs to be considered unlimited.

Quantum correlations present in two-mode squeezed states enable many interesting sensors, including those which do not measure squeezing directly<sup>26</sup> and those which exploit quantum correlations to achieve higher sensitivity in interferometry.<sup>31</sup> In nanoscale devices, sensors cannot benefit indefinitely from increasing the optical power in the readout field. Several quantum sensors that outperform their classical counterparts, and in which the classical power cannot be increased to outperform the quantum sensor, have been recently

<sup>25</sup> Slusher, R.E. et al., "Observation of Squeezed States Generated by Four-Wave Mixing in an Optical Cavity," *Physical Review Letters* **55**, 22 (25 November 1985), pp. 2409–12; <https://doi.org/10.1103/PhysRevLett.55.2409>

<sup>26</sup> Carlton M. Caves, "Quantum-mechanical noise in an interferometer," *Physical Review D* **23**, (15 April 1981), pp. 1693–1708; <https://doi.org/10.1103/PhysRevD.23.1693>

<sup>27</sup> Lawrie, B.J., Evans, P.G., and Pooser, R.C., "Extraordinary Optical Transmission of Multimode Quantum Correlations via Localized Surface Plasmons," *Physical Review Letters* **110** (9 April 2013), 156802; <https://doi.org/10.1103/PhysRevLett.110.156802>

<sup>28</sup> Alexander Huck et al., "Demonstration of Quadrature-Squeezed Surface Plasmons in a Gold Waveguide," *Physical Review Letters* **102**, (19 June 2009), 246802; <https://doi.org/10.1103/PhysRevLett.102.246802>

<sup>29</sup> Seth Lloyd, "Enhanced Sensitivity of Photodetection via Quantum Illumination," *Science* **321**, 5895 (12 September 2008), pp. 1463–1465; <https://doi.org/10.1126/science.1160627>

<sup>30</sup> Si-Hui Tan et al., "Quantum Illumination with Gaussian States," *Physical Review Letters* **101**, 25 (18 December 2008), 253601; <https://doi.org/10.1103/PhysRevLett.101.253601>

<sup>31</sup> Jietai Jing et al., "Realization of a nonlinear interferometer with parametric amplifiers," *Applied Physics Letters* **99**, 011110–011110 (8 July 2011); <https://doi.org/10.1063/1.3606549>

demonstrated.<sup>32,33,34,35,36,37</sup> Quantum noise reduction levels of 4-5 dB are now possible.<sup>30,32</sup> With additional work, progress to 10 dB should be achievable. A reduction in noise by 6 dB could represent a *halving* of the integration or averaging time in some experiments. Similar advances have been made in interferometry.

Optical spectroscopy is used to measure vector electric and magnetic fields within hot plasmas. Time-dependent fluctuations in these plasmas frequently limit the sensitivity of field measurements, but existing classical techniques have been developed to enable measurement of trace signals in the RF sidebands of otherwise noisy fields. These improvements in sensitivity are critical not just because they enable the characterization of smaller field fluctuations, but because they enable multiplexing of field measurements. Ultimately, the program of verification and validation in the magnetic confinement program could benefit greatly from further improvements in sensitivity in scattering systems. An evaluation of diagnostic advances based on quantum optics for tokamak plasmas could reveal an opportunity for using QIS technology for fusion in the near term.

### Potential impact for FES

Advances in quantum sensing and the adaptation of quantum sensing techniques have the potential to advance plasma diagnostics capabilities across Fusion Energy Sciences, from discovery plasma science of astrophysical plasma analogs in the laboratory to precision diagnostics in emerging burning plasma devices. An evaluation and demonstration of applicability would make that potential a reality.

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<sup>32</sup> Ulrich B. Hoff et al., "Quantum-enhanced micromechanical displacement sensitivity," *Optics Letters* **38**, 9 (24 April 2013), pp.1413–1415; <https://doi.org/10.1364/OL.38.001413>

<sup>33</sup> Michael A. Taylor et al., "Biological measurement beyond the quantum limit," *Nature Photonics* **7**, 229–233 (3 February 2013); <https://doi.org/10.1038/nphoton.2012.346>

<sup>34</sup> Raphael C. Pooser and Benjamin Lawrie, "Plasmonic Trace Sensing below the Photon Shot Noise Limit," *ACS Photonics* **3**, 1 (9 December 2015), pp. 8–13; [10.1021/acsphotonics.5b00501](https://doi.org/10.1021/acsphotonics.5b00501)

<sup>35</sup> Wenjiang Fan, Benjamin J. Lawrie, and Raphael C. Pooser, "Quantum plasmonic sensing," *Physical Review A* **92**, 053812 (4 November 2015); <https://doi.org/10.1103/PhysRevA.92.053812>

<sup>36</sup> Raphael C. Pooser and Benjamin Lawrie, "Ultrasensitive measurement of microcantilever displacement below the shot-noise limit," *Optica* **2**, 5 (23 April 2015), pp. 393-9; <https://doi.org/10.1364/OPTICA.2.000393>

<sup>37</sup> Mohammadjavad Dowran et al., "Quantum-Enhanced Plasmonic Sensing," *Optica* **5**, 5 (16 May 2018), pp. 628-633; <https://doi.org/10.1364/OPTICA.5.000628>

### III. PRIORITY RESEARCH OPPORTUNITIES FOR FES TO ADVANCE QIS (FUSION FOR QUANTUM)

#### PRO 4: HIGH ENERGY DENSITY LABORATORY PLASMA SCIENCE FOR NOVEL QUANTUM MATERIALS

##### Scientific challenge for Quantum Information Science

Information is physical; qubits for quantum computing and quantum simulations, as well as quantum systems for quantum communication and sensing, are based on different forms of “quantum materials.” The term “quantum material” was originally coined in condensed matter physics to describe strongly correlated electron systems,<sup>38</sup> mostly at very low temperatures. Advances in all aspects of QIS (computing, communication and sensing) require advances in the synthesis and integration of quantum materials in which, e.g., two-level systems can be implemented as qubits or quantum information can be transferred back and forth between quantum processors and long term quantum memories (e.g., nuclear spins) with flying qubits (i.e., photons). While there are many recent examples of highly impactful quantum materials science (graphene, high temperature superconductors, topological insulators, etc.), the ability to drive materials to extreme areas in their phase diagram followed by rapid quenching and stabilization has disruptive impact potential in the discovery of quantum materials with tailored properties for applications in QIS.<sup>39</sup>

##### Barriers to overcome

Research in High Energy Density Science or High Energy Density Laboratory Plasmas (HEDLP) has recently advanced our ability to drive matter to extreme conditions in pressure, temperature, composition and electromagnetic fields. This extension of our reach of materials physics and materials science now enables us to form novel quantum materials, study them in transient states, and aim at collecting and stabilizing them. A key barrier to overcome is to first discover and characterize novel quantum materials phases and to then stabilize these phases so that the novel quantum properties persist and can be harvested in QIS systems.

