Quantum computing and simulations for nuclear physics

Dean Lee Facility for Rare Isotope Beams Michigan State University

NSAC Long Range Plan Town Hall Meeting on Nuclear Structure, Reactions, and Astrophysics

November 14, 2022





Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

The rule of simulation that I would like to have is that the number of computer elements required to simulate a large physical system is only to be proportional to the space-time volume of the physical system. I don't want to have an explosion. That is, if you say I want to explain this much physics, I can do it exactly and I need a certain-sized computer. If doubling the volume of space and time means I'll need an *exponentially* larger computer, I consider that against the rules (I make up the rules, I'm allowed to do that). Let's start with a few interesting questions.

And I'm not happy with

all the analyses that go with just the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy. Thank you.



NSF Quantum Leap Challenge Institutes



QLCI-CI: NSF Quantum Leap Challenge Institute for Present and Future Quantum Computing University of California-Berkeley; Start Date: 09/01/2020; Award Amount: \$23,936,988

QLCI-CI: NSF Quantum Leap Challenge Institute for Robust Quantum Simulation University of Maryland, College Park; Start Date: 09/01/2021; Award Amount: \$20,950,000

QLCI-CI: NSF Quantum Leap Challenge Institute for Quantum Sensing in Biophysics and Bioengineering University of Chicago; Start Date:09/01/2021; Award Amount: \$20,950,000

QLCI-CI: NSF Quantum Leap Challenge Institute for Enhanced Sensing and Distribution Using Correlated Quantum States University of Colorado at Boulder; Start Date:09/01/2020; Award Amount: \$24,000,000

QLCI-CI: NSF Quantum Leap Challenge Institute for Hybrid Quantum Architectures and Networks University of Illinois at Urbana-Champaign; Start Date:09/01/2020; Award Amount:\$23,536,605 Advances in quantum science and technology have the potential to revolutionize research. The U.S. Department of Energy (DOE) is at the forefront of this burgeoning field. Led by a DOE national laboratory, each National Quantum Information Science Research Center represents a partnership of labs, universities, and private companies. Together, the five centers are developing technologies that go beyond what was previously imaginable.

 At the National QIS Research Centers, scientists and engineers work on designing and building

 • powerful quantum computers
 • ultrasensitive instruments and sensors

 • unhackable communication networks
 • groundbreaking new materials



Website: bnl.gov/quantumcenter Lead laboratory: Brookhaven National Laboratory

The Co-design Center for Quantum Advantage (C²QA) aims to overcome the limitations of today's noisy intermediate scale quantum (NISQ) computer systems to achieve quantum advantage for scientific computations in high-energy, nuclear, chemical, and condensed matter physics. Its technology focus is superconducting microwave circuits and modules for quantum computation and hybrid superconducting/optical devices for quantum communication. The integrated five-year aspirational goal of C²QA is to deliver a factor of 10 improvement in software optimization, underlying materials and device properties, and quantum error correction, and to ensure these improvements combine to provide a factor of 1,000 improvement in appropriate metrics for computation and communication.



Website: q-next.org Lead laboratory: Argonne National Laboratory

Q-NEXT brings together leading experts from national laboratories, academia and the private sector to develop the science and technology to control and distribute quantum information. The center develops technologies to enable: secure communication over long distances using quantum repeaters; quantum sensors to achieve unprecedented sensitivities; and processing and test beds for quantum simulators and future full-stack universal quantum computers. Q-NEXT will also create two national foundries for quantum materials, establish a first-ever National Quantum Devices Database for the standardization of next-generation quantum devices, and train the next-generation quantum workforce through innovative programs with industry, academia, and government.



QUANTUM SYSTEMS ACCELERATOR Catalyzing the Quantum Ecosystem

Website: quantumsystemsaccelerator.org Lead laboratory: Lawrence Berkeley National Laboratory

The Quantum Systems Accelerator (QSA) will catalyze national leadership in quantum information science to co-design the algorithms, quantum devices, and engineering solutions needed to deliver certified quantum advantage in scientific applications. Led by Lawrence Berkeley National Laboratory with lead partner Sandia National Laboratories, the QSA brings together dozens of scientists who are pioneers of many of today's quantum capabilities from 15 institutions. The team pairs advanced quantum prototypes — based on neutral atoms, trapped ions, and superconducting circuits — with algorithms specifically designed for imperfect hardware to demonstrate optimal applications for each platform in scientific computing, materials science, and fundamental physics.





