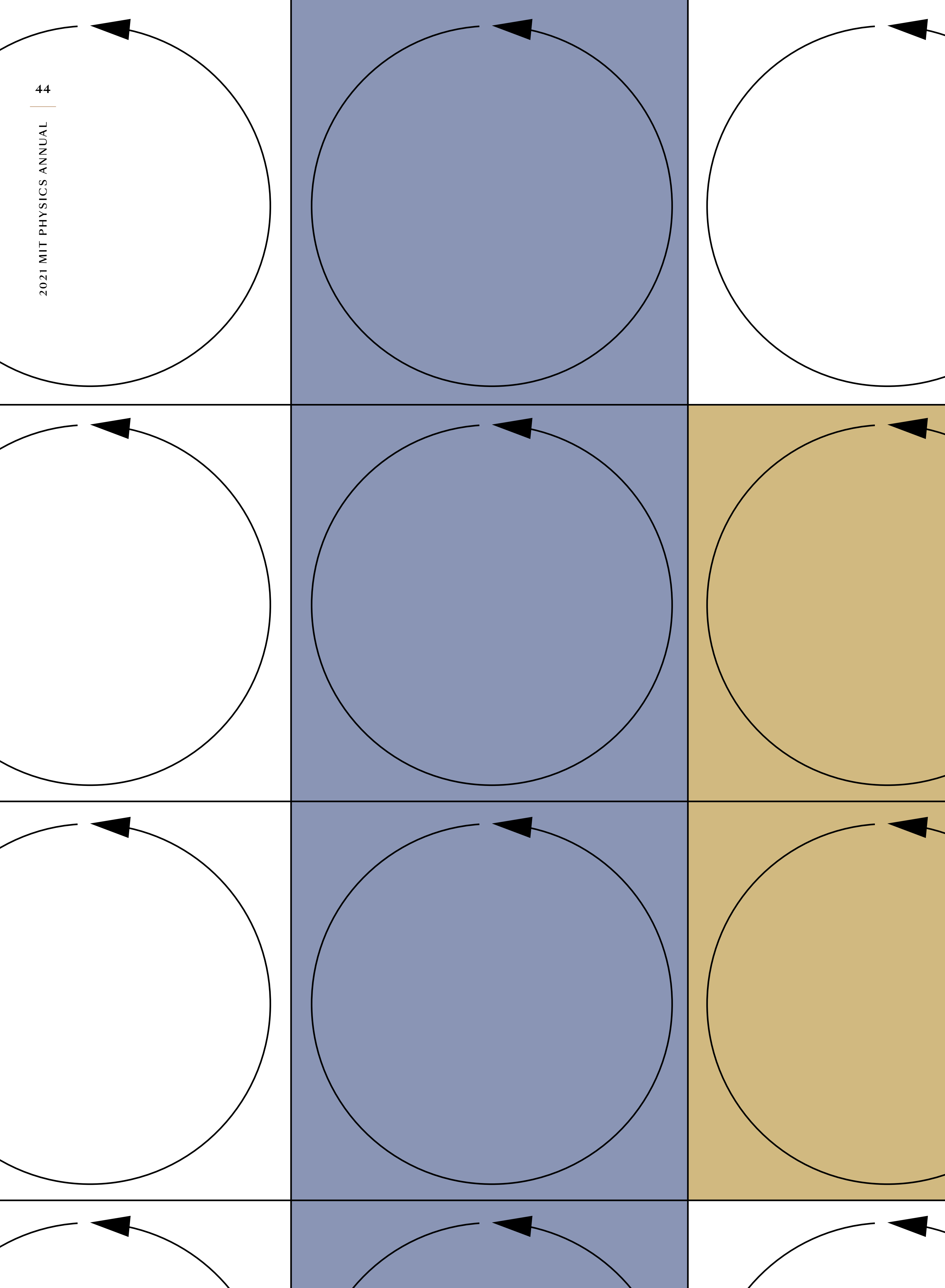

From Quarks to Nuclei

The Building Blocks of Matter

by Phiala Shanahan

Since the 1970s, we have understood three of the four fundamental forces of nature in terms of a unified whole: the Standard Model of particle physics. This theory is elegant, symmetric and compact, and it is inarguably a triumph of modern physics.

