2023 INCITE Proposal Submission
Proposal

Title: Nuclear femtography: parton distribution functions for the Electron-Ion Collider

Principal Investigator: Phiala Shanahan

Organization: Massachusetts Instiutute of Technology

Date/Time Generated: 6/17/2022 12:42:15 PM

Section 1: PI and Co-PI Information

Question #1

Principal Investigator: *The PI is responsible for the project and managing any resources awarded to the project. If your project has multiple investigators, list the PI in this section and add any Co-PIs in the following section.*

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Question #2

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Question #3

Institutional Contact: *For the PI's institution on the proposal, identify the agent who has the authority to review, negotiate, and sign the user agreement on behalf of that institution. The person who can commit an organization may be someone in the contracts or procurement department, legal, or if a university, the department head or Sponsored Research Office or Grants Department.*

Institutional Contact

Institutional Contact Name

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Institutional Contact Phone

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Section 2: Project Information

Question #1

Select the category that best describes your project.

Research Category

Physics: Nuclear Physics

Question #2

Please provide a project summary in two sentences that can be used to describe the impact of your project to the public (50 words maximum)

Project Summary

This project will determine fundamental aspects of the quark and gluon structure of light nuclei for the first time through direct calculations in the Standard Model of particle physics. The results will provide critical theory benchmarks for the science program of the future Electron-Ion Collider and will inform searches for new physics beyond the Standard Model.

Section 3: Early Career Track

Question #1

Early Career

Starting in the INCITE 2022 year, INCITE is committing 10% of allocatable time to an [Early Career Track](#) in INCITE. The goal of the early career track is to encourage the next generation of high-performance computing researchers. Researchers within 10 years from earning their PhD (after December 31st 2012) may choose to apply. Projects will go through the regular INCITE Computational Readiness and Peer Review process, but the INCITE Management Committee will consider meritorious projects in the Early Career Track separately.

***Who Can Apply**: Researchers less than 10 years out from their PhD that need LCF-level capabilities to advance their overall research plan and who have not been a previous INCITE PI.*

How to Apply:

In the regular application process, there will be a check-box to self-identify as early career.

- *The required CV should make eligibility clear.*
- *If awarded, how will this allocation fit into your overall research plan for the next 5 years?*

Projects will go through the regular INCITE review process. The INCITE Program is targeting at least 10% of allocatable time. When selecting the INCITE Career Track, PIs are not restricted to just competing in that track.

- *What is the Early Career Track?*
    - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
    - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*

- *What do I need to do to be considered on the Early Career Track?*
    - *In the application process, select 'Yes' at 'If you are within 10 years of your PhD, would you like to be considered in the Early Career Track?' You will need to write a paragraph about how the INCITE proposal fits into your 5-year research and career goals.*
- *What review criteria will be used for the Early Career Track?*
    - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

Early Career Track

If you are within 10 years of your PhD, would you like to be considered in the Early Career Track? Choosing this does not reduce your chances of receiving an award.

No

If 'yes', what year was your PhD? If 'no' enter N/A

N/A

If 'yes', how will this allocation fit into your overall research plan for the next 5 years? If 'no' enter N/A.

N/A

Section 4: INCITE Allocation Request & Other Project Funding/Computing Resources

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Node Hours

60000

Storage (TB)

50

Off-Line Storage (TB)

0

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Node Hours

899000

Storage (TB)

250

Off-Line Storage (TB)

85

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Node Hours

830000

Storage (TB)

300

Off-Line Storage (TB)

30

Question #4

OLCF Frontier (Cray Shasta) Resource Request – 2025

Node Hours

945000

Storage (TB)

300

Off-Line Storage (TB)

10

Question #5

ALCF Theta (Cray XC40) Resource Request - 2023

Question #6

ALCF Polaris Resource Request - 2023

Question #7

ALCF Polaris Resource Request - 2024

Question #8

ALCF Polaris Resource Request - 2025

Question #9

ALCF Aurora (Intel X^e) Resource Request – 2023

Question #10

ALCF Aurora (Intel X^e) Resource Request – 2024

Question #11

ALCF Aurora (Intel X^e) Resource Request – 2025

Question #12

List any funding this project receives from other funding agencies.

Funding Sources

Funding Source

Dept of Energy

Grant Number

DE- SC0021006

Funding Source

Dept of Energy

Grant Number

DE-SC0011090

Funding Source

Dept of Energy

Grant Number

DE-SC0018121

Question #13

List any other high-performance computing allocations being received in support of this project.

Other High Performance Computing Resource Allocations

Resource	INCITE Summit
Allocation Agency	DOE INCITE
Allocation	600000
Allocation Year	2022

Section 5: Project Narrative and Supplemental Materials

Question #1

Using the templates provided here, please follow the [INCITE Proposal Preparation Instructions]to prepare your proposal. Elements needed include (1) Project Executive Summary, (2) Project Narrative, (3) Personnel Justification and Management Plan, (4) Milestone Table, (5) Publications Resulting from prior INCITE Awards (if appropriate), and (6) Biographical Sketches for the PI and all co-PI's. Concatenate all materials into a single PDF file.   Prior to submission, it is strongly recommended that proposers review their proposals to ensure they comply with the proposal preparation instructions.

Concatenate all materials below into a single PDF file.

1. **Project Executive Summary (One Page Max)**
2. **Project Narrative (15 Pages Max)**
3. **Personnel Justification and Management Plan (1 Page Max)**
4. **Milestone Table**
5. **Publications resulting from prior INCITE Awards (if appropriate)**
6. **Biographical Sketches for the PI and all co-PI's.**

NPLQCD_INCITE_2022_3.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title: Nuclear femtography: parton distribution functions for the Electron-Ion Collider

PI and Co-PI(s): Phiala Shanahan*† (MIT, PI), Zohreh Davoudi*† (UMD), William Detmold (MIT), Assumpta Parreño (Barcelona), Michael Wagman* (Fermilab), Frank Winter (Jefferson Lab)

* indicates applicant less than 10 years post-PhD; † indicates current DOE Early Career awardee

Applying Institution/Organization: Massachusetts Institute of Technology

Number of Processor Hours Requested:
Year 1: 899×10^3 Frontier node hours and 60×10^3 Summit node hours;
Year 2: 830×10^3 Frontier node hours.
Year 3: 944×10^3 Frontier node hours.
Amount of Storage Requested: 500 TB

Executive Summary: We propose to use leadership computing to continue a campaign on Summit and Frontier to determine important aspects of the structure of light nuclei from their fundamental constituents. This work continues our 2022 INCITE award, with the ultimate goal to undertake the first calculations of nuclear parton distribution functions (PDFs) with fully-quantified uncertainties from the underlying theory of the strong interactions between quarks and gluons, Quantum Chromodynamics (QCD). The PDFs that we target through variational lattice QCD calculations are fundamental quantities that encapsulate our knowledge of nuclear structure. The proposed work will be used in global PDF fits and markedly increase the precision with which nuclear PDFs are known. This will enable:

- The uncertainties on the nuclear PDFs to be reduced by a factor of 3 or more in specific kinematic regions, as is necessary for experiments at the Electron-Ion Collider (EIC) which aim to achieve new understanding of novel QCD dynamics at high parton density;
- The development of QCD benchmarks that define theory predictions and precision goals for measurements of gluonic contributions to nuclear structure at the EIC;
- Precise quark flavor separation of proton PDFs, thereby enabling precision tests of electroweak interactions, and searches for physics beyond the Standard Model, at the EIC and elsewhere;
- Improvements in studies characterizing the quark-gluon plasma via hard probes at the Relativistic Heavy Ion Collider and at the Large Hadron Collider;
- First insight into the QCD mechanisms that drive the modifications of proton and neutron structure in the nuclear medium, constraining models of nuclear effects in the PDFs.

This project thus constitutes timely and essential theoretical support for the science program of the EIC, for which Department of Energy site selection occurred in 2020 and design is under rapid development. It will lead to the first calculations of nuclear structure with controlled systematic uncertainties from QCD. The results of the proposed work will thus directly impact the DOE experimental program, and in particular the design, and future science program, of the EIC.

This proposal is submitted by the Nuclear Physics from Lattice QCD (NPLQCD) collaboration, which has led the development of lattice QCD for nuclear physics. The project director is less than 10 years post-PhD and has successfully led large-scale allocations on NSF Bluewaters, ALCC, USQCD, and INCITE resources. Two other members of the project team are early career scientists, and two team members are current DOE Early Career award holders. This proposed work builds on our demonstrated progress towards lattice-QCD calculations of nuclei and on the long-term investment in lattice-QCD software and algorithms through the USQCD SciDAC and ECP software projects that have ensured readiness for Frontier when allocations begin.

PROJECT NARRATIVE

1 SIGNIFICANCE OF RESEARCH

The Electron-Ion Collider (EIC) [1], being constructed at Brookhaven National Laboratory over the next decade, will transform our knowledge of strongly interacting matter and Quantum Chromodynamics (QCD), enabling new insights into QCD dynamics in the regime of high parton density, and will shed new light on nuclear structure through 3-dimensional *femtography* of the proton and nuclei. Key to the success of the EIC mission are improved constraints on nuclear parton distribution functions (PDFs). Nuclear PDFs describe how the longitudinal momentum and spin of a nucleus are distributed among its quark and gluon constituents (partons) and, as such, are some of the most fundamental quantities encoding nuclear structure. As discussed in the following section, more precise theory constraints on these quantities are important for the design and future successful science prospects of the EIC.

With this proposal, we will continue the first calculation of the moments of the spin-independent and spin-dependent nuclear PDFs of light nuclei from QCD that was begun under our 2022 INCITE allocation. This calculation will use the numerical technique of lattice QCD (LQCD), which is the only known approach to study QCD with quantified uncertainties in the relevant energy regimes. Variational calculations of nuclear spectroscopy and of the matrix elements of the relevant operators will provide statistically precise determinations of the physical PDF moments that explicitly account for low-energy excited-state effects. Since this approach presents a massive computational challenge, previous LQCD studies of nuclear structure have been limited to investigations with heavier quarks than in nature for reasons of computational expediency. The investments in the development of LQCD through SciDAC, the Exascale Computing Project, and the LQCD infrastructure project over the last decade have transformed what is possible, and the stage is now set for the work proposed here. This study will be the first through which LQCD calculations of nuclei at the physical quark masses will provide critical input for experiment with quantified uncertainties, beginning a new era of QCD understanding of the physics of nuclei. Calculations with multiple volumes and lattice spacings as well as close-to-physical quark masses will enable quantification of all systematic uncertainties.