Website: qscience.org Lead laboratory: Oak Ridge National Laboratory

The Quantum Science Center (QSC) performs cutting edge research at national laboratories, universities, and industry partners to overcome key roadblocks in quantum state resilience, controllability, and ultimately the scalability of quantum technologies. QSC researchers are designing materials that enable topological quantum computing; implementing new quantum sensors to characterize topological states and detect dark matter; and designing quantum algorithms and simulations to provide a greater understanding of quantum materials, chemistry, and quantum field theories. These innovations will enable the QSC, headquartered at ORNL, to accelerate information processing, explore the previously unmeasurable, and better predict quantum performance across technologies.





Website: sqms.fnal.gov Lead laboratory: Fermi National Accelerator Laboratory

The Superconducting Quantum Materials and Systems Center (SQMS) brings together partners from national laboratories, academia, and industry to make revolutionary advances in quantum information science, including the building and deployment of the first quantum computer at Fermilab. A key SQMS goal is to extend the 'coherence time' of quantum states – the lifetime of a qubit or a quantum sensor. Building on a world-record coherence time, demonstrated at Fermilab in superconducting devices, and drawing on world-class expertise in materials science, condensed matter physics, particle physics, and computational science, SQMS will deliver new national QIS platforms for scientific discovery.



approximately \$115,000,000 over five years

QIS Crosses the Technical Breadth of the Office of Science



Nuclear Physics and Quantum Information Science



Summary of Recommendations

• R1A: We recommend establishing one or more multiinstitutional Quantum Co-Development Consortia for simulation. These Co-Development Consortia should pursue and facilitate the development of quantum simulation capabilities for NP research and utilize NP expertise in quantum many-body physics and quantum field theory to impact quantum information science and quantum computing;

• R1B: We recommend establishing one or more multiinstitutional Quantum Co-Development Consortia for sensors focused on targeted, prioritized, cross-disciplinary developments in quantum-enhanced sensing for NP research;

• R2: We recommend that DOE and NSF encourage and support selected exploratory technologies and techniques that have promise to be of mutual benefit to NP and QIS research activities;

• R3: With the expectation of mutual benefit, we recommend strengthening the QIS and QC expertise in the NP workforce.





InQubator for Quantum Simulation

About Us 🗸

Science

Nuclear physics is expected to advance and be advanced by quantum information science research in quantum many-body systems, quantum field theories and fundamental physics.

People

Seminars

Our Mission

IQuS aims to improve understanding of strongly interacting, correlated matter and complex quantum systems of importance to nuclear physics and quantum information science, from the familiar to the exotic, using quantum simulations and emerging theoretical techniques where quantum entanglement and coherence are essential ingredients. Local researchers, visitors, and community-driven workshops at the Institute of Nuclear Theory, along with close connections with national laboratories and technology companies, will help create and disseminate new ideas and grow a quantum-ready workforce.

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QUANTUM HORIZONS: QIS RESEARCH AND INNOVATION FOR NUCLEAR SCIENCE

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER: DE-FOA-0002110

> FOA TYPE: INITIAL CFDA NUMBER: 81.049

FOA Issue Date:	April 8, 2019
Submission Deadline for Applications:	May 31, 2019, at 5 PM Eastern

QUANTUM HORIZONS: QIS RESEARCH AND INNOVATION FOR NUCLEAR SCIENCE

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER: DE-FOA-0002514

> FOA TYPE: INITIAL CFDA NUMBER: 81.049

FOA Issue Date:	May 6, 2021		
Submission Deadline for Letters of Intent:	May 21, 2021, at 5:00 PM Eastern Time		
	A Letter of Intent is encouraged		
Letter of Intent Response Date	May 26, 2021, at 5:00 PM Eastern Time		
Submission Deadline for Applications:	June 18, 2021, at 5:00 PM Eastern Time		

up to \$6,800,000

up to \$10,000,000

Qubits

The basic element in quantum computation is the qubit, which is a simply a two-level quantum system.

$$|0\rangle = \begin{bmatrix} 1\\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0\\ 1 \end{bmatrix}$$

There are also extensions to systems with more than two levels, known as qudits. But we will focus on qubits in these lectures.

In general, our qubit will be in a general superposition of the two states.

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \qquad |\psi\rangle = \alpha \begin{bmatrix} 1\\0 \end{bmatrix} + \beta \begin{bmatrix} 0\\1 \end{bmatrix} = \begin{bmatrix} \alpha\\\beta \end{bmatrix}$$

With proper normalization we have

$$|\alpha|^2 + |\beta|^2 = 1$$

Single-Qubit Gates

Since the evolution of quantum systems is unitary, all quantum gates are unitary.