Encoding the strong, electromagnetic and weak interactions of the 17 fundamental particles, we believe that the Standard Model describes the structure and interactions of matter at all distance and energy scales we can access, from high energy particle collisions at the Large Hadron Collider, to the decays of heavy nuclei, to the properties of matter under extreme conditions, such as in the core of a neutron star. It is also clear, however, that this theory does not describe everything that we observe about the universe; there has not yet been a successful unification of gravity (which is described by the separate theory of general relativity) into the framework, and the Standard Model does not explain other "beyond-Standard-Model" phenomena, from the masses of neutrinos to the abundant gravitational evidence for dark matter and dark energy.

In this context, direct studies of our fundamental theory serve two purposes, both complementary and entwined. First, they give us a window on the complexity of nature: Can we truly reveal the emergence of the structure of matter, explaining observations from the mass of a single proton through to nuclear reactions, neutron stars and supernovae, all from the simple rules of the underlying theory? Can we learn how sensitive the existence of atomic structure, and ultimately life, is to the free parameters of the theory, such as the masses of the fundamental particles like electrons and quarks?

Second, terrestrial experiments searching to constrain beyond-Standard-Model physics are built from protons, neutrons, and nuclei, themselves composed of fundamental particles. Understanding their structure and interactions is thus crucial to determine the necessary backgrounds and benchmarks for our searches for new physics beyond that which we understand. These questions, and their answers, reach across particle physics, nuclear physics and cosmology, and their pursuit drives a rich program of theory investigations that leverages high-performance computing at the most extreme scales.

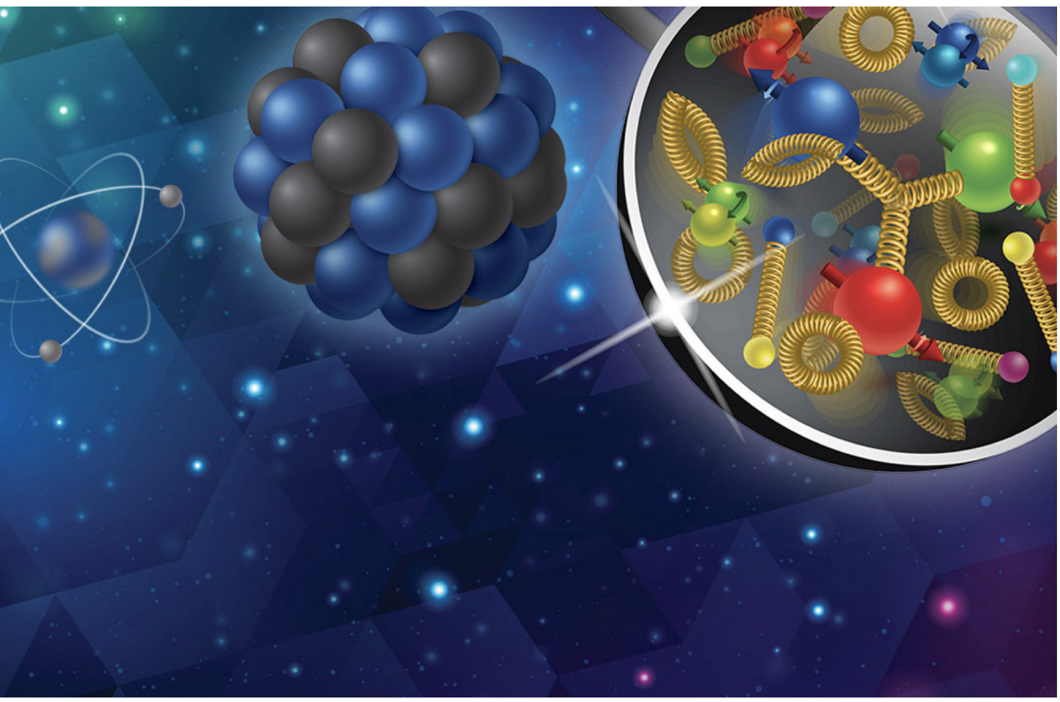

FIGURE 1:
At the core of atoms (left) are atomic nuclei made of protons and neutrons (center). The protons and neutrons are themselves composed of fundamental particles called quarks and gluons (right). Credit: Brookhaven National Laboratory and Thomas Jefferson National Accelerator Facility