1.1 Nuclear PDFs and their impact

The utility and importance of PDFs comes from their universality; they encode the process-independent partonic structure of protons and nuclei. Once determined, either experimentally, from some limited set of reactions, or from theory calculations, the PDFs can be used for the analysis of other processes, ranging from deep inelastic scattering to Drell-Yan processes or $W^{\pm}$ production. They are also essential to experimental programs searching for physics beyond the Standard Model, for example through the scattering of ultra-high-energy cosmic ray particles, or at fixed target and collider experiments. In the infinite-momentum frame, PDFs represent the number density of partons of each type (gluons or the various flavors of quarks) carrying a fraction x of the longitudinal momentum of the nucleus. It has been known for more than three decades that nuclear PDFs are different from those of free protons; this nuclear modification, termed the EMC effect, was first revealed by the pioneering studies of the European Muon Collaboration in 1983 [2]. Since MeV-scale nuclear binding effects might be expected to be negligible compared to the typical many GeV-scale momentum transfers in hard-scattering reactions, this modification was surprising at the time. Even now, despite decades of innovative experiments and theory efforts, the underlying mechanisms that generate these modifications are not yet fully understood [3, 4, 5].

Including the constraints on nuclear PDFs achieved through the proposed project into global PDF fits will advance our understanding of nature in three key directions. The results will:

- **Reveal the QCD origin of nuclear effects in PDFs:** The calculations proposed here will give first insight into how the dynamics of QCD in nuclei generate nuclear effects in the PDFs. In particular, the calculations will determine the spin and flavor dependence of the EMC effect from QCD for the first time. In addition, they will predict the magnitude of a "gluonic EMC effect" from LQCD. The EIC will have the ability to measure gluonic properties of nuclei with unprecedented precision and will dramatically improve our knowledge of these important components of nuclear structure. An analogue of the EMC effect for gluons, in which the distributions of gluons in a nucleus differ from the sum of the gluon distributions of the constituent protons and neutrons [6], has not been observed but would be a milestone discovery of the EIC [7]. Our proposed calculation will be influential in the planning of the EIC program by providing a precision target for this key measurement. Moreover, experiments at the Thomas Jefferson National Accelerator Facility (JLab) over the last decade have uncovered an interesting correlation between short-range nuclear interactions and the EMC effect [8, 5], and this study will constrain theoretical explanations of this correlation [9, 10, 11] from QCD for the first time.

- **Constrain nuclear PDFs for experimental nuclear physics programs:** The constraints on nuclear PDFs which will be achieved through this proposal will be systematically controlled, and will provide critical information to a range of experimental programs, in particular to the future EIC. This, and other future facilities, will probe nuclear structure in the region of small x to reveal novel QCD dynamics such as gluon saturation and the accompanying conjectured universal properties of QCD matter at high partonic density. This will only be achievable if improved determinations of nuclear PDFs and a reliable estimate of their uncertainties can be attained [12]. Nuclear PDFs are also an essential ingredient for the interpretation of heavy ion collisions at the Relativistic Heavy Ion Collider (RHIC) and the Large Hadron Collider (LHC), in particular for the characterization of the Quark-Gluon Plasma (QGP) via hard probes. Here, well-determined PDFs are needed to separate the hot nuclear-matter effects from the presence of a QGP from cold nuclear-matter effects in the initial stages of the heavy ion collision, such as nuclear shadowing [13, 14].

- **Control uncertainties from nuclear PDFs in studies of proton structure:** Since nuclear targets are also used in experiments aiming to determine the PDFs of the *proton*, the improved constraints on nuclear PDFs generated through this project will impact diverse physics studies involving the proton. In particular, knowledge of the nuclear effects in the PDFs of the deuteron and ^{3}He are crucial for disentangling the flavor-separated quark and antiquark distributions of the proton via scattering from these light nuclei. Given the precision of the latest generation of proton PDF fits, neglecting the nuclear uncertainties associated with this scattering, as has been done in the past, is likely no longer justifiable [15]. The improved constraints on proton PDFs will, in turn, impact precision studies of electroweak interactions and searches for new physics at the EIC [16].

With the EIC having entered an intense planning and development phase since site selection in early 2020, it is important that the timely studies we propose are undertaken in the next few years.

1.2 LQCD input in global PDF fits

The current constraints on nuclear PDFs come from global fits to experimental data. Naturally, the most challenging aspects of the PDFs to constrain are those which are difficult to probe or resolve experimentally. For example, experimental information on neutral current structure functions obtained from deep inelastic scattering experiments does not in practice enable a full quark flavor separation of the PDFs, and the region of x over which nuclear PDFs have been constrained is limited. The nuclear gluon PDFs are difficult to probe experimentally, and spin-dependent nuclear PDFs are almost entirely unconstrained. As a result, additional assumptions must be made when the PDFs are used for phenomenological applications. Current nuclear PDF fits [17, 18, 19, 20, 21, 22, 23, 24, 15] also necessarily rely on model-dependent assumptions for the parameterization of the dependence of the PDFs on x and atomic mass number A, resulting in systematic uncertainties or biases whose magnitudes are difficult to assess.[1] The LQCD calculations which are proposed here will provide additional constraints on the nuclear PDFs, including their flavor separation, the gluon PDFs, and spin-dependent PDFs. Including these constraints in global fits to experimental data will significantly reduce PDF uncertainties.

The approach of combining global fits of experimental data and LQCD constraints to extract improved PDFs has been used in the past for the PDFs of the proton with great success. For the proton transversity PDFs, Ref [25] demonstrated that including LQCD constraints on the lowest Mellin moment of the PDFs into global fits to experimental data from semi-inclusive deep inelastic scattering (SIDIS) experiments results in a significant reduction of the PDF uncertainties, at some parameter values by more than a factor of 5. Similarly, improved constraints on nuclear PDFs will result from the moment computations that are proposed here.

As further elaborated in Sec. 2, through this project we will calculate the lowest nontrivial Mellin moment of the spin-independent and spin-dependent nuclear PDFs of light nuclei with $A \leq 4$. The nuclear PDFs at a renormalization scale μ are defined as

$$\begin{aligned} q^A(x,\mu^2) &= q^A_\uparrow(x,\mu^2) + q^A_\downarrow(x,\mu^2), \\ \Delta q^A(x,\mu^2) &= q^A_\uparrow(x,\mu^2) - q^A_\downarrow(x,\mu^2), \end{aligned} \tag{1}$$

where $q^A_{\uparrow(\downarrow)}(x,\mu^2)$ represents the number density of quarks with momentum fraction x whose spin is parallel (antiparallel) to the longitudinal spin direction of the nucleus A. Similar expressions are defined from the antiquark, $\overline{q}^A_{\uparrow(\downarrow)}(x,\mu^2)$, and gluon, $g^A(x,\mu^2)$, distributions. The Mellin moments are defined as

$$\begin{aligned} \langle x^{n-1}\rangle^q_A\Big|_{\mu^2} &= \int_0^1 dx\, x^{n-1}(q^A(x,\mu^2) + (-1)^n\overline{q}^A(x,\mu^2)), \\ \langle x^{n}\rangle^{\Delta q}_A\Big|_{\mu^2} &= \int_0^1 dx\, x^{n}(\Delta q^A(x,\mu^2) + (-1)^n\Delta\overline{q}^A(x,\mu^2)), \\ \langle x^{n}\rangle^{g}_A\Big|_{\mu^2} &= \int_0^1 dx\, x^{n} g^A(x,\mu^2), \end{aligned} \tag{2}$$

for $n \geq 1$ (our proposed study will focus on $n = 1$ initially). Constraints on the lowest moments of the light quark and gluon nuclear PDFs will provide critical information about their *integrated* x-dependence. As in the example of nucleon transversity, incorporating this information into global nuclear-PDF fits will substantially improve constraints on these quantities. Fig. 1 shows the impact of our recent proof-of-principle study following this approach in calculations at heavy quark masses [26] to constrain the isovector flavor combination of the nuclear PDFs of ^{3}He, from the inclusion of the lowest moment of the nuclear PDF. The studies of light nuclei at close-to-physical quark masses proposed here, including the deuteron, ^{3}He, and ^{4}He, will significantly improve these constraints.

The LQCD framework which will be used for these studies, described further in subsection 2.1, is the only known first-principles method of calculating QCD matrix elements and, as such, is the appropriate tool for the calculations that we propose. LQCD is a key source of information for studies of proton structure and for many tests of the Standard Model as it provides results for hadronic matrix elements that are systematically improvable and model independent. For example, many LQCD matrix elements are used in studies of unitarity in the CKM paradigm in the quark sector as summarized in Ref. [27]. The proposed

[1] Approaches based on neural networks ameliorate these particular concerns and have recently been applied to nuclear PDFs [15].