Pauli-X gate (NOT gate)
$$\mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
 $\mathbf{X} = \begin{bmatrix} \mathbf{X} \\ \mathbf{X} \end{bmatrix}$
Pauli-Y gate $\mathbf{Y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ $\mathbf{Y} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{Y} \end{bmatrix}$

Hadamard gate $\mathbf{H} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$ \mathbf{H}

Phase gate

$$\mathbf{R}_{\phi} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} - \mathbf{R}_{\phi}$$

Two-Qubit Gate

Controlled-NOT (C-NOT) gate









rigetti







Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu, A. J. McCaskey, G. Hagen, G. R. Jansen, T. D. Morris, T. Papenbrock, R. C. Pooser, D. J. Dean, and P. Lougovski Phys. Rev. Lett. **120**, 210501 – Published 23 May 2018

PhySICS See Viewpoint: Cloud Quantum Computing Tackles Simple Nucleus



FIG. 2. (Color online) Experimentally determined energies for H_2 (top) and expectation values of the Pauli terms that enter the two-qubit Hamiltonian H_2 as determined on the QX5 (center) and 19Q (bottom) chips. Experimental (theoretical) results are denoted by symbols (lines).

	E from exact diagonalization				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$	
2	-1.749	-2.39	-2.19		
3	-2.046	-2.33	-2.20	-2.21	
E from quantum computing					
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$	
2	-1.74(3)	-2.38(4)	-2.18(3)		
3	-2.08(3)	-2.35(2)	-2.21(3)	-2.28(3)	

Variational approaches to constructing the many-body nuclear ground state for quantum computing

I. Stetcu, A. Baroni, and J. Carlson Phys. Rev. C **105**, 064308 – Published 21 June 2022

$$\begin{split} |\Psi(\vec{\theta})\rangle &= \exp\left(U(\vec{\theta})\right) |\Psi_{0}\rangle \\ U(\vec{\theta}) &= \sum_{i,m} \theta_{im} \left(a_{i}^{\dagger} a_{m} - a_{m}^{\dagger} a_{i}\right) \\ &+ \sum_{i < j;m < n} \theta_{ij;mn} \left(a_{i}^{\dagger} a_{j}^{\dagger} a_{n} a_{m} - a_{m}^{\dagger} a_{n}^{\dagger} a_{j} a_{i}\right) + \cdots, \end{split} \qquad \begin{array}{c} 1.5 \\ 0.0 \\ 0.0 \\ -1.5 \end{array}$$

 $heta_{0123}/\pi$

Quantum computing of the $^{6}\mathrm{Li}$ nucleus via ordered unitary coupled clusters

Oriel Kiss, Michele Grossi, Pavel Lougovski, Federico Sanchez, Sofia Vallecorsa, and Thomas Papenbrock Phys. Rev. C **106**, 034325 – Published 29 September 2022



TABLE II. Hardware results of the QBE-UCC ansatz for the ground state (g.s.) and first excited state (1st es), alongside the number of parameters and CNOT gates after transpilation. The exact result, obtained with exact diagonalization, are reproduced up to one standard deviation.

hardware	No. parameters	No. CNOT	mean	st. deviation	exact	error ratio
ibmq_mumbai raw (g.s.)	9	209	-6.27	0.269	-5.529	13.36%
ibmq_mumbai mitigated (g.s.)	9	209	-5.319	0.24	-5.529	3.81%
ibmq_mumbai raw (1st es)	3	41	-2.907	0.87	-3.420	14.97%
ibmq_mumbai mitigated (1st es)	3	41	-3.424	0.08	-3.420	0.12%

Dynamic linear response quantum algorithm

Alessandro Roggero and Joseph Carlson Phys. Rev. C **100**, 034610 – Published 13 September 2019



Preparation of excited states for nuclear dynamics on a quantum computer

Alessandro Roggero, Chenyi Gu, Alessandro Baroni, and Thomas Papenbrock Phys. Rev. C **102**, 064624 – Published 28 December 2020

$$|\Phi_E
angle = rac{1}{\eta} O |\Psi_0
angle ~~ ext{with}~~~\eta = \|O|\Psi_0
angle\|~,$$





FIG. 6. (Color online) Results on the transition probability P_t for time dependent method with the VM run (a) and QPU run (b) and exact analysis (green line). Results are given with (red squares) and without (black squares) full mitigation.