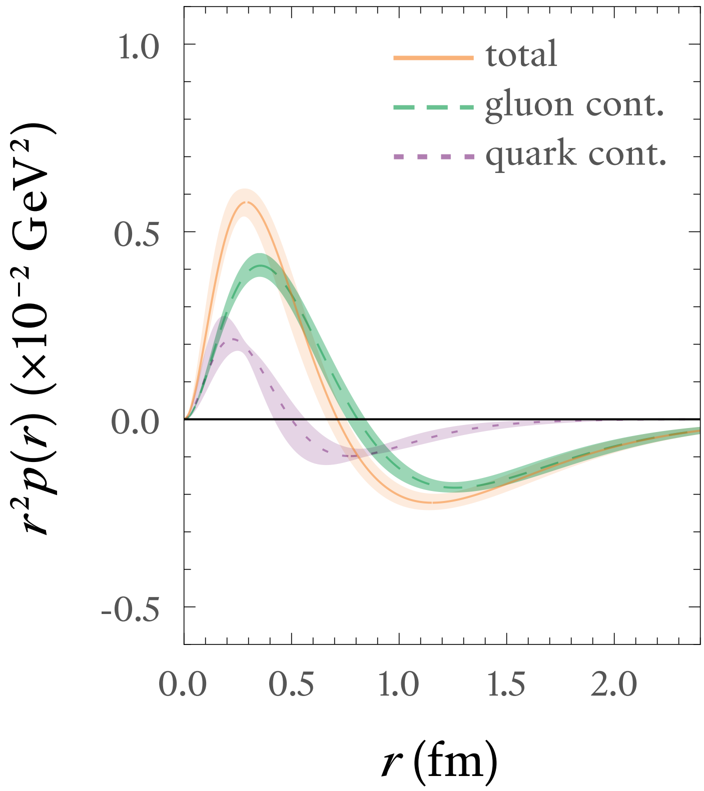

FIGURE 2:
Quark and gluon contributions to the radial pressure distribution in the proton, calculated using lattice field theory. The horizontal axis shows the radial distance from the center of the proton, while the vertical axis shows that distance squared times the pressure. This quantity must integrate to zero for the stability of the proton. Credit: Shanahan Group; Copyright: American Physical Society

Computing the strong interactions

Within the Standard Model, the strong nuclear force, responsible for binding fundamental particles called quarks and gluons together into protons and neutrons, and for binding the protons and neutrons together into nuclei, presents a particular obstacle to theory calculations. At the low energy-scales relevant, for example, to nuclei at rest in a detector, the only known systematically-improvable approach to calculation is a numerical method named "lattice field theory." Over the last 20 years, lattice field theory computations, which proceed by discretizing space and time onto a four-dimensional grid (a lattice), have become an extraordinarily powerful and versatile tool. They can accurately describe how the masses of the proton and neutron arise (and importantly for the stability of atoms, how they differ), and have been used to make predictions of the masses of new composite particles later discovered by experiments at CERN. More complicated quantities are also accessible: calculations I have undertaken with my colleague Will Detmold have revealed that the pressure generated by the quarks and gluons inside a proton is larger than that inside neutron stars, and have shown for the first time how nuclear reactions, such as the proton-proton fusion process that initiates the chain reaction that powers the sun, emerges from our most fundamental understanding of particle physics.

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Nevertheless, there are significant limitations imposed on the lattice field theory approach by its computational demands. Even with approximately 10% of open-science supercomputing in the United States devoted to such studies, many calculations that would elucidate new details about the structure and formation of the matter in our universe remain quite simply too expensive to pursue. In particular for nuclei, the computational challenge presented by such calculations is daunting; naively, there are compounding factorial and exponential growths in computational cost with the atomic number of the nucleus under study. As a result, while direct calculations of the structure of the proton are now extremely precise, with theory calculations in some cases competitive with or better than the best experimental measurements, for nuclear physics the era of controlled calculations through this framework is only now beginning.