Dynamic compression can now control the thermodynamic path from Mbar (100 GPa or a million atmospheres) to Gbar (billion atmospheres) pressures, producing to 1000-fold

<sup>38</sup> Joe Orenstein, “Ultrafast spectroscopy of quantum materials,” *Physics Today* **65**, 9, 44 (01 September 2012); <https://doi.org/10.1063/PT.3.1717>

<sup>39</sup> *Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology*, Department of Energy Office of Science, 9 December 2016; [https://science.energy.gov/~media/bes/pdf/reports/2016/BRNQM\\_rpt\\_Final\\_12-09-2016.pdf](https://science.energy.gov/~media/bes/pdf/reports/2016/BRNQM_rpt_Final_12-09-2016.pdf)



compression and the control of interatomic distances. Such conditions are predicted to produce very-high-temperature superconductors, topological insulators, superfluidity, new chemical bonding, and other novel “quantum properties.”<sup>40</sup> Quantum matter and discoveries usually occur at low temperatures,  $T$ , where the de Broglie wavelength,  $\lambda_{deBroglie}$ , becomes comparable to the interatomic distance,  $a_{nn}$ .

$$\lambda_{deBroglie} = \frac{h}{\sqrt{3mk_B T}} \sim a_{nn}$$

Helium, which has an interatomic spacing of about 0.9 nm, undergoes a transition to a quantum superfluid state at  $\sim 2\text{K}$ , which is where  $\lambda_{deBroglie}$  is comparable to this interatomic spacing. In the same way Onnes once controlled temperature to reach the quantum behavior seen in superfluid helium, HEDLP experiments can now control the energy density to be comparable to the quantum forces of constituent atoms. For example, through compression, we control  $a_{nn}$  to be  $< \lambda_{deBroglie}$  to bring quantum behavior to high temperature and perhaps even to  $< a_{Bohr}$  to break foundational building blocks of quantum mechanics, bringing quantum behavior to the macroscale.

Experiments and theory to date have explored only the incipient conditions accessible with today’s HEDLP facilities, yet these results are rich with discovery. Discoveries include a new class of hydrogen-rich superconductors with measured critical temperature  $T_c = 203\text{ K}$ ,<sup>41</sup> predicted superconductors with  $T_c > 300\text{ K}$ ,<sup>42</sup> a combined superconducting-superfluid state of hydrogen,<sup>43</sup> exotic chemical bonding,<sup>44</sup> “electride” insulators characterized by interstitial electron localization,<sup>45,46,47</sup> and new topological materials.<sup>48</sup> Tuning the energy density allows access to a wide variation of novel phases, quantum behavior, transition mechanisms, and pathways not easily accessed or simply out of reach with traditional synthesis techniques.

<sup>40</sup> Francesco Capitani et al., “Spectroscopic evidence of a new energy scale for superconductivity in  $\text{H}_3\text{S}$ ,” *Nature Physics* **13** (19 June 2017), pp. 859–863; <https://doi.org/10.1038/nphys4156>

<sup>41</sup> A.P. Drozdov et al., “Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system,” *Nature* **525** (03 September 2015), pp. 73–76; <https://doi.org/10.1038/nature14964>

<sup>42</sup> Ashcroft, N.W., “Metallic Hydrogen: A High-Temperature Superconductor?,” *Physical Review Letters* **21**, 26 (3 May 1968), pp. 1748–9; <https://doi.org/10.1103/PhysRevLett.21.1748>

<sup>43</sup> Egor Babaev, Asle Sudbø and N.W. Ashcroft, “A superconductor to superfluid phase transition in liquid metallic hydrogen,” *Nature* **431**, (07 October 2004), pp. 666–8; <https://doi.org/10.1038/nature02910>

<sup>44</sup> Wojciech Grochala, “Atypical compounds of gases, which have been called ‘noble’,” *Chemical Society Reviews* **36**, 1632 (2007); <https://doi.org/10.1039/B702109G>

<sup>45</sup> Mao-Sheng Miao and Roald Hoffmann, “High Pressure Electrides: A Predictive Chemical and Physical Theory,” *Accounts of Chemical Research* **47**, 4 (5 April 2014), pp. 1311–17; <https://doi.org/10.1021/ar4002922>

<sup>46</sup> J.B. Neaton and W. Ashcroft, “Pairing in dense lithium,” *Nature* **400** (8 July 1999), pp. 141–4; <https://doi.org/10.1038/22067>

<sup>47</sup> Chris J. Pickard and R.J. Needs, “Aluminium at terapascal pressures,” *Nature Materials* **9** (11 July 2010), pp. 624–7; <https://doi.org/10.1038/nmat2796>

<sup>48</sup> Ivan I. Naumov and Russell J. Hemley, “Metallic surface states in elemental electrides,” *Physical Review B* **96**, 3 (18 July 2017), 035421; <https://doi.org/10.1103/PhysRevB.96.035421>

Atomic pressures,  $P=E_H/a_0^3$  (where  $E_H$  is the Hartree energy and  $a_0=50$  picometers is the Bohr radius), are where the traditional core orbitals of atoms are significantly changed. For many materials at modest temperatures it is where atoms are compressed to within a Bohr orbit. For many low-Z elements and compounds, at even a fraction of this pressure, core electron orbitals are forced to engage in bonding, structure, and transport, thereby inducing in calculations a quantum phenomenon unexplored in the laboratory. As the core electrons begin to interact and valence electrons are squeezed into the interstitial regions, symmetry-breaking distortions and unique short- and mid-range order reminiscent of the liquid state appear. In a number of systems, the solid phase undergoes an evolution towards structural complexity and sometimes reveals a sharp decrease in the melting temperature above a critical pressure. This is an area rich for discovery and that has only recently become accessible at HEDLP facilities.