Optimal control for the quantum simulation of nuclear dynamics

Eric T. Holland, Kyle A. Wendt, Konstantinos Kravvaris, Xian Wu, W. Erich Ormand, Jonathan L DuBois, Sofia Quaglioni, and Francesco Pederiva Phys. Rev. A **101**, 062307 – Published 3 June 2020

Demonstration of noise-resilient real-time evolution of two interacting neutrons on the LLNL quantum testbed

- Prepare QPU initial state: e.g., | + +
- Perform time evolution by dividing into small time steps: repeat same gate at each time step
- Due to the nucleons' interaction, with time the QPU evolves into an entangled superposition of the 3 states
- Measure time-dependent probability with which QPU occupies each spin state



[from Sofia Quaglioni]

Quantum state preparation by adiabatic evolution with custom gates

Eduardo A. Coello Pérez, Joey Bonitati, Dean Lee, Sofia Quaglioni, and Kyle A. Wendt Phys. Rev. A **105**, 032403 – Published 2 March 2022



Ab initio nuclear structure via quantum adiabatic algorithm

Weijie $Du^{a,b}$, James P. Vary^a, Xingbo Zhao^{b,c}, and Wei Zuo^{b,c}

arXiv:2105.08910



Imaginary-time propagation on a quantum chip

F. Turro, A. Roggero, V. Amitrano, P. Luchi, K. A. Wendt, J. L. Dubois, S. Quaglioni, and F. Pederiva Phys. Rev. A **105**, 022440 – Published 28 February 2022

$$\hat{U}(\tau) = \begin{pmatrix} \hat{Q}_{\rm ITP}(\tau) & \frac{1}{\sqrt{1 + e^{-2(\hat{H} - E_T)\tau}}} \\ \frac{1}{\sqrt{1 + e^{-2(\hat{H} - E_T)\tau}}} & -\hat{Q}_{\rm ITP}(\tau) \end{pmatrix} \qquad \hat{Q}_{\rm ITP}(\tau) = \left(1 + e^{-2(\hat{H} - E_T)\tau}\right)^{-1/2} e^{-(\hat{H} - E_T)\tau}$$



An Alternative Approach to Quantum Imaginary Time Evolution

Pejman Jouzdani,^{1,*} Calvin W. Johnson,² Eduardo R. Mucciolo,³ and Ionel Stetcu⁴

arXiv: 2208.10535



FIG. 3. (a) Relative difference between the computed ground state energy and the exact value for the ITE (blue circle) and MQITE (orange cross) methods as a function of the imaginary time. Real (b) and imaginary (c) parts of the components of the quantum state $|\psi_{\tau}\rangle$ at the final time evolution time step ($\tau = 3/J$) for the ITE and MQITE methods.

Radiative processes on a quantum computer

Paulo F. Bedaque,^{1, *} Ratna Khadka,^{2, †} Gautam Rupak,^{2, ‡} and Muhammad Yusf^{2, §}

arXiv:2105.08910

$$H_{T} = \mathbb{1} \otimes H + \frac{\omega}{2} (\mathbb{1} - Z) \otimes \mathbb{1} + c_{0} X \otimes O_{T},$$
$$\hat{H} = -\frac{1}{2\hat{m}} \sum_{l} [\hat{\psi}_{l}^{\dagger} \hat{\psi}_{l+1} + \hat{\psi}_{l+1}^{\dagger} \hat{\psi}_{l} - 2\hat{\psi}_{l}^{\dagger} \hat{\psi}_{l}] + \sum_{l} \hat{V}_{l} \hat{\psi}_{l}^{\dagger} \hat{\psi}_{l} + \frac{\omega}{2} (\mathbb{1} - Z) + qe\sigma^{2} X \sum_{l} l \hat{\psi}_{l}^{\dagger} \hat{\psi}_{l}, \quad (4)$$



Improving Hamiltonian encodings with the Gray code

Olivia Di Matteo, Anna McCoy, Peter Gysbers, Takayuki Miyagi, R. M. Woloshyn, and Petr Navrátil Phys. Rev. A **103**, 042405 – Published 2 April 2021

$000 \rightarrow \mathbf{100} \rightarrow 1\mathbf{10} \rightarrow \mathbf{010} \rightarrow 01\mathbf{1} \rightarrow \mathbf{111} \rightarrow 1\mathbf{01} \rightarrow \mathbf{001} \rightarrow 00\mathbf{0}.$