One concrete example of the computational challenge posed by lattice field theory for nuclear physics is offered by a recent calculation that my collaborators and I undertook, which revealed unexpectedly large nuclear effects in the scattering cross-sections of a class of dark matter candidates with the Helium-3 nucleus. While the calculation was performed with values of the quark masses larger than they are in nature (given the limitation of computing resources), it revealed that there are important corrections to the standard "Born approximation," which models the nucleus as a collection of free protons and neutrons and neglects any correlations between them. If similar effects exist in the larger nuclei, such as Xenon, used as detectors in experiments searching for direct evidence of dark matter, these corrections will have important impact on the interpretation of the experimental results. However, while we in principle know how, there is not enough computing capacity in the world to calculate predictions for the scattering of dark matter from such large nuclei directly. Matching lattice field theory calculations to models of nuclear physics, which involve protons and neutrons as the effective degrees of freedom—so-called "nuclear effective theories"—provides some information, but clearly there are compelling reasons to develop new methods that circumvent the computational limitations of lattice field theory to enable an understanding of larger nuclei directly from the Standard Model.

Faced by computational challenges of this extreme scale, the only solution is to develop novel approaches in the form of new types of computing hardware or more efficient algorithms. From custom silicon devices to quantum computing, all avenues are being pursued at MIT, but the fantastic success of machine learning (ML) and artificial intelligence (AI) in recent years across applications from the game of Go to image recognition presents a tantalizing new possibility on the algorithmic side. Can we use AI not as a black box to achieve tasks that typically require human intelligence, but in a provably-exact way to accelerate the algorithms we use in first-principles physics calculations?

New possibilities with *ab-initio* artificial intelligence

For more than 70 years, since Turing's 1950 paper, "Computing Machinery and Intelligence," asked the question: *Can machines think?*, the branch of computer science described as AI has sought to design algorithms which mimic human intelligence and learning. Whether we can use similar algorithms in a different context, to enable theoretical physics calculations that are currently computationally intractable, is one of the questions that motivates the new National Science Foundation Institute for Artificial Intelligence and Fundamental Interactions (*iaifi.org*), launched this year as a collaboration between physics and AI researchers at MIT, Harvard, Northeastern and Tufts Universities. The interdisciplinary team, which includes 12 MIT physics faculty, is developing the new field of "*ab-initio* AI": approaches to artificial intelligence