The potential for new chemistry under extreme conditions emerges as the electronic structure responds to high density, and needs to be explored both experimentally and theoretically. In order to adapt to the geometric changes induced by a decrease in the volume, atoms must adopt new bonding strategies such as the formation of electron-rich or electron-poor multicenter bonds. Even in simple elemental systems at extremes, changes in electronic configuration, orbital ordering, oxidation states are still unclear.<sup>49</sup> The fact that core orbitals can become involved in bonding opens a new energy scale for chemistry. A key effort is needed to explore the potential for a universal phase diagram, pressure dependent periodic table both for equilibrium and metastable systems.

To explore this new HEDS quantum realm, new generations of measurement capabilities are needed. Dynamic compression can achieve 10s of Mbar (multi-terapascal) pressures, with nanosecond duration, whereas static compression can achieve multi-Mbar (hundreds of GPa) for longer duration but only for nanoliter volumes.<sup>50</sup> New techniques in x-ray and electron diffraction, extended x-ray absorption fine structure, magnetic properties and conductivity (electrical, thermal, etc.), as well as techniques to measure the bonding and atomic to mesoscale behavior of such matter can be developed to enable in situ, time resolved measurements.<sup>51,52</sup> While such experiments are underway, a multidisciplinary effort is needed to fully explore the quantum nature of matter at HEDLP conditions and to connect it with potential applications in QIS.

In addition to understanding new quantum behavior, there is the potential for recovering such states at near standard conditions for engineering purposes. Developing dynamic

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<sup>49</sup> Hiroshi Fujihisa et al., "Ca-VII: A Chain Ordered Host-Guest Structure of Calcium above 210 GPa," *Physical Review Letters* **110**, 23 (4 June 2013), 235501; <https://doi.org/10.1103/PhysRevLett.110.235501>

<sup>50</sup> Reinhard Boehler, J. J. Molaison, and Bianca Haberl, "Novel diamond cells for neutron diffraction using multi-carat CVD anvils," *Review of Scientific Instruments* **88**, 083905 (17 August 2017); <https://doi.org/10.1063/1.4997265>

<sup>51</sup> O. V. Gotchev et al., "Laser-Driven Magnetic-Flux Compression in High-Energy-Density Plasmas," *Physical Review Letters* **103**, 21 (18 November 2009), 215004; <https://doi.org/10.1103/PhysRevLett.103.215004>

<sup>52</sup> A.E. Gleason et al., "Ultrafast visualization of crystallization and grain growth in shock-compressed SiO<sub>2</sub>," *Nature Communications* **6**, 8191 (4 September 2015); <https://doi.org/10.1038/ncomms9191>

synthesis, path manipulation, and real time monitoring may allow tuning of kinetic barriers for opening and locking in new states of quantum matter. Such recovery from extreme dynamic compression conditioning has of course been the main technique for producing diamonds (a metastable form of carbon) for tooling for decades. A more recent calculation for stabilizing yet a more extreme form of carbon with perhaps still more useful properties was put forth by Sun, Klug and Mortonak.<sup>53</sup> New collaborations engaging *ab initio* calculations with HEDLP experiments may provide a more rapid predictive manipulation and recovery of such new quantum materials.

Critical barriers for HEDLP based research to overcome in order to contribute to emerging QIS include:

- Improved modeling of materials evolution under extreme conditions of pressure, temperature, electrical and magnetic fields, the equation of states and structural and compositional evolution under these conditions; improved predictive power of models (with possible adaptation of emerging quantum simulation and quantum computation techniques).
- Design experiments at HEDLP facilities to drive materials into desired phases, advance the *in situ* characterization of materials in transient states and develop techniques and methods to quench, stabilize, capture and recover novel materials with tailored quantum properties. These facilities can be large-scale, such as Omega, NIF and Z, or mid-scale, such as petawatt lasers, available, for instance, through LaserNetUS, a U.S. collaborative network of high-power laser facilities.
- Connect with QIS practitioners in computation/simulations, sensing and communication to test novel quantum materials in QIS applications.

### Potential impact for QIS

Discovery and tailoring of quantum materials using the toolbox of HEDLP can lead to the discovery of novel quantum materials for QIS applications.

An example of a highly promising research direction is in the discovery, understanding, and potential recovering a new class of stable or metastable superconductors through significant manipulation of the free energy landscape by tuning pressure-temperature and electromagnetic field conditions, uniquely accessible with HEDLP facilities. Exploring and characterizing for example, superconductors with transition temperatures at or well beyond room temperature offers a new window into quantum coherence and quantum materials. Recent observations of H<sub>3</sub>S with its spectacular new record T<sub>c</sub> of 203 K occurs at ~200 GPa. A large isotope effect on T<sub>c</sub> is observed suggesting that the superconducting mechanism is mediated by phonons<sup>54</sup> with the

<sup>53</sup> Jian Sun, Dennis D. Klug, and Roman Martoňák, "Structural transformations in carbon under extreme pressure: Beyond diamond," *Journal of Chemical Physics* **130**, 19 (21 May 2009), 194512; <https://doi.org/10.1063/1.3139060>

<sup>54</sup> A.P. Drozdov et al., "Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system," *Nature* **525** (03 September 2015), pp. 73–76; <https://doi.org/10.1038/nature14964>

possibility to control  $T_c$  with pressure. Several materials are now predicted to have high  $T_c$  superconducting behavior at HED conditions, and the preponderance of these predictions are for hydrogen rich superconductors.<sup>55,56,57,58,59,60,61</sup> Very high temperature superconductors observed in transient high-pressure experiments might show paths for stabilization of new phases of materials with persistent superconductivity near room temperature with much lower applied pressures. These materials would have high impact in solid state qubit integration for low noise, low loss electrical control of qubits.

Hydrogen is an archetypal system for study of quantum matter.<sup>62</sup> We can now gain access to the phase diagram of hydrogen to new extremes of pressure and density; this can provide a window to the discovery of novel quantum behaviors in a model system that then guides the discovery of novel quantum effects in other materials with potential applications in QIS.