Classical and quantum evolution in a simple coherent neutrino problem

Joshua D. Martin, A. Roggero, Huaiyu Duan, J. Carlson, and V. Cirigliano Phys. Rev. D **105**, 083020 – Published 27 April 2022

$$H = \sum_{i} \left[\frac{\omega_{i}}{2} \vec{B} \cdot \vec{\sigma}_{i} \right] + \frac{\sqrt{2}G_{\rm F}}{2V} \sum_{i < j} \left(1 - \mathbf{v}_{i} \cdot \mathbf{v}_{j} \right) \vec{\sigma}_{i} \cdot \vec{\sigma}_{j}$$



Simulation of collective neutrino oscillations on a quantum computer

Benjamin Hall, Alessandro Roggero, Alessandro Baroni, and Joseph Carlson Phys. Rev. D **104**, 063009 – Published 3 September 2021



Time-dependent Hamiltonian Simulation Using Discrete Clock Constructions

Jacob Watkins¹, Nathan Wiebe^{2,3,4}, Alessandro Roggero^{5,6,7}, Dean Lee¹



arXiv: 2203.11353

Accessing ground-state and excited-state energies in a many-body system after symmetry restoration using quantum computers

Edgar Andres Ruiz Guzman and Denis Lacroix Phys. Rev. C **105**, 024324 – Published 22 February 2022

Filtering states with total spin on a quantum computer

Pooja Siwach and Denis Lacroix Phys. Rev. A **104**, 062435 – Published 21 December 2021

Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers

A quantum many-body perspective

arXiv:2208.11567

Denis Lacroix^{a,1}, Edgar Andres Ruiz Guzman^{b,1}, Pooja Siwach^{c,2}

Simulating excited states of the Lipkin model on a quantum computer

Manqoba Q. Hlatshwayo¹,* Yinu Zhang¹, Herlik Wibowo², Ryan LaRose³, Denis Lacroix⁴, and Elena Litvinova^{1,5}

arXiv: 2203.01478



Rodeo algorithm



Choi, D.L., Bonitati, Qian, Watkins, PRL 127, 040505 (2021)



	Exact	IBM Perth	IBM Perth	Quantinuum H1-2
		Three Cycles	Five Cycles	Five Cycles
$ \psi_0 angle$	-4.0000	-4.0022(49)	-4.0006(42)	-3.9982(21)
$ \psi_1 angle$	-1.0000	-0.9829(56)	-0.9927(40)	-1.0083(39)
$ \psi_2 angle$	1.0000	1.0007(26)	1.0008(19)	1.0028(22)
$ \psi_3 angle$	4.0000	4.0093(84)	3.9982(25)	4.0036(17)

Bee-Lindgren, Qian, DeCross, Brown, Gilbreth, Watkins, Zhang, D.L., arXiv:2208.13557

Vision for the future



Real time dynamics and spectral functions

Vision for the future



Vision for the future

Example: lattice effective field theory on quantum computers



error rate $< 0.05 L^{-3}$

qubits $=4L^3$

New Computing Technologies (QC, AI/ML)

Program for 15 November 2022

Quantum Computing (QC)

15:20 Kyle Wendt – Overview – 15 min
15:35 Joe Carlson – 5 min
15:40 Gautam Rupak – 5 min (via Zoom)
15:45 James Vary – 5 min (via Zoom)
15:50 Discussion – 20 min
16:10 End of QC part

Artificial Intelligence/Machine Learning (AI/ML)

16:15 Michelle Kuchera – Overview – 15 min
16:30 Yue Hao – 5 min (via Zoom)
16:35 Alessandro Lovato – 5 min (via Zoom)
16:40 Witek Nazarewicz – 5 min
16:45 Michael Smith – 5 min (via Zoom)
16:50 James Vary – 5 min (slides presented by Dean Lee)
16:55 Xilin Zhang – 5 min
17:00 Discussion – 20 min
17:20 End of AI/ML part

IQUS InQubator for Quantum Simulation

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Quantum Information Science for US Nuclear Physics Long Range Planning – 2022

Organizing Committee: Douglas Beck (UIUC), Joe Carlson (LANL), Zohreh Davoudi (U of Maryland), Joe Formaggio (MIT), Sofia Quaglioni (LLNL), Martin Savage (UW)

This meeting will gather experts to consider the current state of quantum information science in nuclear physics research. It is expected to provide information to be considered during the current nuclear physics long-range planning process.

This workshop is jointly-sponsored by Los Alamos National Laboratory (LANL) and the InQubator for Quantum Simulation (IQuS), and will be held in the Hilton Hotel in Santa Fe. The New Mexico Consortium (NMC) has kindly agreed to handle the logistics.

To register for this event : **REGISTRATION**



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