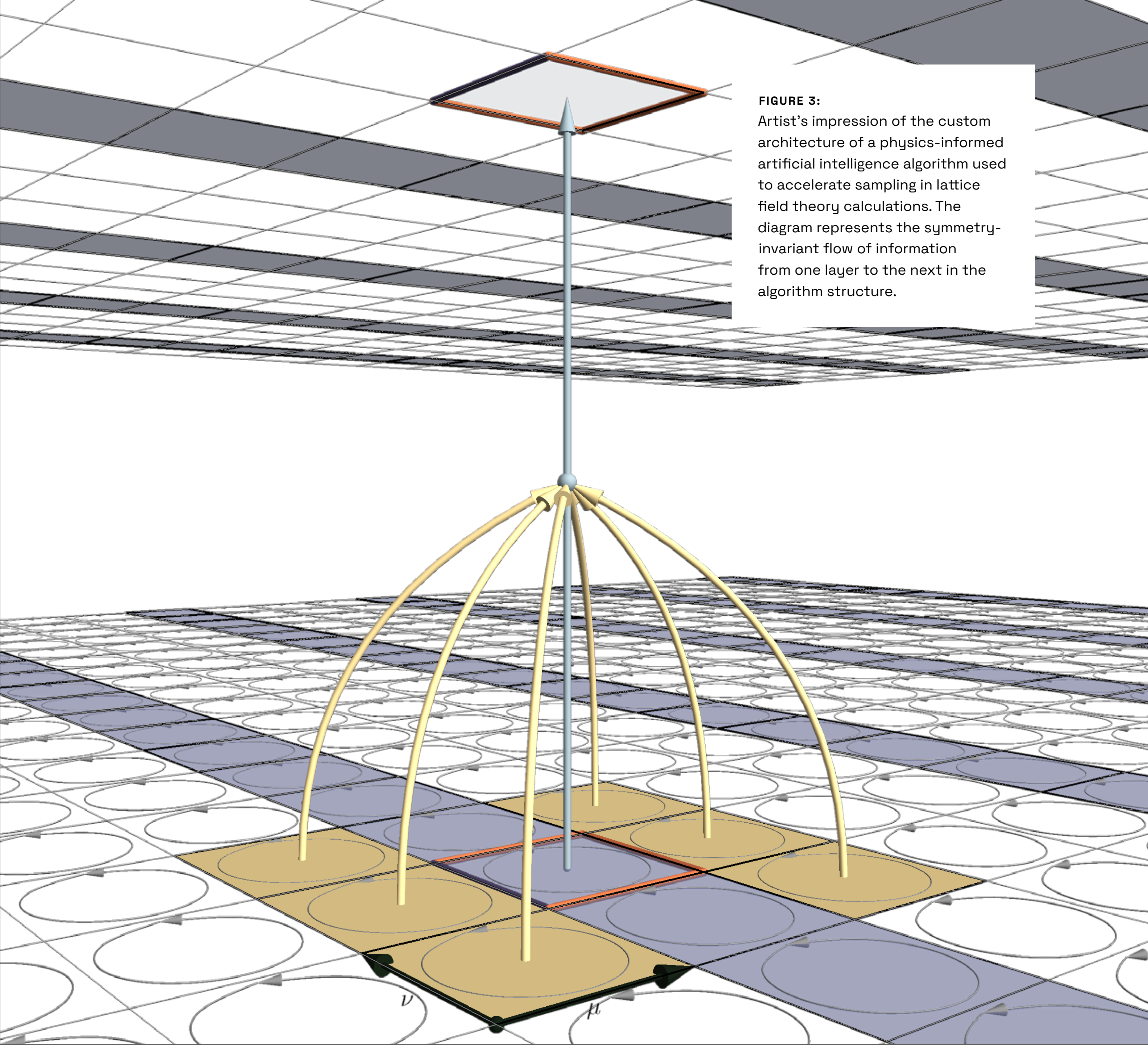

FIGURE 3:
Artist's impression of the custom architecture of a physics-informed artificial intelligence algorithm used to accelerate sampling in lattice field theory calculations. The diagram represents the symmetry-invariant flow of information from one layer to the next in the algorithm structure.

that build in and incorporate the fundamental physics principles that underpin our understanding of the universe.

The development of *ab-initio* AI addresses the unique challenges that arise in the application of AI or ML to fundamental physics, including within lattice field theory calculations. We require calculations or analyses to obey precise principles, for example symmetries, conservation laws, scaling relations, limiting behaviors, locality or causality. We demand rigor in the computation of systematic uncertainties, as well as reproducibility, verifiability, and crucially, guarantees of exactness for applications which require them. In some cases, there might be no "training data" available with which to optimize the algorithms; generating that data might in fact be the task at hand, requiring the development of self-training approaches. All of these challenges arise in the application of AI to lattice field theory calculations of nuclei, where it is crucial to the integrity of the approach (as a direct first-principles theoretical study of our underlying theory), to maintain mathematical rigor.

Over the last few years, my group has developed provably-exact algorithms exploiting *ab-initio* AI for first-principles nuclear physics. Exciting progress has been made to address one computational challenge in lattice field theory calculations in particular: Studying physical quantities in the theory requires sampling over contributions to extremely high-dimensional integrals (over up to 10^{12} variables in state-of-the-art calculations). Developing an efficient, provably-exact, self-training approach to generate these samples that precisely incorporates all of the symmetries of the underlying strong interactions has led my group to an intense interdisciplinary collaboration with researchers at Google DeepMind. The result has been a number of groundbreaking ML algorithms that achieve results orders of magnitude faster than traditional algorithms when applied to simplified versions of the Standard Model. To impact state-of-the-art particle and nuclear physics studies, the approach must be scaled to the first exascale supercomputing systems in the United States, which are currently under construction. The new machines, named Aurora (*alcf.anl.gov/aurora*) and Frontier (*olcf.ornl.gov/frontier/*), will compute a billion billion (*i.e.*, a quintillion) operations each second, making them many thousands of times faster than a high-end desktop computer.