An early example for the formation of QIS relevant quantum materials with tools for HEDS are color center qubits. Here, a recent report shows that local excitation of diamond to a temperature of  $\sim 0.5$  eV ( $\sim 5000$  K) for a few picoseconds, followed by rapid quenching, leads to the direct formation of nitrogen-vacancy color centers without any global thermal annealing.<sup>63</sup> Novel combinations of high pressure, temperature and electronic excitation might lead to the formation of stable color centers for efficient spin-photon conversion in the telecom band, with very high impact potential in quantum communication and the linking of local quantum computer nodes.

There are broad areas of high impact opportunities for quantum materials discoveries enabled by HEDLP to impact emerging applications in QIS, including novel superconductors with very high transition temperatures, designer topological insulators, high temperature Bose-Einstein condensates, quantum-nuclear reactions (e.g., pycnonuclear reactions) and tailored spin-photon qubits.

<sup>55</sup> Xiaolei Feng et al., *RSC Advances* **5**, (2 July 2015), pp. 59292-6; <https://doi.org/10.1039/C5RA11459D>

<sup>56</sup> Hui Wang et al., "Superconductive sodalite-like clathrate calcium hydride at high pressures," *Proceedings of the National Academy of Sciences* **109**, 17 (April 24, 2012), pp. 6463-6; <https://doi.org/10.1073/pnas.1118168109>

<sup>57</sup> Hanyu Liu et al., "Potential high- $T_c$  superconducting lanthanum and yttrium hydrides at high pressure," *Proceedings of the National Academy of Sciences* **114**, 27 (published ahead of print 19 June 2017), pp. 6990-6995; <https://doi.org/10.1073/pnas.1704505114>

<sup>58</sup> Feng Peng et al., "Hydrogen Clathrate Structures in Rare Earth Hydrides at High Pressures: Possible Route to Room-Temperature Superconductivity," *Physical Review Letters* **119** (8 September 2017), 107001; <https://doi.org/10.1103/PhysRevLett.119.107001>

<sup>59</sup> Zachary M. Geballe et al., "Synthesis and Stability of Lanthanum Superhydrides," *Angewandte Chemie* **57**, 3 (29 November 2017), pp. 688-92; <https://doi.org/10.1002/anie.201709970>

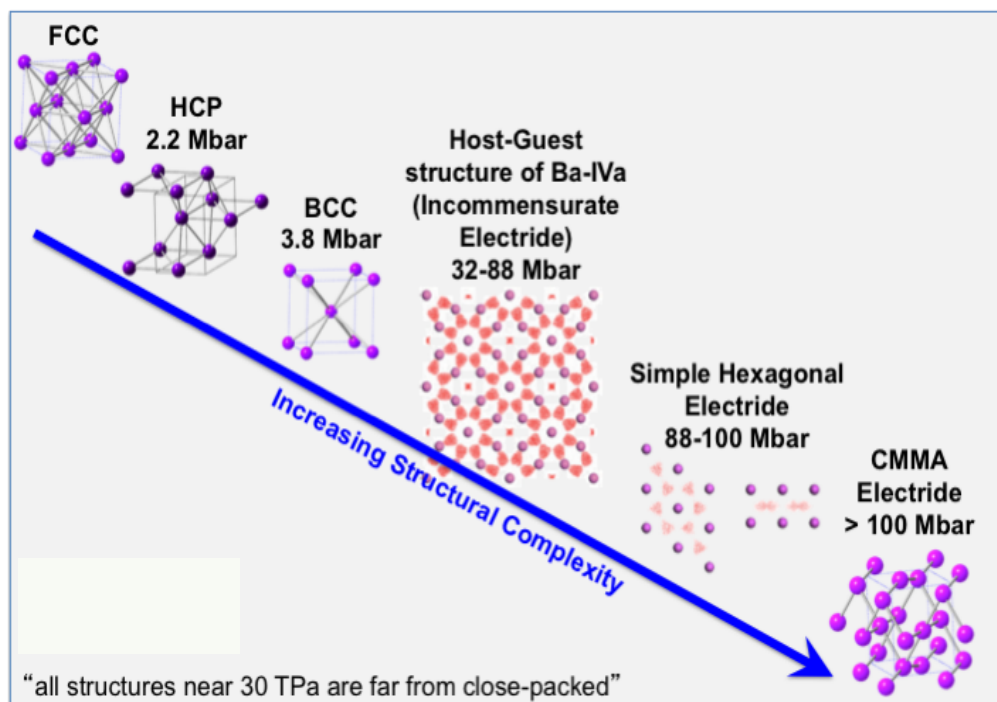
<sup>60</sup> M. Somayazulu et al., personal communication (paper in preparation), 2018.

<sup>61</sup> Siyu Lu et al., "Superconductivity in dense carbon-based materials," *Physical Review B* **93**, (8 March 2016), 104509; <https://doi.org/10.1103/PhysRevB.93.104509>

<sup>62</sup> Jeffrey M. McMahon et al., "The properties of hydrogen and helium under extreme conditions," *Reviews of Modern Physics* **84**, 4 (13 November 2012), 1607; <https://doi.org/10.1103/RevModPhys.84.1607>

<sup>63</sup> J. Schwartz et al., "Local formation of nitrogen-vacancy centers in diamond by swift heavy ions," *Journal of Applied Physics* **116**, 21 (3 December 2014), 214107; <https://doi.org/10.1063/1.4903075>

Tuning the structural order of atoms can create very different properties in materials. Pioneering experiments—inspired by computations and understood with theory—are needed to explore novel ordering of elemental combinations. An example is the structure of Al,<sup>64</sup> as a function of pressure (Figure 2).<sup>65</sup> HEDLP facilities provide a new and unique way to explore these new quantum phenomena.