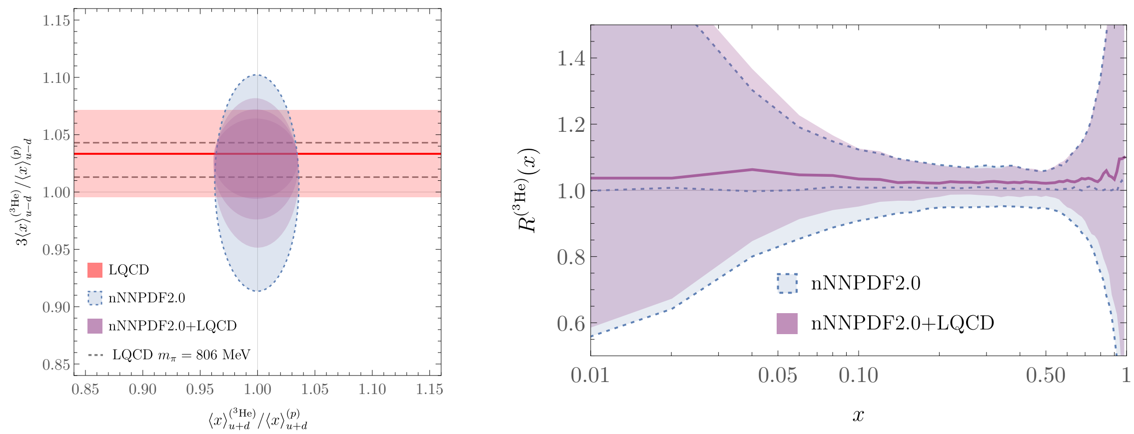

Figure 1. Left: The ratio of the isovector momentum fractions of ^{3}He and p determined in our proof-of-principle calculation [26], compared to constraints on the isovector and isoscalar momentum fraction ratios from the nNNPDF2.0 [15] global analysis before and after the LQCD constraint is imposed. Both axes are normalized to unity in the absence of nuclear effects. The red band, and central purple ellipse, correspond to LQCD results taking 100% of the value of the LEC as an additional systematic uncertainty to account for its unconstrained mass-dependence. The inner and outer purple ellipses show the results of instead taking 50% and 200% of the LQCD result as the additional systematic uncertainty before incorporating LQCD as a constraint into the global fit. The LQCD constraint on the isovector ratio at $m_\pi = 806$ MeV is also displayed. In all cases, 68% confidence intervals are shown. Right: The corresponding impact of the moment constraint on the ratio of isovector x-dependent PDFs in ^{3}He and the proton.

calculations build upon our successful studies of aspects of the structure and spectroscopy of light nuclei from LQCD at larger-than-physical values of the quark masses [28, 29, 30, 31, 32, 33, 34], which were enabled in part by previous INCITE awards. In particular, a large part of the methodology we propose has been demonstrated in our aforementioned proof-of-principle calculation of the isovector combination of nuclear PDFs at unphysical quark masses that was recently published in Physical Review Letters [26]. Our proposed study is made possible by recent advances in LQCD algorithms and software enabled by the SciDAC4 project “Computing the Properties of Matter with Leadership Computing Resources” of which a number of co-PIs are members.

1.3 Relevance to DOE mission

The goals of this proposal are aligned with the strategic plans of the high-energy [35] and nuclear physics [36] communities in the US, and will have particular impact on the planning and development of the EIC, while also having important consequences for experiments at JLab, RHIC, and the LHC. Implementing the calculations in this proposal will also provide important opportunities for training graduate students and postdocs in high-performance computing and nuclear physics, preparing them for future careers in academia, national labs, and industry.

1.4 Contribution to community resources

This proposal necessarily includes the production of gauge-field configurations to be used in the LQCD calculations. Such field configurations are costly to generate, and once produced, can be used for a range of physics studies. We plan to extend existing ensembles of configurations produced by us (and by others in the USQCD Collaboration through previous INCITE awards) to achieve the statistics necessary for the calculation proposed here. The configurations generated through this project will be made available immediately after generation to the broader community under the terms of the USQCD charter (see https://www.usqcd.org/documents/charter.pdf).

1.5 Previous INCITE awards

Our project team received a 2022 INCITE award on the current topic. Our application was submitted as a three-year request but the award was for the first year only. We are on track to significantly surpass the milestones of the first year of our proposal, having developed additional code and workflow optimizations. We are submitting the current proposal to complete the calculations that have begun under the 2022 award and in year 3 have added calculations at an additional set of parameters to fully control systematic uncertainties. As this project is currently in the production phase, no publications have yet been generated, but preliminary results from the data generated to date are provided in the following sections.

In addition to the 2022 INCITE award to this project team, a number of co-PIs have been co-PIs on previous earlier INCITE awards, titled “Lattice QCD”, in 2017-9 (PI Paul Mackenzie) and 2020 (PI Andreas Kronfeld). These were large community efforts from the USQCD Collaboration, focused on LQCD calculations to address research priorities in high-energy and nuclear physics. One of the main objectives of these awards was to generate gauge configurations; the configurations generated through those allocations are exploited in the current proposal. The broad suite of physics calculations undertaken under the previous allocations included efforts in quark and lepton flavor physics, neutrino physics, QCD thermodynamics, and hadron structure and spectroscopy. Calculations of nuclear structure were undertaken with support from these allocations at larger-than-physical values of the quark masses, setting the stage for the physical calculations proposed here. Major accomplishments that have arisen from these awards include precision hadronic inputs to the determination of the anomalous magnetic moment of the muon [37], rare kaon decays [38] and heavy quark physics [39], along with determination of the QCD phase transition temperature [40], various aspects of the structure of the proton [41] and categorization of exotic mesons [42]. Of direct relevance to this proposal, gauge configurations produced using INCITE resources have been essential to all our previous LQCD calculations of nuclear structure [29, 30, 31, 32, 33, 34, 26].

2 RESEARCH OBJECTIVES AND MILESTONES

The following subsections describe the computational method that we will use to constrain the PDFs of light nuclei, and detail the goals and milestones for this project.

2.1 Computational Methods: Lattice QCD for PDFs

LQCD is a numerical technique with which properties of strongly interacting particles are calculated by a Monte-Carlo (probabilistic) evaluation of the Euclidean-spacetime path integral, as first introduced by Wilson in 1974 [43]. As an intermediate step in this approach, space-time is discretized to a finite 4-dimensional lattice, with the quarks residing on the lattice sites and gluons residing on the links between sites. The lattice spacing, i.e., the distance between adjacent lattice sites, is required to be much smaller than the characteristic length scale of the system under study (typically the size of hadrons such as the proton), and the limit of zero lattice spacing must be systematically approached by combining calculations at several lattice spacings to recover physical results. In order to numerically evaluate the path integral, boundary conditions are imposed so that the lattice volume is finite in all four space-time directions, with spatial and temporal extents, L and T, large compared to characteristic hadronic length scales. Calculations in multiple volumes can be reliably extrapolated to the infinite-volume limit using effective field theory. In addition, the bare quark masses, which are parameters of QCD, must be determined by comparison of simple quantities to experiment. Values of the quark masses which are larger than those in nature are sometimes used in calculations because it is computationally more efficient, necessitating a further extrapolation; a key feature of the proposed calculations is the use of near-physical values of the quark masses, significantly reducing this uncertainty.

Deep inelastic scattering and related processes are dominated by physics that is light-like, and as such PDFs themselves are challenging to access in the Euclidean spacetime in which LQCD calculations are necessarily performed. Over the last few years, several methods have been suggested to access the x-dependence of PDFs using LQCD [44, 45, 46]. Since lightcone quantities can not be calculated directly on a Euclidean lattice, these approaches involve a transformation to a 'quasi' or 'pseudo' PDF, defined in Euclidean spacetime, and an extrapolation back to the physical quantity in the large-momentum limit. While these calculations are promising [47, 48, 49], the systematics are very challenging to control [50], and are too numerically costly to perform for nuclei. Mellin moments of PDFs, Eq. (2), can on the other hand be evaluated using calculations of nuclear matrix elements of local operators [51, 52, 53, 54, 55, 56]. The methodology of such calculations for both single hadrons and nuclei is now well established, and it is this approach which we pursue in the proposed program.

The NPLQCD Collaboration has achieved a number of significant milestones in calculations of nuclear physics from LQCD within the past few years and our studies have demonstrated that calculations of nuclear matrix elements from LQCD are feasible. For example, we calculated the magnetic moments and polarizabilities of light nuclei at $m_\pi \sim 806$ MeV and $m_\pi \sim 450$ MeV [57, 29, 58]. With the same suite of calculations, the cross section for the low-energy inelastic nuclear reaction $np \to d\gamma$, the first nuclear reaction in the evolution of the universe, was determined [30]. The correlated two-nucleon interaction with the magnetic field in this process was found to be essentially independent of the quark masses, similar to the trend seen for the magnetic moments. To extend these calculations, we developed a new algorithm with which to calculate the interactions of nuclei with axial currents, as found in weak interactions. Weak interactions dictate the rate of the proton-proton fusion process that initiates the solar burning cycle in the Sun, and contribute significantly to tritium β-decay; we have performed the first QCD calculations of these processes [31]. which became a science highlight of the DOE and were summarized in an APS *Physics* Synopsis. Furthermore, second-order interactions with the axial current determine the rate of the $\beta\beta$-decay processes of nuclei. Such processes are now being used to search for lepton-number violation, and there is significant uncertainty in the requisite nuclear matrix elements. Our calculations of the two-neutrino $\beta\beta$-decay matrix elements of two nucleons [32, 33] revealed a new feature that indicates that these uncertainties may be even larger than previously thought. In ongoing work [59], the neutrinoless process is also being constrained. We have also computed the scalar, axial, and tensor current matrix elements of light nuclei [34, 32], at quark masses that are larger than those of nature, resolving nuclear effects with important phenomenological consequences. Furthermore, we undertook the first LQCD calculations of the gluon structure of light nuclei [60] and have recently completed a first calculation of the first moment of the isovector combination of quark PDFs in $A \in \{2, 3\}$ nuclei [26], albeit at unphysically large quark masses and at a single lattice volume and discretization scale. This study demonstrated essentially all of the techniques necessary for the proposed calculations and shows the feasibility of the proposed work and our ability to carry it out at the physical point.