With exascale computing under development, the ultimate impact of AI on state-of-the-art lattice field theory calculations remains to be seen, but the novel algorithm developments that the challenge of AI for first-principles nuclear theory has inspired have already found broad interdisciplinary applications. The same work that enables ML architectures to be defined for the mathematical group structures needed in lattice field theory enables architectures to work with the angles that define the positions of a multi-jointed robot arm. The same algorithmic approaches that provide guarantees of exactness in the relevant limits of the theory are being applied to studies of molecular design and protein folding in computational chemistry. Already it is clear that the nascent field of *ab-initio* AI is only beginning to reveal its full potential.

Nuclear physics calculations at the exascale and beyond

As we consider the history and future of first-principles Standard Model calculations, it is apparent that we are at a turning point: We have begun to connect the Standard Model to nuclear physics in a robust and systematically controlled way, through calculations that we are only now beginning to have the algorithmic technology, and the supercomputers, to undertake. We have recently demonstrated this potential by accomplishing the very first first-principles calculations of simple nuclear reactions, and beautiful examples of the critical role that theory input plays in searches for new physics beyond the Standard Model. Over the next decades we can expect that first-principles theory calculations will allow us to answer questions about the fine-tunings in nuclear physics that are deeply important for our existence. We will be able to see, from the underlying Standard Model, how sensitive the production of carbon in the universe via the triple-α process is to the free parameters of the theory, and to answer why we see clustering in nuclei. We will be able to compute not just the first step, but the entire chain of Big Bang nucleosynthesis reactions to understand how the elements formed in the first minutes of the universe's existence. As we continue to push the physics frontier, a new generation of provably-exact physics-informed ML algorithms promises to enable calculations that were previously intractable and to usher-in the grounding of nuclear physics in the Standard Model, as we continue our ages-old quest to understand the universe from its most fundamental building blocks.

FIGURE 4:
Aurora, currently under construction, will be the first exascale computing system in the United States. It will compute a billion billion (*i.e.*, a quintillion) operations each second. Credit: Argonne Leadership Computing Facility

PHIALA SHANAHAN is the Class of 1957 Career Development Assistant Professor of Physics in MIT's Center for Theoretical Physics. Her research is focused on particle and nuclear theory, as well as on the development of novel computational and algorithmic tools for theoretical physics.

In particular, Shanahan works to understand the structure and interactions of hadrons and nuclei from the fundamental (quark and gluon) degrees of freedom encoded in the Standard Model of particle physics. Her recent work has focused in particular on the role of gluons, the force carriers of the strong interactions described by Quantum Chromodynamics (QCD). Using analytic tools and high-performance supercomputing, Shanahan recently achieved the first calculation of the gluon structure of light nuclei, making predictions which will be testable in new experiments proposed at Jefferson National Accelerator Facility and at the planned Electron-Ion Collider. She has also undertaken extensive studies of the role of strange quarks in the proton and light nuclei, which sharpen theory predictions for dark matter cross-sections in direct detection experiments. To overcome computational limitations in QCD calculations for hadrons and in particular for nuclei, Shanahan is pursuing a program to integrate modern machine learning techniques in computational nuclear physics studies.

A native of Adelaide, Australia, Phiala Shanahan earned her BSc from the University of Adelaide in 2012, and her PhD from the same institution in 2015. In 2015–2017 she held a postdoctoral position within the MIT Center for Theoretical Physics, followed by joint appointments at The College of William & Mary (faculty) and the Thomas Jefferson National Accelerator Facility (senior staff scientist). In July 2018, Shanahan returned to MIT Physics as an Assistant Professor. Her research has been recognized with numerous awards and fellowships including Early Career Awards from both the National Science Foundation and the Department of Energy, the 2021 Maria Goeppert Mayer Award from the American Physical Society, a Simons Foundation Emmy Noether fellowship, and she was listed in Forbes Magazine's "30 Under 30 in Science" in 2017.