**Figure 2.** Evolution of the structure of aluminum as a function of pressure. We show this example to illustrate opportunities for the formation of novel quantum materials with tailored properties and potential impact in QIS using techniques from HEDLP.<sup>60, 61</sup>

<sup>64</sup> Chris J. Pickard and R.J. Needs, "Aluminium at terapascal pressures," *Nature Materials* 4 9 (11 July 2010), pp. 624–7; <https://doi.org/10.1038/nmat2796>

<sup>65</sup> Ivan I. Naumov and Russell J. Hemley, "Metallic surface states in elemental electrides," *Physical Review B* 96, 3 (18 July 2017), 035421; <https://doi.org/10.1103/PhysRevB.96.035421>



## PRO 5: RELATIVISTIC PLASMA SCIENCE FOR QUBIT CONTROL AND QUANTUM COMMUNICATION

### Scientific challenge for Quantum Information Science

Photons are ubiquitously used for measurement, sensing and communication. A long-term QIS mission goal is to gain the capability to generate and manipulate multiple entangled photons for quantum sensing, quantum communication, and quantum computing. The field of “quantum sensing”<sup>66</sup> (as also explored in the section on PRO 3, above) offers the potential to dramatically increase measurement sensitivity. Using entangled states or squeezed states, the signal to noise ratio can be enhanced from  $1/\sqrt{N}$  to  $1/N$ , where  $N$  is the number of photons. Hence, in principle, a quantum communications channel has double the channel capacity of a classical communication channel, since the capacity is proportional to the logarithm of the signal to noise ratio. Ultimately, photons may also be used to transmit and even store qubits in scaled quantum computational systems, which offer the potential to dramatically increase computational efficiency for many types of computational problems.

The generation of entangled photon states requires generating efficient nonlinear photon interactions. The ability to individually address and manipulate quantum states also requires nonlinear interactions in order to ensure that the spacing between energy levels is not constant. Optical parametric generators, oscillators and amplifiers can be designed to generate entangled and squeezed states of light. For example, squeezed states were first generated via four-wave mixing in an optical cavity<sup>67</sup> and parametric down-conversion (half-harmonic frequency generation).<sup>68</sup> These methods rely on nonlinear light-matter interactions where the dielectric constant depends on light intensity. The present state-of-the-art uses nonlinear optical crystals to mediate parametric down-conversion and, hence, generate two entangled photons at half the frequency of the incoming photon. However, conversion efficiencies are quite low and the resulting photon intensity is limited by the power handling capabilities of the crystal.

Plasmas and laser-plasma interactions have significant potential to be used as both linear and nonlinear optical elements. Two main advantages are that (i) a plasma can handle very high intensity power fluxes, which cannot be handled by condensed matter systems, and (ii) light-plasma interactions can be switched on and off at pico- or femtosecond timescales, over 1000x faster than solid state counterparts. These capabilities may be essential for a number of applications such as high bandwidth optical communications and ultra-fast optical switches that could help enable large-scale quantum networks.

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66 M.A. Nielsen and I.L. Chuang, *Quantum Computation and Quantum Information*, London: Cambridge University Press, 2000; ISBN: 9781107002173

67 Slusher, R.E. et al., “Observation of Squeezed States Generated by Four-Wave Mixing in an Optical Cavity,” *Physical Review Letters* **55**, 22 (25 November 1985), pp. 2409–12; <https://doi.org/10.1103/PhysRevLett.55.2409>

68 Ling-An Wu et al., “Generation of squeezed states by parametric down-conversion,” *Physical Review Letters* **57**, 20 (17 November 1986), pp. 2520-3; <https://doi.org/10.1103/PhysRevLett.57.2520>

### Barriers to overcome for relativistic laser-plasma interactions to advance QIS

Plasma-light interactions have undergone intensive study for many years and much of this research has been supported by the FES program. Plasma physics research has enabled experimental demonstration and application of plasma-based mirrors,<sup>69</sup> diffraction gratings,<sup>70,71</sup> and laser amplifiers and compressors.<sup>72,73,74</sup> Recently, plasma physicists have gained the ability to manipulate the polarization of light using plasma-based polarizers and wave-plates<sup>75,76,77</sup> that can both generate polarized light and change the polarization of light, e.g., from linearly polarized to circularly polarized (Figure 3). In principle, laser-plasma-based wave-plates allow construction of ultrafast damage-resistant Pockels cells and optical switches. Early research in this area is highly promising and it maps to critical gaps in QIS in the areas of quantum sensing and quantum communication, especially for scaling to larger bandwidth.

Plasma absorption resonances at the electron plasma and ion acoustic frequencies may have to the potential to “slow” light and strongly enhance parametric down-conversion processes, which would boost the rate of entangled photon pair production. Theory, simulations and experimental research in relativistic laser-plasma science can advance control and precision in novel plasma optical elements for QIS applications in specific areas, such as sensing and communication. Barriers to applications of plasma photonics to QIS can be overcome by addressing specific QIS problem areas and by integration of plasma optical elements into quantum sensing and quantum communications experiments of increasing complexity, starting with basic demonstrations, e.g., of ultrafast switching or enhanced production of entangled photon pairs in plasma based nonlinear optical elements.

<sup>69</sup> C. Thaury et al., “Plasma mirrors for ultrahigh-intensity optics,” *Nature Physics* **3**, 424 (15 April 2007); <https://doi.org/10.1038/nphys595>

<sup>70</sup> P. Michel et al., “Tuning the Implosion Symmetry of ICF Targets via Controlled Crossed-Beam Energy Transfer,” *Physical Review Letters* **102**, 2 (14 January 2009), 025004; <https://doi.org/10.1103/PhysRevLett.102.025004>

<sup>71</sup> J. D. Moody et al., “Multistep redirection by cross-beam power transfer of ultrahigh-power lasers in a plasma,” *Nature Physics* **8** (26 February 2012), pp. 344-9; <https://doi.org/10.1038/nphys2239>

<sup>72</sup> G. Shvets et al., “Superradiant Amplification of an Ultrashort Laser Pulse in a Plasma by a Counterpropagating Pump,” *Physical Review Letters* **81**, 22 (30 November 1998), 4879; <https://doi.org/10.1103/PhysRevLett.81.4879>

<sup>73</sup> V. M. Malkin, G. Shvets, and N. J. Fisch, “Fast Compression of Laser Beams to Highly Overcritical Powers,” *Physical Review Letters* **82**, 22 (31 May 1999), 4448; <https://doi.org/10.1103/PhysRevLett.82.444>

<sup>74</sup> Jun Ren et al., “A new method for generating ultraintense and ultrashort laser pulses,” *Nature Physics* **3** (9 September 2007), pp. 732-6; <https://doi.org/10.1038/nphys717>

<sup>75</sup> P. Michel et al., “Optical Wave Mixing in Plasmas,” *Physical Review Letters* **113**, 20 (14 November 2014), 205001; <https://doi.org/10.1103/PhysRevLett.113.205001>