2.2 Objectives and Milestones

The goals of the proposed program are to constrain the lowest non-trivial Mellin moments ($n = 1$ in Eq. (2)) of the spin-independent and spin-dependent quark PDFs of light nuclei with $A \leq 4$, in a controlled calculation with 5% precision for the deuteron and ^{3}He and produce a result for ^{4}He which may be less precise. This target precision is determined so that the calculations meet the needs of studies of saturation phenomena at small x at the EIC. Taking correlated ratios of the nuclear and nucleon PDFs will allow an

Identifier	β	a [fm]	m_π [MeV]	$L^3 \times T$	Status	N_{cfgs} on 1st June 2022
A	6.3	0.091	170	$48^3 \times 96$	Complete	3000
B	6.3	0.091	170	$64^3 \times 128$	Complete	4000
C	6.5	0.072	170	$72^3 \times 192$	In progress	600
D	6.5	0.072	170	$96^3 \times 192$	In progress	250

Table 1. Ensembles of LQCD gauge-field configuration to be used in this project. Ensembles will be referred to by the identifier. The parameter β denotes the inverse strong coupling, a the lattice spacing, m_π the pion mass, and $L^3 \times T$ the space-time volume of the calculations. All ensembles have been generated, in part, through our previous INCITE allocations (including under our 2022 INCITE award).

even more precise constraint on the nuclear modifications to the PDFs than on the PDFs themselves. We will achieve this goal via computations at a single, close-to-physical, set of values of the quark masses that use four lattice volumes at two different lattice spacings to enable a crude continuum and infinite volume extrapolation to be undertaken. The ensembles of LQCD gauge fields to be used are detailed in Table 1 and all ensembles were generated in part with our previous INCITE allocation. The A and B ensembles have the same value of the lattice spacing $a = 0.091$ fm, and the same quark masses corresponding to an almost-physical pion mass $m_\pi \sim 170$ MeV. The C and D ensembles have a finer lattice spacing, $a = 0.072$ fm, and a similar almost-physical pion mass. Our calculations will be based on variational set of correlation functions discussed below. This will allow us to improve our spectroscopy extractions and ameliorate the problem of excited-state contamination that is a significant challenge at the near-physical quark masses that are considered here (Fig. 3 below shows preliminary results for variational spectroscopy on the A ensemble achieved so far using our in-progress 2022 INCITE allocation). Our calculations will also make use of background-field methods to determine the requisite operator matrix elements in a variational approach and will be non-perturbatively renormalized using the RI-SMOM scheme [26]. The binding energies and matrix elements of the various systems will be extrapolated to infinite volume by matching to effective field theory [61, 62] formulated in the same finite volumes as the numerical calculations, using techniques already shown to work at larger quark masses. To estimate the remaining systematic uncertainties due to the slightly unphysical quark masses, we will compare the results of this study with those from our recent calculation of the isovector moments at a larger set of quark masses and a different lattice spacing. A summary of the results of that study, in which we have computed the lowest nontrivial moment of the spin-independent PDFs of nuclei with $A \leq 3$, at quark masses corresponding to an unphysically heavy pion $m_\pi \sim 800$ MeV, is shown in Fig. 2. The isovector results appeared in Physical Review Letters [26] and are non-perturbatively renormalized. The precision achieved in that study, with momentum-fraction ratios determined at the 1–2% level, serve as a proof-of-principle that the computation proposed here can be achieved, and constitute an end-to-end test of the proposed computational workflow.

The key milestones that must be met to achieve our objectives correspond to calculations on each of the for ensembles, and for two ensembles the generation of additional gauge-field configurations to reach the required statistics. Work on the first ensemble will be completed under our 2022 INCITE award.

- **Milestone 1 - Spectroscopy on the B ensemble** [labeled as $64^3 \times 128$ Spectroscopy task]: Determine the ground state and low-energy excited state spectrum on the B ensemble employing large sets of interpolating operators using the variational method [63, 64] as implemented in Ref. [65] and propagator sparsening techniques [66]. Preliminary calculations for two-nucleon variational spectroscopy on this ensemble are underway under our 2022 INCITE award. In the dineutron (deuteron) channel, 22 (48) interpolating operators are used in the variational matrix and extensions of the approach to three- and four-nucleon systems are underway. Based on the initial

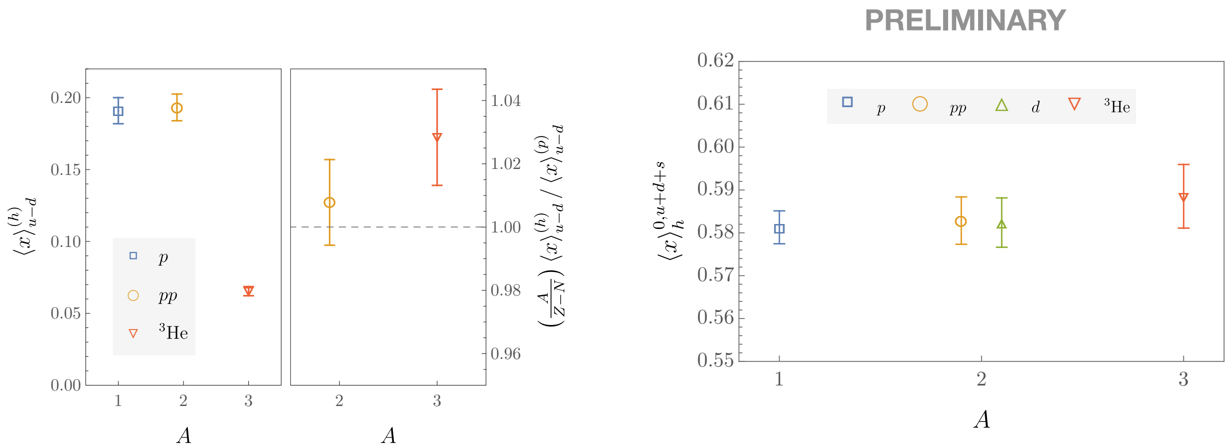

Figure 2. Mellin moments of the flavor-separated spin-independent PDFs of the proton, deuteron, diproton (which is bound at the unphysical masses used in this calculation) and ^{3}He, computed on an ensemble with lattice volume $L^3 \times T = 32^3 \times 64$, lattice spacing $a = 0.12$ fm, and $m_\pi \sim 800$ MeV. The left figure shows the isovector combination from Ref. [26] while the right figure shows preliminary unrenormalized results for the isoscalar case.

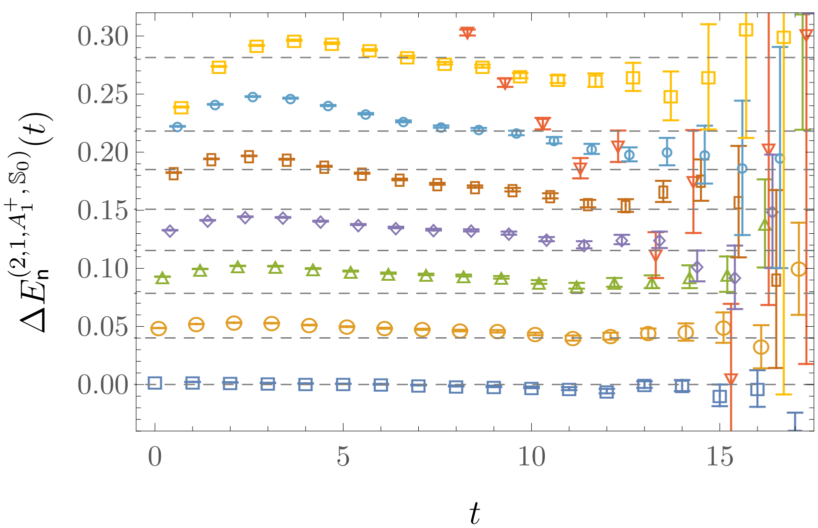

Figure 3. Preliminary analysis of dineutron correlation functions at $m_\pi = 170$ MeV using $N_{\mathrm{cfgs}} = 426$ with the variational approach and a subset of the operator basis for the spectroscopy studies proposed here. Shown are effective-mass functions of the lowest eight principal correlation functions that result from the variational diagonalization of a set of 22 interpolating operators.

study and preliminary results at larger quark masses, we plan to add spectroscopy on an additional ~ 1200 configurations to reach the target precision. This milestone is targeted in year 1 and will run on Frontier with contractions evaluated on Summit.

- **Milestone 2 - Generation of gauge fields in the C ensemble** [corresponds to $72^3 \times 192$ Gauge generation task]: To achieve the target precision of Milestone 3 and 5, it is necessary to generate an additional 1400 decorrelated gauge-field configurations in the larger-volume stream (corresponding

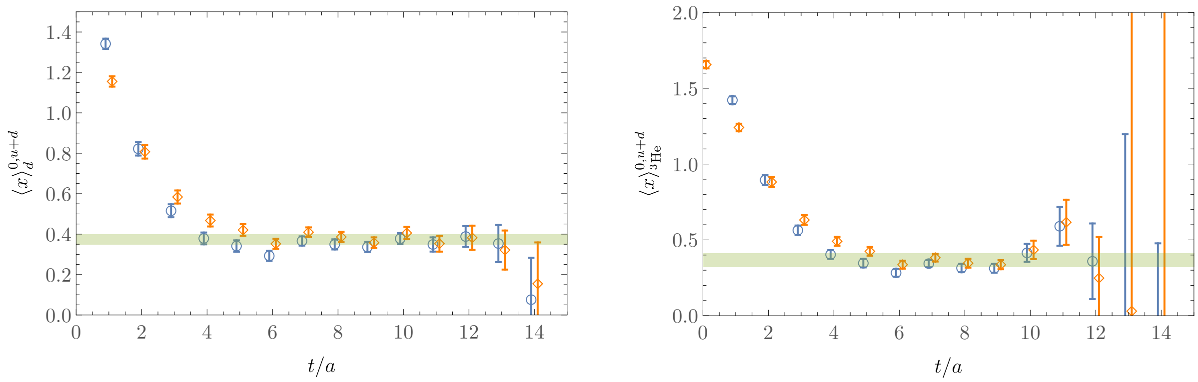

Figure 4. Preliminary results for the unrenormalized connected quark contributions to the Mellin moment of the sum of the spin-independent up and down quark PDFs of the deuteron and ^{3}He, computed on the $48^3 \times 96$ A ensemble. The different colors show results obtained with different propagator smearings (not yet a variational analysis). The calculations used 512 sources on each of 300 configurations. The figures show 'effective matrix elements' in which signals are revealed by flat behavior at large Euclidean times t/a, and early times suffer exponential contamination from excited states. The green bands show the results of multi-exponential fits to the effective matrix elements.

to 28,000 Monte-Carlo trajectories). This task will be undertaken in year 1 on Frontier.

- **Milestone 3 - Spectroscopy on the C ensemble** [labeled as $72^3 \times 192$ Spectroscopy task]: Similar to the task in milestone 1 but for the C ensemble. Statistical requirements are estimated to be slightly increased for the C ensemble due to the finer lattice spacing and longer-range correlations. Resources are requested for spectroscopy on 2000 configurations in year 1 on Frontier. Insufficient configurations to achieve this precision currently exist, and completing this Milestone will thus rely on additional configurations being generated, as proposed in Milestone 2.

- **Milestone 4 - Generation of gauge fields in the D ensemble** [corresponds to $96^3 \times 192$ Gauge generation task]: To achieve the target precision of Milestone 7 and 8, it is necessary to generate approximately 750 additional decorrelated gauge-field configurations in this large-volume fine lattice-spacing ensemble (corresponding to 15,000 Monte-Carlo trajectories). This task will be undertaken in year 1 on Frontier and this ensemble will be widely used by other groups for other physics projects.

- **Milestone 5 - Calculation of Mellin moments of nuclear PDFs on the B ensemble** [labeled as $64^3 \times 128$ Measurement task]: On the B ensemble, determine the lowest non-trivial moments of the unpolarized and polarized PDFs for the proton, deuteron, ^{3}He and ^{4}He, enabling correlated ratios of nuclear and nucleon PDF moments to be formed. The target statistical precision for moments of the $A \in \{1, 2, 3\}$ nuclei is 3%. This target precision is defined by the goal of 5% overall precision, as needed to meet the needs of studies for the EIC, after the continuum, physical mass, and infinite volume extrapolations have been performed (our estimates are that these effects lead to a 4% uncertainty). To determine the computational requirements for meeting this precision goal, we have performed preliminary calculations of the connected quark contributions to the lowest non-trivial Mellin moment of the spin-independent nuclear PDFs on the A ensemble. The results of that study are shown in Fig. 4 (analysis not yet using the variational approach). Achieving signals with half the statistical uncertainties to those in the preliminary study, requiring four times the statistical samples, would meet the target precision. The calculations of the connected and disconnected quark contributions requested in subsection 3.1 are sufficient to meet this milestone through measurements on 2000 configurations. This milestone is targeted in year 2 on Frontier.

- **Milestone 6 - Calculation of Mellin moments of nuclear PDFs on the C ensemble** [labeled as $72^3 \times 192$ Measurement task]: Matrix-element calculations as in Milestone 5 but for the C ensemble. These runs will enable the continuum extrapolation to be controlled. This task will run on Frontier in year 2. Insufficient configurations to achieve this precision currently exist, and completing this Milestone will thus rely on additional configurations being generated, as proposed in Milestone 2.
- **Milestone 7 - Spectroscopy on the D ensemble** [labeled as $96^3 \times 192$ Spectroscopy task]: Similar to the task in milestone 1 and 3 but for the D ensemble. Resources are requested for spectroscopy on 1000 configurations in year 2 on Frontier and calculations require the configurations proposed in Milestone 4. Less statistics are expected to be required on this large volume ensemble because of significant gains from volume averaging.
- **Milestone 8 - Calculation of Mellin moments of nuclear PDFs on the D ensemble** [labeled as $96^3 \times 192$ Measurement task]: calculations as in Milestone 5 and 6 but for the D ensemble. This milestone will enable the continuum and infinite-volume limits to be reached for the moments, and will be accomplished in year 3 on Frontier.

The non-perturbative renormalization of the local operators which determine the quark and gluon Mellin moments, including their mixing, and the computation of the gluon operator matrix elements themselves, are smaller computational components which are vital to the final physics results. The renormalization will use the RI-SMOM scheme as in our pilot study [26]. Two additional computational tasks are involved in the analysis required to connect the LQCD calculations to experiment. First, the extrapolation of nuclear matrix elements to infinite volume using effective field theory is an involved task for $A \in \{3, 4\}$ nuclei, in particular, and requires solving the many-nucleon problem numerically. Matching to effective field theory [9, 26] and other many-body approaches that have been pursued in the literature [67, 68, 69, 70, 71] will also allow for constraint of the PDFs of heavier nuclei such as those used in the Deep Underground Neutrino Experiment. Similarly, global PDF fitting is a complicated optimization task and imposing our constraint onto such fits will require coordination and collaboration with the established groups [20, 15]. These smaller tasks are not part of this computing request and can be performed on local resources.

3 COMPUTATIONAL READINESS

3.1 Use of Resources Requested

As discussed in Section 2, LQCD calculations are based on Monte-Carlo importance sampling evaluations of very high dimensional integrals over the quark and gluon degrees of freedom defined on a 4-dimensional spacetime grid. Calculations can be divided into two stages i) *gauge-field generation* which refers to the creation of the appropriate configurations to enable sampling of these integrals; ii) *measurements* which involve calculations of particular building blocks known as *propagators* and the subsequent *contractions* of sets of propagators to determine quantities of physical interest. Both tasks are undertaken in this proposal, allowing for controlled calculations of the partonic structure of nuclei. The tasks to be accomplished (corresponding to project milestones) are as follows:

- $64^3 \times 128$ **Spectroscopy and Measurement tasks:** using existing gauge-field configurations available within the USQCD collaboration, compute propagators and contractions allowing for extraction of the moments of unpolarized and polarized PDFs for nuclei including the deuteron, ^{3}He and ^{4}He. These tasks are proposed for year 1 and 2, respectively.

- $72^3 \times 192$ **Gauge-field generation task:** using the HMC algorithm generate 28000 trajectories. This task will be accomplished in year 1 and will extend existing ensembles at the requisite parameter values. Gauge fields will be saved every 5 trajectories with approximately independent samples generated every 20 trajectories. Combined with existing configurations, this will result in 2000 independent samples.

- $72^3 \times 192$ **Spectroscopy and Measurement tasks:** perform measurements on the finer lattice spacing ensemble using the same procedure as for the $64^3 \times 128$ Measurement task. These tasks will be undertaken in year 1 and 2, respectively.

- $96^3 \times 192$ **Gauge generation task:** using the HMC algorithm generate 15000 trajectories of gauge field configurations. This task will be undertaken in year 1 and will provide necessary extensions of an existing ensembles at the requisite parameter values. Gauge fields will be saved every 5 trajectories with approximately independent samples generated every 20 trajectories. Combined with existing configurations, this will result in 1000 independent samples.

- $96^3 \times 192$ **Spectroscopy and Measurement tasks:** perform measurements on the larger volume fine lattice spacing ensemble using the same procedure as for the smaller ones. These tasks will be undertaken in years 2 and 3, respectively.

The computationally demanding components of the calculation have been explicitly optimized and benchmarked on Crusher and Summit at OLCF (see Section 3.3 for detailed investigations of timings). The computational costs are determined by taking the optimal timings presented in Table 3 in Section 3.3 and scaling to the requisite level of statistics. Table 2 summarizes the request in Frontier node-hours. In year 1, a small request for Summit is also included to perform necessary contractions as we are in the process of porting our contraction codes from NVIDIA GPUs to AMD GPUs (see below) and may not be ready at the start of 2023. Year 2 and 3 requests are for Frontier.

Responses to specific computational readiness and resource utilization questions:

1. **Computational run plan:** The calculations to be undertaken are enumerated in Table 2. Tasks break down into those associated with the milestones: the gauge-field generation tasks, and the various spectroscopy and measurement tasks. Since some of the necessary gauge configurations already exist, the measurement tasks for each ensemble can begin immediately, with the newly generated gauge fields being used for measurements in Year 2 and 3.

2. **Processor/node use:** The $72^3 \times 192$ and $96^3 \times 192$ gauge-field generation tasks will be executed as streams of 108 and 512 Frontier-node jobs, respectively, that are set up to resubmit themselves. The $64^3 \times 128$, $72^3 \times 192$ and $96^3 \times 192$ spectroscopy and measurement tasks comprise the bulk of the computational load and will be executed through 500–2000 Frontier-node jobs that last $O(24)$ hours. All tasks make full use of GPU resources for their floating-point workload, while we utilize the CPU to drive inter-node communications for grid boundary (halo) transfers, global reductions and IO.

3. **Computation of requested number of node hours:** This is determined from explicit timing runs on the Crusher testbed on desired partition sizes. For the $96^3 \times 192$ calculations, timings are extrapolated using known volume scalings.

4. **Annual burn rate:** As the workflow and and software are already set up, the burn rate is expected to be approximately linear throughout each year until the allocation is exhausted.

Year	Milestone	Task	Cost/cfg [node-hrs]	$N_{\rm config}$	Total Cost [node-hrs]
0		$48^3 \times 96$ Spectroscopy	1	900	|
0		$48^3 \times 96$ Measurements	2	900	Performed
0		$64^3 \times 128$ Gauge Generation	2	6000	in 2022
0		$64^3 \times 128$ Spectroscopy	15	1200	|
1	1	$64^3 \times 128$ Spectroscopy	15	1200	18,400
1	2	$72^3 \times 192$ Gauge Generation	8	28000	232,600
1	3	$72^3 \times 192$ Spectroscopy	74	2000	148,500
1	4	$96^3 \times 192$ Gauge Generation	33	15000	499,000
1	1+3	$96^3 \times 192$ Summit contractions†	–	–	60,000
2	5	$64^3 \times 128$ Measurements	31	2000	61,200
2	6	$72^3 \times 192$ Measurements	157	2000	297,000
2	7	$96^3 \times 192$ Spectroscopy	472	1000	472,200
3	8	$96^3 \times 192$ Measurements	945	1000	945,000
				Total	**2,673,900**

Table 2. Costs for the gauge-field generation, spectroscopy, and matrix-element measurement tasks planned for this proposal Time is requested in Frontier node hours except for the Summit contractions milestone which will run on Summit and is in Summit node-hours (†). Year 0 correspond to tasks undertaken using our 2022 INCITE allocation.

5. **Uniqueness to LCF resources:** The GPU resources, inter-node parallelism, and fast and reliable storage systems are key features that make Summit and Frontier at OLCF critical to undertaking the proposed computations. The optimal job partition sizes for the majority of the proposed work is 500–2000 Frontier nodes. Coupled with the amount of integrated computing involved, this project is only possible with the resources available under the INCITE program.

6. **Data requirements and usage:** It is anticipated that during active production, scratch storage will be $\mathcal{O}$(500 TB) at a given point in time. Input data (gauge-field configurations for the measurement task) will also be kept on tape, but this amounts to only $\mathcal{O}$(50 TB). The scratch data for a given run will persist for a few weeks while subsequent processing and reduction is undertaken. The outputs of the gauge-field generation task and subsets of the scratch data from the measurement task will be transferred (using `globus`) to NERSC, JLab, and local resources for long-term storage. Further reduction and analysis of data needed to extract the physics quantities that are the goals of this proposal will be performed on local resources using `python`, `julia` and `mathematica`.