<sup>76</sup> D. Turnbull et al., “High Power Dynamic Polarization Control Using Plasma Photonics,” *Physical Review Letters* **116**, 20 (18 May 2016), 205001; <https://doi.org/10.1103/PhysRevLett.116.205001>

<sup>77</sup> D. Turnbull et al., “Refractive Index Seen by a Probe Beam Interacting with a Laser-Plasma System,” *Physical Review Letters* **118**, 1 (5 January 2017), 015001; <https://doi.org/10.1103/PhysRevLett.118.015001>

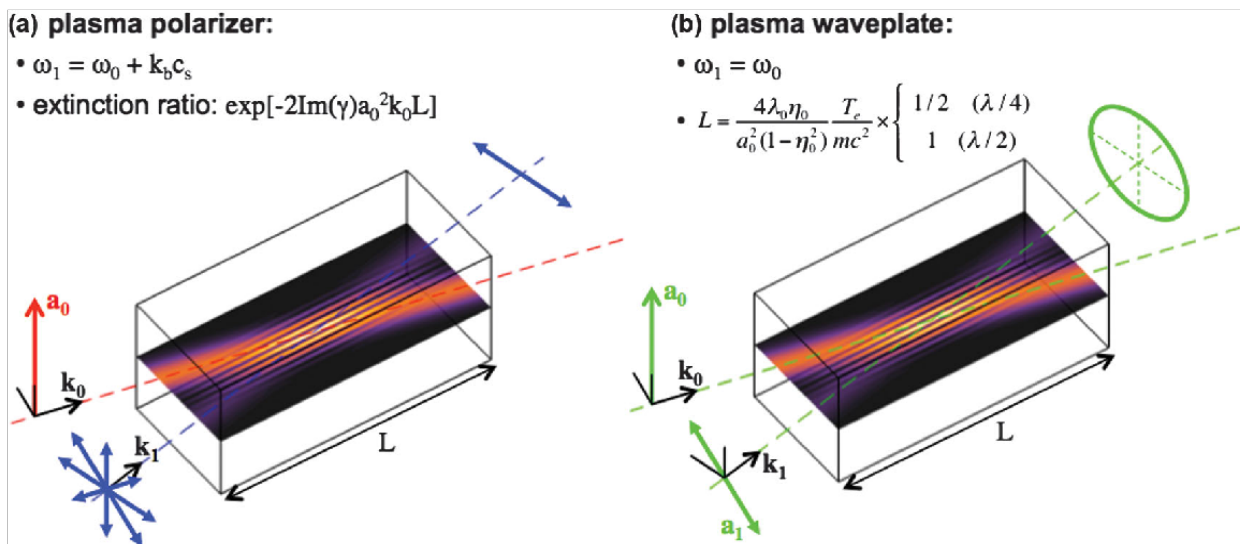


Figure 3. Laser-plasma interactions can dynamically control polarization of light on ultrafast timescales. (From P. Michel et al., "Optical Wave Mixing in Plasmas," *Physical Review Letters* **113**, 20 (14 November 2014), 205001; <https://doi.org/10.1103/PhysRevLett.113.205001>).

### Potential Impact for QIS

Plasma photonics has the potential to efficiently generate and manipulate high intensity beams of entangled and squeezed states of light on ultrafast timescales. Development of optical quantum sensors with a high signal-to-noise ratio could revolutionize measurement capabilities in many fields of science. Using nonlinear light-plasma interactions could ultimately enable optical qubits to become a routine means to transfer and store information in quantum computers. Exploiting light-plasma interactions may provide a route to damage-resistant optics that can simultaneously achieve high beam intensity and high entanglement/squeezing amplitude. Developing high intensity entangled light sources could have a major impact on high-bandwidth secure quantum communications.

## PRO 6: PLASMA SCIENCE TOOLS FOR SIMULATION AND CONTROL OF QUANTUM SYSTEMS

### Scientific challenge for Quantum Information Science

Particles in traps are both idealized plasmas and promising qubit systems, connecting core areas of Fusion Energy Sciences and Quantum Information Science. Ion traps are among the most advanced quantum technologies with exquisite control of states in strings of ions that are trapped by electromagnetic potentials. Recent studies of trapped anti-hydrogen atoms for tests of standard model physics were enabled by advanced classical particle-in-cell simulations.<sup>78</sup> It is a critical QIS challenge to design ion traps with high fidelity quantum gates and possibility for scaling to large numbers of qubits. Further, efficient coupling to “flying qubits” for coherent communication between quantum computing nodes will likely be essential for scaling of quantum computers to more than a few thousand physical qubits. This development relies on advanced simulations of particle confinement and control fields. Applied mathematics and software tools and techniques developed in Fusion Energy Sciences that are widely used in the plasma science community can play a crucial role in the advancement of trapped particle qubits (both ions and electrons).

Enormous progress has been made in manipulating qubits using ion traps, including demonstration of a scalable quantum Fourier transform,<sup>79</sup> and 14-qubit entanglement.<sup>80</sup> The scalable designs for quantum computing involve RF surface electrode ion traps, which are a surface variant of the more conventional Paul trap. Additionally, many-ion plasma crystals in one or two dimensions utilizing either a Paul or Penning trap configuration are beginning to demonstrate analog quantum simulation,<sup>81,82</sup> as well as sensing zero-point quantum fluctuations.<sup>83</sup> Understanding the motional dynamics of the ions is critical for proper operation and success of these quantum science experiments. The energy spectrum of the normal mode

<sup>78</sup> M. Ahmadi et al., “Characterization of the 1S–2S transition in antihydrogen,” *Nature* **557** (4 April 2018), pp. 71-5; <https://doi.org/10.1038/s41586-018-0017-2>

<sup>79</sup> J. Chiaverini et al., “Implementation of the Semiclassical Quantum Fourier Transform in a Scalable System,” *Science* **308**, 5724 (13 May 2005), pp. 997-2000; <https://doi.org/10.1126/science.1110335>

<sup>80</sup> Thomas Monz et al., “4-Qubit Entanglement: Creation and Coherence,” *Physical Review Letters* **106**, 13 (31 March 2011), 130506; <https://doi.org/10.1103/PhysRevLett.106.130506>

<sup>81</sup> R. Blatt and C.F. Roos, “Quantum simulations with trapped ions,” *Nature Physics* **8** (2 April 2012), pp. 277-284; <https://doi.org/10.1038/nphys2252>