7. **Public Data availability:** As discussed in Section 1, the gauge-field configurations that are generated in this proposal will be made freely and immediately available to all members of the national USQCD collaboration (approximately 150 researchers). Gauge-field configurations are the foundation of any LQCD calculations so these are expected to be widely used by the community for multiple different scientific projects. Configurations will be copied using `globus` to JLab where then will be archived for the community. The subset of stored sparse quark propagators will also be made available on request for non-competing research and replicated on local storage. Storage needs in the scratch filesystems will not exceed 500 terabytes.

3.2 Computational Approach

The gauge field generation task will be carried out using the `chroma` lattice field theory library [72], developed under the USQCD SciDAC software project, which implements a state of the art Hybrid Monte Carlo (HMC) [73, 74] algorithm which is a Hybrid Molecular-Dynamics Markov-Chain Monte-Carlo (MCMC) approach and has been tuned specifically for Summit and Frontier through efforts within the USQCD collaboration ECP and SciDAC projects (primarily K. Clark, F. Winter and B. Joò). The majority (~ 90%) of the computational cost is in computing the Molecular Dynamics (MD) forces and the majority of those computations (roughly 60%-80% of the total run-time) is in the solution of the Dirac equation in the computation called at each step of the algorithm. Throughout our project we use a Wilson-Clover [75] formulation of the fermion action and a stout-smeared [76, 77, 78] gauge action. Our state-of-the-art simulations utilize sophisticated *multiple time-scale, higher order MD time-step integrators* [79, 80, 81, 82, 83], advanced linear solvers such as Adaptive Aggregation Multi-Grid (AAMG) [84, 85, 86], and sophisticated determinant break-up schemes to construct the pseudo-fermion action [87, 88, 74].

The determination of quark propagators on each gauge-field configuration constitutes a significant part of the required computation. Using the background-field technology that we have developed, we will calculate various types of compound propagators [31, 33] that implement the local matrix elements needed for our calculations. These propagator calculations require the solution of a large sparse system of linear equations with the problem formulated so that the coefficient matrix is Hermitian positive definite. Here, we will also use the `chroma` library coupled to the highly optimized `quda` library [89, 90] to perform propagator calculations on GPUs. The code has been optimized, tested and used in many super-computing environments and simple load balancing extensions to `chroma` that enable full concurrent use of the CPUs and GPUs have been developed. All calculations are performed in double precision (making use of single/half precision within the solves where appropriate) and propagators are inverted to a precision of 10^{-14}, as high-precision solves are critical in calculations of multi-baryon systems. The disconnected contributions to the matrix elements will be computed using the hierarchical probing techniques introduced in Refs. [91, 92] and correlated with nuclear two-point functions. For the gauge ensembles considered here, the quark masses and volumes are such that the algebraic multigrid inverter in the `quda` library is the most efficient approach (an order of magnitude faster than Krylov methods such as biCG [90]). Extensive studies of the performance of this inverter have been undertaken on Summit, and the relevant details are presented in Section 3.3. Our production runs will parallelize further over the different configurations in the ensembles at the script level, bundling multiple tasks together as discussed below.

Chroma is on the application level of the USQCD software stack and borrows its data types and operations from QDP++, the C++ QCD Data Parallel layer. In Chroma, algorithms are written in terms of expressions using operator infix form (C++ global operators) and are processed by QDP++'s expression template engine PETE, initially to enhance memory locality on CPUs and consequently improve performance. In order to efficiently execute the `chroma` software on GPU-enabled architectures, we build our software stack on top of the `QDP-JIT` framework [93]. This library is a re-implementation of the QDP++ API and was in fact the first library that brought C++ expression template execution to NVIDIA GPUs without calling NVCC in a child process. It did so by generating PTX directly and using the CUDA driver interface to JIT-compile the kernels to GPU code. Since this first implementation, the library has been transitioned to generate LLVM IR [94] which opened the way to target more architectures. The first fully supported target was the LLVM NVPTX backend used for NVIDIA GPUs. Recently the library was extended to fully include the LLVM AMDGPU backend used for AMD GPUs and is fully tested and functional on the Crusher testbed. QDP-JIT produces high-performing GPU kernels from a high-level representation of the computation. Many optimizations have made it into the library: consequent coalesced memory accesses, JIT-compilation occurs only once per expression (repeated calls are simply kernel launches), fast memory allocation through use of memory pools (avoids CUDA/HIP's slow memory allocator), auto-tuning of thread block/workgroup size, and a direct GPU memory interface to `quda`. Furthermore, the use of JIT compilation enables the library to specialize kernels to given runtime parameters, such as for the virtual 4D machine geometry derived from the allocated nodes. Working with QDP-JIT enables us to execute the entire analysis (source creation, propagators, baryon building blocks, contraction) with a single execution of the program.

The contraction codes for studies of nuclear systems make use of automated and recursive techniques [95, 96] and are implemented in parallel over `mpi` using the `tiramisu` compiler [97]. The automated construction of the (dense tensor) contraction codes allows for generation of correlation functions for a large number of interpolating fields of a given set of quantum numbers, vital for the application of the variational method. At present these contraction codes run on CPU and NVIDIA GPU, but efforts are underway to extend the `tiramisu` compiler to generate code for AMD GPUs using the LLVM AMDGPU backend. Since this port may not be ready at the start of 2023, we have also requested time on Summit to perform contractions in Year 1.

Responses to specific computational approach questions:

1. **Libraries languages, and other software requirements:** GCC, LLVM, fftw.
2. **Parallel programming models:** MPI/OpenMP, CUDA (Summit), ROCm (Frontier).
3. **Project workflow:** main computational tasks on Summit and Frontier, followed by small analysis tasks on local resources.
4. **Software workflow solutions:** we anticipate that a few hundred large jobs will be be run to achieve the project goals. This is a sufficiently small number that it can be managed manually by the 4 scientists who will be actively managing the project execution.
5. **I/O requirements:** significant temporary storage (O(500 TB)) is required during active runs but can be reduced quickly thereafter once data is copied remotely.

3.3 Parallel Performance

In terms of readiness for Frontier, QUDA and QDP-JIT have been successfully tested and optimized on the Crusher testbed for Frontier. Kernels generated with QDP-JIT for the AMD system have been benchmarked and achieve performance similar to their NVIDIA counterparts. Our production workflow has been benchmarked and tested for the proposed computational campaign directly on Summit. Below we discuss specifics of Crusher benchmarking; additional benchmarking on Frontier will be performed as it becomes available, but we are ready to run on Frontier as soon as the allocation begins.

Configuration generation task: In preparation for Frontier (and previously Summit), very significant efforts within the USQCD collaboration ECP and SciDAC projects (primarily K. Clark, F. Winter and B. Joò) have gone into optimization of gauge configuration generation using the `chroma` lattice field theory library built on top of the `quda` inverter library and the `qdp-jit` framework discussed above. These improvements, and the expertise within the NPLQCD and USQCD collaborations, allow for the configuration task to be executed very efficiently. Weak and strong scaling studies of this task have been presented for Summit, leading to an OLCF highlight[2]. For Frontier, strong scaling studies on the Crusher testbed are shown in Fig. 5. For the $72^3 \times 192$ geometry included in this proposal, the optimal partition size is 4 streams of configuration generation running in a 108 node partition of Frontier. For the $96^3 \times 192$ geometry, a 512 Frontier node partition is expected to be used.

[2]`https://www.olcf.ornl.gov/2018/09/17/summit-speeds-calculations-in-the-search-for-exotic-particles/`

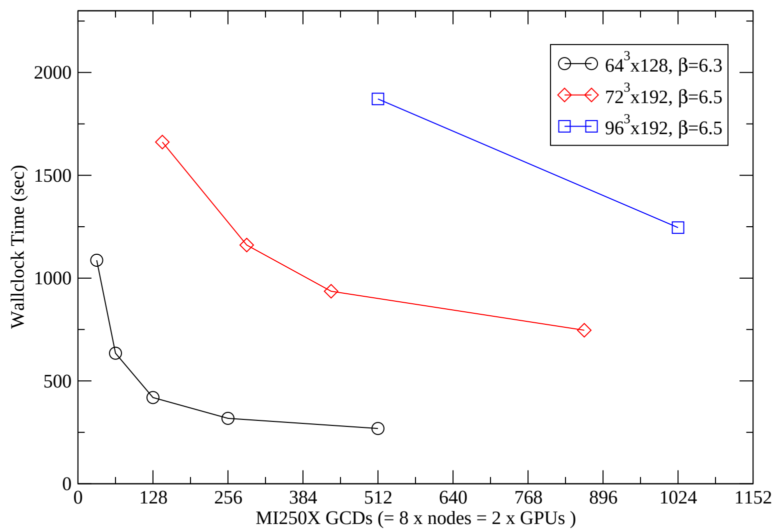

Figure 5. Time per trajectory for the $64^3 \times 128$, $72^3 \times 192$ and $96^3 \times 192$ gauge generation tasks as a function of the number of MI250X GCDs on Crusher [created by B. Joó (OLCF)].

Identifier	MI250X GCDs	Frontier Nodes	Light propagator inversion time [s]
$48^3 \times 96$	8	1	6.5
$64^3 \times 128$	16	2	41.3
$64^3 \times 128$	32	4	26.8
$72^3 \times 192$	48	6	191.4
$72^3 \times 192$	72	9	144.6
$96^3 \times 192$*	128	16	192.8

Table 3. Timing for a single light quark propagator inversion (12 spin-color components) for various ensembles and computational geometries. The result for the largest $96^3 \times 192$ ensemble is projected from volume scaling.

Spectroscopy and measurement tasks: The computational geometries of the proposed work are 4D grids of size $64^3 \times 128$, $72^3 \times 192$, and $96^3 \times 192$. The algebraic multigrid inverter in the `quda` library is used for the propagator inversions that dominate these tasks. Table 3 compiles timings on various partitions of Crusher for single light quark propagator inversion tasks. On each configuration either 216 (C ensemble) or 512 (B and D ensembles) propagators are required for spectroscopy and approximately twice that for the momentum fraction measurement task. Since these calculations need to be performed on 1000–2000 configurations, we will execute them in jobs that run 10 or 20 configurations in parallel. Thus we anticipate partition sizes of up to 640 Frontier nodes for the largest volume ensemble.

3.4 Developmental Work

The gauge generation and propagator calculation tasks are already running on the Crusher testbed and are ready to run on Frontier immediately. The tiramisu-generated contraction codes will need to be ported to AMD GPUs for use in years 2 and 3 on Frontier. Current work to extend the code generator to ROCm will ensure this is possible on the necessary timescale.

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PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

PERSONNEL JUSTIFICATION

The NPLQCD (Nuclear Physics with Lattice QCD) collaboration was formed in 2004 and has pioneered the study of nuclear and hyper-nuclear systems from QCD, developing the necessary theoretical understanding, algorithms and analysis tools to pursue these goals. Our primary objective is to provide a quantitative bridge between nuclear physics and the underlying theory of fundamental forces using LQCD. Our efforts directly address the 2014 Nuclear Science Advisory Committee Performance Measure HP10, and our previous work on this topic has been extensively highlighted in the 2015 Long Range Plan in Nuclear Science. The members of this collaboration have a long history of successful contributions to nuclear and high-energy particle physics, in both formal and numerical contexts, and are experts in LQCD, numerical algorithms and computational paradigms, GPU programming, and effective field theory and finite-volume methods. They are well supported by a number of group and individual grants from the DOE and the NSF. Those who will be responsible for the execution of the current proposal are listed below. Three are early creer tenure-track faculty/scientists.

- **Phiala Shanahan*** is an Assistant Professor at MIT and project PI. She is supported by NSF CAREER award 1841699 and DOE Early Career Award DE-SC0021006. She will be responsible for overseeing project goals and will work on production, data analysis, and effective field theory. Shanahan is an **early career researcher** with her PhD in 2015.
- **Zohreh Davoudi** is an Assistant Professor at the University of Maryland supported by the Alfred P. Sloan Foundation and DOE Early Career award DE-SC0020271. She will work on data analysis and effective field theory. Davoudi is an **early career researcher** with her PhD in 2014.
- **William Detmold*** is an Associate Professor at MIT. He is supported by DOE grant DE-SC0011090 and by the SciDAC4 award DE-SC0018121. He will work on production and data analysis.
- **Assumpta Parreño** is an Associate Professor of Physics at the University of Barcelona in Spain. She is supported by the Spanish Ministerio de Economia y Empresa (MINECO) under project FIS2017-87534-P. She will work on data analysis.
- **Michael Wagman*** is an Associate Staff Scientist at Fermi National Accelerator Laboratory (FNAL). He will work on production and data analysis. Wagman is an **early career researcher** with his PhD in 2017.
- **Frank Winter**† is a Staff Member at the Thomas Jefferson National Accelerator Facility (JLab). He will optimize production codes for Summit and Frontier and ensure best use of GPU resources.

Associated postdoctoral researchers and graduate students will also contribute. All the senior members listed above are in positions that are stable for the course of the proposal. Those indicated with an asterisk will be tasked with day to day running of the calculations while a † indicates resonsibility for code optimization and Frontier-readiness.

MANAGEMENT PLAN

The leadership of the project consists of the PI and a core group of co-PIs who will be involved in the running of the requested computing resources: Shanahan, Detmold, and Wagman. PI Shanahan has successfully led large-scale computing allocations on NSF Bluewaters, ALCC, INCITE and USQCD resources. This group will make day-to-day decisions about scheduling of jobs and defining appropriate checkpoints for intermediate analysis. Within this group, each member will take month-long turns in being responsible for the management of batch jobs, data movement to/from the LCF and archival. This group will also be responsible for communications with the LCF and submission of appropriate reports and science highlights. The larger group of co-PIs will contribute to subsequent stages of data analysis and processing. Critical tasks here are extrapolations to physical results and feeding these results into global PDF fits. The entire team will contribute to manuscript writeups and highlights that arise from the proposed calculations.

Proposal Title: Nuclear femtography: parton distribution functions for the Electron-Ion Collider

Year 1			
Milestone	**Details**	**Dates**	**Status (renewals only)**
$72^3 \times 192$ Gauge generation	**Resources:** Frontier **Node hours:** 232,600 **Filesystem storage (TB and dates):** 50 TB **Archival storage (TB and dates):** 50 TB **Software Application:** chroma/quda **Tasks:** Extend generation of ensemble of configurations **Dependencies:** None	1/1/23-6/30/23	
$64^3 \times 128$ Spectroscopy	**Resources:** Frontier **Node hours:** 18,400 **Filesystem storage (TB and dates):** 80TB intermittently **Archival storage (TB and dates):** 0 **Software Application:** chroma/quda **Tasks:** Compute propagators **Dependencies:** None	1/1/23–3/31/23	
$72^3 \times 192$ Spectroscopy	**Resources:** Frontier **Node hours:** 148,500 **Filesystem storage (TB and dates):** 250TB intermittently **Archival storage (TB and dates):** 0 **Software Application:** chroma/quda/tiramisu **Tasks:** Compute propagators **Dependencies:** $72^3 \times 128$ Gauge generation year 2 task	3/1/23–8/31/23	
Few-body contractions	**Resources:** Summit **Node hours:** 60,000 **Filesystem storage (TB and dates):** 10 TB **Archival storage (TB and dates):** 5 TB **Software Application:** tiramisu **Tasks:** Contract $64^3 \times 128$ and $72^3 \times 128$ quark propagators into hadronic correlation functions **Dependencies:** None	3/1/23-8/1/23	
$96^3 \times 192$ Gauge generation	**Resources:** Frontier **Node hours:** 499,000 **Filesystem storage (TB and dates):** 30 TB **Archival storage (TB and dates):** 30 TB **Software Application:** chroma/quda **Tasks:** Extend generation of ensemble of configurations **Dependencies:** None	6/1/23-12/31/23	

Year 2			
Milestone	**Details**	**Dates**	**Status (renewals only)**
$64^3 \times 128$ Measurements	**Resources:** Frontier **Node hours:** 61,200 **Filesystem storage (TB and dates):** 100TB intermittently **Archival storage (TB and dates):** 10TB **Software Application:** chroma/quda **Tasks:** Compute propagators and contractions **Dependencies:** $64^3 \times 128$ Gauge generation year 1 task	1/1/24–6/30/24	
$72^3 \times 192$ Measurements	**Resources:** Frontier **Node hours:** 297,000 **Filesystem storage (TB and dates):** 200TB intermittently **Archival storage (TB and dates):** 10TB **Software Application:** chroma/quda **Tasks:** Compute propagators and contractions **Dependencies:** $72^3 \times 128$ Gauge generation year 2 task	1/1/24–12/31/24	
$96^3 \times 192$ Spectroscopy	**Resources:** Frontier **Node hours:** 472,200 **Filesystem storage (TB and dates):** 200TB intermittently **Archival storage (TB and dates):** 10TB **Software Application:** chroma/quda **Tasks:** Compute propagators and contractions **Dependencies:** $96^3 \times 128$ Gauge generation year 1 task	1/1/24–12/31/24	

Year 3			
Milestone	**Details**	**Dates**	**Status (renewals only)**
$96^3 \times 192$ Measurements	**Resources:** Frontier **Node hours:** 945,000 **Filesystem storage (TB and dates):** 300TB intermittently **Archival storage (TB and dates):** 10TB **Software Application:** chroma/quda/tiramisu **Tasks:** Compute propagators and contractions **Dependencies:** $96^3 \times 128$ Gauge generation year 1 task	1/1/25–12/31/25	

PUBLICATIONS RESULTING FROM INCITE AWARDS

The PI and co-PIs have benefited from USQCD INCITE awards in 2017-20 (PIs were either Mackenzie or Kronfeld). These awards involved large community efforts from the USQCD consortium and only the publications involving the PI and co-PIs of this application are reported.

1. **"Lattice QCD Constraints on the Parton Distribution Functions of ^{3}He,"**
   W. Detmold *et al.* [NPLQCD],
   Phys. Rev. Lett. **126**, no.20, 202001 (2021).

2. **"Axial charge of the triton from lattice QCD,"**
   A. Parreño *et al.* [NPLQCD],
   Phys. Rev. D **103**, no.7, 074511 (2021).

3. **"Low-energy scattering and effective interactions of two baryons at $m_\pi \sim 450\,$MeV from lattice quantum chromodynamics,"**
   M. Illa *et al.* [NPLQCD],
   Phys. Rev. D **103**, no.5, 054508 (2021)

4. **"Sparsening Algorithm for Multi-Hadron Lattice QCD Correlation Functions,"**
   W. Detmold, D. Murphy, A. Pochinsky, M. Savage, P. Shanahan and M. Wagman,
   arXiv:1908.07050 [hep-lat]

5. **"Nuclear modification of scalar, axial and tensor charges from lattice QCD"**
   E. Chang, Z. Davoudi, W. Detmold, A. S. Gambhir, K. Orginos, M. J. Savage, P. E. Shanahan, M. L. Wagman, F. Winter
   arXiv:1712.03221 [hep-lat]
   Phys. Rev. Lett. **120**, no 15, 152002 (2018)

6. **"First lattice QCD study of the gluonic structure of light nuclei"**
   F. Winter, W. Detmold, A. S. Gambhir, K. Orginos, M. J. Savage, P. E. Shanahan and M. L. Wagman.
   arXiv:1709.00395 [hep-lat]
   Phys. Rev. D **96**, no. 9, 094512 (2017)

7. **"Baryon-Baryon Interactions and Spin-Flavor Symmetry from Lattice Quantum Chromodynamics"**
   M. L. Wagman, F. Winter, E. Chang, Z. Davoudi, W. Detmold, K. Orginos, M. J. Savage and P. E. Shanahan.
   arXiv:1706.06550 [hep-lat]
   Phys. Rev. D **96**, no. 11, 114510 (2017)

8. **"Double-β Decay Matrix Elements from Lattice Quantum Chromodynamics"**
   B. C. Tiburzi, M. L. Wagman, F. Winter, E. Chang, Z. Davoudi, W. Detmold, K. Orginos, M. J. Savage, P. E. Shanahan
   arXiv:1702.02929 [hep-lat]
   Phys. Rev. D **96**, no. 5, 054505 (2017)

9. **"The isotensor axial polarisability and lattice QCD input for nuclear double-β decay phenomenology"**
   P. E. Shanahan, B. C. Tiburzi, M. L. Wagman, F. Winter, E. Chang, Z. Davoudi, W. Detmold, K. Orginos, M. J. Savage

arXiv:1701.03456 [hep-lat]
Phys. Rev. Lett. **119**, no. 6, 062003 (2017)

10. **"Proton-proton fusion and tritium β-decay from lattice quantum chromodynamics"**
M. J. Savage, P. E. Shanahan, B. C. Tiburzi, M. L. Wagman, F. Winter, S. R. Beane, E. Chang, Z. Davoudi, W. Detmold, K. Orginos
arXiv:1610.04545 [hep-lat]
Phys. Rev. Lett. **119**, no. 6, 062002 (2017)

Curriculum Vitae
PHIALA SHANAHAN

Contact Information

Center for Theoretical Physics
Massachusetts Institute of Technology
77 Massachusetts Ave, 6-303
Cambridge, MA 02139

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Professional Preparation

The University of Adelaide	Adelaide, South Australia	Physics	BSc (Hons), 2012
The University of Adelaide	Adelaide, South Australia	Physics	PhD, 2015
Massachusetts Institute of Technology	Cambridge, MA, USA	Physics	postdoctoral, 2015–2017

Appointments

2018 – Assistant Professor of Physics, Massachusetts Institute of Technology.