<sup>82</sup> Justin G. Bohnet et al., “Quantum spin dynamics and entanglement generation with hundreds of trapped ions,” *Science* **352**, 6291 (10 June 2016), pp. 1297-1301; <https://doi.org/10.1126/science.aad9958>

<sup>83</sup> K.A. Gilmore et al., “Amplitude Sensing below the Zero-Point Fluctuations with a Two-Dimensional Trapped-Ion Mechanical Oscillator,” *Physical Review Letters* **118**, 26 (29 June 2017), 263602; <https://doi.org/10.1103/PhysRevLett.118.263602>

vibrations is a nonlinear problem and can be addressed to high accuracy using classical and semi-classical simulation including a fairly detailed Doppler or sub-Doppler<sup>84</sup> laser cooling model. Both the linear ion-chains and two-dimensional ion plasma crystals are of particular interest and these experiments can benefit enormously from computational support using applied mathematics and software tools widely available within the plasma science community. The culture of plasma theory supported by FES includes a longer-term focus on developing first-principles models of nonlinear plasmas using long-time integration with high accuracy and proper conservation properties utilizing the fastest supercomputers.

For Penning type ion traps used in quantum simulation that employ a circular disk-shaped ion crystal (Figure 4), equipartition is often assumed and the coupling between the axial and planar directions are not well understood. Though the ion crystal is extremely cold (a fraction of a millikelvin) the coupling between normal modes is still a nonlinear process mediated by the Coulomb interaction between ions. Axial (along the confining B-field) motion can be well diagnosed, but planar (perpendicular to B) motion cannot. Planar cooling requires balancing the torque from the cooling laser and a time-dependent rotating wall potential, and has subtleties which may be better understood with direct numerical simulation.<sup>85</sup> Other important problems include the modeling of infrequent background neutral collisions, the non-adiabatic motion of trapped ions in anharmonic ponderomotive potential<sup>86</sup> and transporting of ions within a RF surface trap circuit.

In the plasma science context, simulations track both linear and non-linear dynamics in quantum systems that are often open and dissipative. For qubits, uncontrolled coupling to their environment causes loss of coherence, and managing controlled couplings to qubit environments is a central theme in scaling qubit systems and in extending their operation coherence times. Tools and techniques developed in plasma science, such as active feedback control techniques, can be highly impactful in advancing our understanding and control of more open quantum systems with nonlinear dynamics.

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<sup>84</sup> Y. Lin et al., “Sympathetic Electromagnetically-Induced-Transparency Laser Cooling of Motional Modes in an Ion Chain,” *Physical Review Letters* **110**, 15 (8 April 2013), 153002; <https://doi.org/10.1103/PhysRevLett.110.153002>

<sup>85</sup> Steven B. Torrioni et al., “Perpendicular laser cooling with a rotating-wall potential in a Penning trap,” *Physical Review A* **93**, 4 (26 April 2016), 043421; <https://doi.org/10.1103/PhysRevA.93.043421>

<sup>86</sup> J. Mikosch et al., “Evaporation of Buffer-Gas-Thermalized Anions out of a Multipole rf Ion Trap,” *Physical Review Letters* **98**, 22 (30 May 2007), 223001; <https://doi.org/10.1103/PhysRevLett.98.223001>



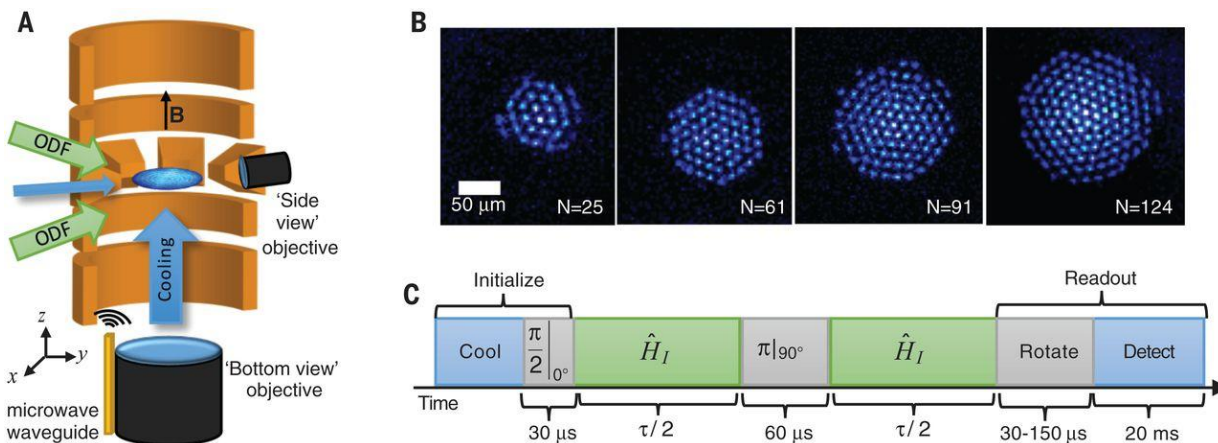


Figure 4. Quantum simulation of entanglement dynamics using an ion plasma crystal. From Justin G. Bohnet et al., “Quantum spin dynamics and entanglement generation with hundreds of trapped ions,” *Science* **352**, 6291 (10 June 2016), pp. 1297-1301; <https://doi.org/10.1126/science.aad9958>

### Barriers to overcome to advance QIS

Powerful particle-in-cell codes and (semi)-classical solvers for electromagnetic simulations already exist, but refinement of computational methods and the development of advanced simulation approaches is needed to be able to track particle traps with increasing number of qubits and increasing complexity of interaction dynamics. Going from proof-of-concept demonstrations with a few to tens of qubits to scaling to many hundreds of qubits is required in order for particle-trap-based qubits to realize their potential as viable platforms for quantum simulations (near term) and error corrected quantum computing (long term). Investments in the development of these advanced (semi)-classical simulations tools promises to significantly increase the rate of progress in the trapped ion qubit platforms. It will also advance emerging qubit concepts such as trapped electron qubits,<sup>87</sup> which have complementary advantages and challenges compared to trapped ions (e.g., potential for faster gate times due to the lighter electron mass, but increased difficulty in reliable trapping and addressing). For trapped electrons, a hybrid system has electron qubits floating on the surface of liquid helium, where ultra-low spin-orbit coupling in a nuclear-spin-free environment leads to very long spin coherence times.<sup>88</sup> Again, advanced simulation tools from the plasma community can greatly enhance the rate of progress in these qubit platforms. One underlying assumption is that it is too early to pick winners in the race for the “best” qubit system. Indeed, complementary advantages from a series of approaches are likely going to lead to fundamental scientific discoveries and show paths to practical applications in selected areas.

<sup>87</sup> P. Peng, C. Matthiesen, and H. Häffner, “Spin readout of trapped electron qubits,” *Physical Review A* **95**, 1 (12 January 2017), 012312; <https://doi.org/10.1103/PhysRevA.95.012312>

<sup>88</sup> F.R. Bradbury et al., “Efficient Clocked Electron Transfer on Superfluid Helium,” *Physical Review Letters* **107**, 26 (23 December 2011), 266803; <https://doi.org/10.1103/PhysRevLett.107.266803>

Communication between the QIS communities that drive the development of trapped particle qubits and the plasma science community may be a trivial barrier; yet enhancing opportunities of information exchange will likely lead to increased awareness of challenges and opportunities for fruitful exchange and collaboration.

Viewing trapped particles as idealized plasmas lets us consider transitions to non-linear and dissipative conditions as they pertain to large scale fusion relevant plasmas. A barrier to overcome to advance QIS is to make the connection across time and length scales from fusion relevant plasmas and to transpose concepts to the trapped particle environments. Processes that lead to loss of phase coherence of qubits have analogies with the phenomenon of Landau damping in plasma physics. Here, information is never actually “lost”; it is mixed to finer and finer scales in phase space. The fine-scale mixing process accelerates the generation of entropy through particle collisions. Information can be recalled by using a plasma “echo” technique up to the point at which the information is finally permanently scrambled by collisions, and these tools and concepts could be applied to the idealized plasmas of trapped particle qubits to develop methods for coherence protection.

### **Potential Impact for QIS**

Development of advanced (semi)-classical simulation tools and applying them to trapped particle qubits has the potential to greatly enhance the rate of progress in our fundamental understanding of control and decoherence limiting factors in trapped particle qubits and to develop viable paths for scaling of trapped particle qubit systems from tens to potentially hundreds and thousands of qubits.

Adapting control theory and feedback methods that are being developed in plasma science for non-linear, dissipative plasmas to the idealized trapped particle environment can lead to great advances in our fundamental understanding of coherence limiting factors across many time and lengths scales and can potentially impact the development of efficient error correction schemes for trapped particle qubits. Understanding noise sources and ways to mitigate uncontrolled interactions with their environment is required for large scale integration of trapped particle qubits, e.g., beyond nearest neighbor coupling, with proposals for shuttling of ions in traps where increased decoherence due to heating is a critical problem.

New strategies for maintaining quantum coherent states in the presence of control errors and decoherence-inducing processes could lead to improved performance and novel approaches to error correction and mitigation. Ultimately, this research could lead to a fundamentally new understanding of extremely open quantum systems.

A perhaps ironic twist is that early quantum simulations with trapped ion qubits can simulate model interaction Hamiltonians whose results can be compared to (semi)-classical simulations of ions in traps. The high degree of control in trapped ion qubits can enable discoveries of fundamental plasma dynamics with iterative application of advancing classical and emerging quantum simulation tools.

## APPENDIX A. AGENDA

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### 2018 FES Roundtable on Quantum Information Science

Hilton Gaithersburg, 620 Perry Parkway, Gaithersburg, Maryland 20877, May 01 – 02, 2018

#### Monday, April 30

7 pm, Optional working dinner

#### Tuesday, May 01

8:30 am	Opening remarks, Jim Van Dam and John Mandrekas
8:45	Emerging opportunities in Quantum Information Science, Steve Binkley
9:20	FES for QIS, Thomas Schenkel
9:40	QIS for FES, Bill Dorland
10 – 10:30	Coffee break
10:30	Discussion led by panel members (10 minutes each)
12:30 – 1:30 pm	Working lunch
1:30	Breakout sessions – FES for QIS, QIS for FES
3 – 3:30	Coffee break
4:30	Panel session, joint discussion of results from breakout sessions
5:30	Adjourn
7	Working dinner

#### Wednesday, May 02

8:30 am	Panel session – reports from breakout sessions
10 – 10:30	Coffee break
12 – 1 pm	Working lunch
1	Breakout sessions
3	Sum-up: Challenges, Opportunities, Assignments, Next steps
4	Adjourn

## APPENDIX B. PARTICIPANTS

### Chairs

Thomas Schenkel                      Lawrence Berkeley National Laboratory

### Co-Chair

Bill Dorland                              University of Maryland

### Panel members

Andrew Baczewski	Sandia National Laboratories
Malcolm Boshier	Los Alamos National Laboratory
Rip Collins	University of Rochester
Jonathan Dubois	Lawrence Livermore National Laboratory
Andrew Houck	Princeton University
Travis Humble	Oak Ridge National Laboratory
Nuno Loureiro	Massachusetts Institute of Technology
Chris Monroe	University of Maryland
Scott Parker	University of Colorado
Francis Robicheaux	Auburn University
Edward Startsev	Princeton Plasma Physics Laboratory
Matt Trevithick	Google Research
George Vahala	College of William and Mary

### Observers

Amitava Bhattacharjee	Princeton Plasma Physics Laboratory
John Canik	Oak Ridge National Laboratory
Ilon Joseph	Lawrence Livermore National Laboratory
David Schissel	General Atomics
Xianzhu Tang	Los Alamos National Laboratory

### DOE Office of Science

Kramer Akli	Fusion Energy Sciences
Steve Binkley	Office of Science
Atlaf Carim	High Energy Physics
Claire Cramer	Advanced Scientific Computing Research
Jim Horwitz	Basic Energy Sciences
John Mandrekas	Fusion Energy Sciences
Gulshan Rai	Nuclear Physics
James Van Dam	Fusion Energy Sciences

### Web links:

- <https://science.energy.gov/fes/community-resources/workshop-reports/>
- [https://science.energy.gov/fes/community-resources/workshop-reports/QIS FES Roundtable Report 2018](https://science.energy.gov/fes/community-resources/workshop-reports/QIS_FES_Roundtable_Report_2018)



*Roundtable participants*

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