2017 – 2018 Assistant Professor of Physics, William & Mary,
Senior Staff Scientist, Thomas Jefferson National Accelerator Facility.

Five Publications Most Relevant to This Proposal

1. W. Detmold, M. Illa, D. J. Murphy, P. Oare, K. Orginos, P. E. Shanahan, M. L. Wagman, F. Winter, "Lattice QCD Constraints on the Parton Distribution Functions of ^{3}He," Phys. Rev. Lett. **126**, no.20, 202001 (2021) doi:10.1103/PhysRevLett.126.202001 [arXiv:2009.05522 [hep-lat]].
2. P. E. Shanahan and W. Detmold, "The pressure distribution and shear forces inside the proton," Phys. Rev. Lett. **122**, no. 7, 072003 (2019), *cover feature*.
3. E. Chang, Z. Davoudi, W. Detmold, A. S. Gambhir, K. Orginos, M. J. Savage, P. E. Shanahan, M. L. Wagman, and F. Winter, "Nuclear modification of scalar, axial and tensor charges from lattice QCD", Phys. Rev. Lett. 120, 152002 (2018) [arXiv:1712.03221].
4. M. J. Savage, P. E. Shanahan, B. C. Tiburzi, M. L. Wagman, F. Winter, S. R. Beane, E. Chang, Z. Davoudi, W. Detmold, and K. Orginos, "Proton-proton fusion and tritium β-decay from lattice quantum chromodynamics", Phys. Rev. Lett. 119 (2017) 062002, [arXiv:1610.04545].
5. P. E. Shanahan et al., "Determination of the strange nucleon form factors," Phys. Rev. Lett. 114, no. 9, 091802 (2015), [arXiv:1403.6537 [hep-lat]].

Synergistic Activities

- *Outreach to High Schools*
  NSF Theory Net Partner scientist for Reading Memorial High School, Reading, MA 2015–present.
  Scientist in residence at Wilderness School for girls, Medindie, South Australia 2014–2015.
- *Outreach to the General Public*
  Regular science panellist for ABC Radio National 2015–present.
  6 public lectures since 2014; e.g., "The building blocks of the Universe" >60k views
  https://www.youtube.com/watch?v=YkymlrUL0Sw

- *Community Service*
  Elected member-at-large of the Executive Committee of the Group on Hadronic Physics of the American Physical Society 2020–2022.
  Program Committee Member for the American Physical Society Division of Nuclear Physics 2018–2020.
  Convenor for the Snowmass 2021 process; topical group on machine learning in the Computational Frontier 2021.
  Center for Frontiers in Nuclear Science Program Advisory Committee 2019–present.
  International Symposium in Lattice Field Theory International Advisory Committee 2019–present.

- *Mentoring*
  Mentoring of undergraduate summer research students from underrepresented minorities and underserved backgrounds through the MIT summer research program 2017–present.

- *Recognition*
  2021 APS Maria Goeppert Mayer Award.
  2020 DoE Early Career Award.
  2020 Kenneth Wilson Award in Lattice Gauge Theory.
  2018 NSF CAREER Award.
  2018 Simons Foundation Emmy Noether Fellowship, Perimeter Institute for Theoretical Physics.
  2017 Forbes Magazine 30 under 30 in Science.
  2016 APS Dissertation Award in Hadronic Physics.
  2016 Australian Institute of Physics Bragg Gold Medal.

Collaborators (past 5 years including name and current institution)

- Albergo, Michael, New York University;
- Avkhadiev, Artur, MIT;
- Beane, Silas R, University of Washington;
- Bickerton, Jacob, The University of Adelaide;
- Chang, Emmanuel, unknown;
- Cooke, Ashley;
- Davoudi, Zohreh, University of Maryland;
- Detmold, William, MIT;
- Erben, Felix;
- Gong, Ming, Beijing Institute for High Energy Physics;
- Horsley, Roger, Edinburgh University;
- Kanwar, Gurtej, MIT;
- Lian, Jian, Kentucky University;
- Lin, Huey-Wen, Michigan State University;
- Liu, Keh-Fei, Kentucky University;
- Maxwell, James, TJNAF;
- Myhrer, Fred, University of South Carolina;
- Nakamura, Yoshifumi, RIKEN;
- Orginos, Kostas, The College of William and Mary;
- Parreno, Assumpta, Barceloa U, ECM;
- Pefkou, Dimitra, MIT;
- Pleiter, Dirk, Regensburg University;
- Rakow, Paul E L, Liverpool University;
- Savage, Martin J, Institute for Nuclear Theory;
- Schierholz, Gerrit, DESY;
- Schiller, Arwed, Leipzig University;
- Stuben, Hinnerk, Hamburg University;
- Thomas, Anthony, The University of Adelaide;
- Tiburzi, Brian C, City college of NY, CUNY;
- Trewartha, Daniel, UC Berkeley;
- Tsushima, Kazuo, Cruzeiro do Sul University;
- Wagman, Michael, MIT;
- Winter, Frank T, TJNAF;
- Yang, Yi-Bo, Michigan State;
- Young, Ross, The University of Adelaide;
- Zanotti, James, The University of Adelaide

Curriculum Vitae
ZOHREH DAVOUDI

Contact Information
Department of Physics 3162 Physical Science Complex phone: (301) 405 48591
University of Maryland (College Park) email: davoudi@umd.edu
3162 Physical Science Complex
College Park, MD 20742-4111

Professional Preparation

Ph. D., Physics, University of Washington, 2014 (Advisor: Martin Savage)
M. Sc., Physics, Sharif University of Technology, 2009
B. Sc., Physics, Sharif University of Technology, 2007

Appointments

2017-present, University of Maryland, College Park, Assistant Professor
2017-present, RIKEN Center for Accelerator Based Sceinces, Research Fellow
2014-17, Massachusetts Institute of Technology, Post-doc Research Associate

Five Publications Most Relevant to This Proposal

1. E. Chang *et al.* [NPLQCD], "Scalar, Axial, and Tensor Interactions of Light Nuclei from Lattice QCD," Phys. Rev. Lett. **120**, no.15, 152002 (2018) [arXiv:1712.03221 [hep-lat]].

2. P. E. Shanahan, B. C. Tiburzi, M. L. Wagman, F. Winter, E. Chang, Z. Davoudi, W. Detmold, K. Orginos and M. J. Savage, "Isotensor Axial Polarizability and Lattice QCD Input for Nuclear Double-β Decay Phenomenology," Phys. Rev. Lett. **119**, no.6, 062003 (2017) [arXiv:1701.03456 [hep-lat]].

3. M. J. Savage, P. E. Shanahan, B. C. Tiburzi, M. L. Wagman, F. Winter, S. R. Beane, E. Chang, Z. Davoudi, W. Detmold and K. Orginos, "Proton-Proton Fusion and Tritium β Decay from Lattice Quantum Chromodynamics," Phys. Rev. Lett. **119**, no.6, 062002 (2017)

4. R. A. Briceno and Z. Davoudi, "Three-particle scattering amplitudes from a finite volume formalism," Phys. Rev. D **87**, no.9, 094507 (2013) [arXiv:1212.3398 [hep-lat]].

5. R. A. Briceno and Z. Davoudi, "Moving multichannel systems in a finite volume with application to proton-proton fusion," Phys. Rev. D **88**, no.9, 094507 (2013) [arXiv:1204.1110 [hep-lat]].

Research Interests and Expertise

I study strongly interacting systems using analytical and computational methods including effective field theories, lattice quantum chromodynamics, quantum simulation, and quantum computing. Since 2015, I am a member of NPLQCD collaboration which focuses on first-principles numerical determinations of nuclear-physics quantities in the light-nuclear sector, such a nuclear and hypernuclear interactions and spectroscopy, nuclear reaction cross sections, nuclear matrix elements in rare processes such as double-beta decays, and in nuclear responses to external probes in search for dark matter candidates or for violation of fundamental symmetries such as CP violation using nuclear targets. I have also developed formal frameworks for extracting and interpreting multi-hadron observables from numerical calculations based in lattice QCD.

Synergistic Activities

Elected topical co-convener of the U.S. particle physics 10-year planning process (Snowmass) on the topic of Lattice Gauge Theory, 2020-2022.

Co-Lead of the USQCD collaboration 5-year planning process and lead editor of the USQCD whitepaer in Fundamental Symmetries in 2019.
Program organizer of the IQuS workshops on "Quantum Simulation of Strong Interactions (QuaSI I and II)" (2021), INT program organizer on "Nuclear Forces for Precision Nuclear Physics" (2021), INT workshop on "LQCD input for 0vBB decay" (2017), lead organizer of the INT program on "Nuclear physics from LQCD" (2016), and the program organizer of the INT workshop on "Nuclear reactions from LQCD" (2013).
Invited lecturer of the advanced training course on "Nuclear Forces", Institute for Nuclear Theory, Seattle (2013), the Odense Winter School on "Theoretical Physics", CP3-Origins Institute, Odense, Denmark (2017), the TALENT course on "From Quarks and Gluons to Nuclear Forces and Structure", ECT*, Trento, Italy (2019), and the Summer School on "The Physics of the Future Electron Ion Collider", Center for Frontiers in Nuclear Science, Stony Brook University (2019). International advisory committee of the EuroPLEx School, Edinburgh, UK (2021).
Reviewer and panelist of the U.S. Department of Energy's Office of Science and the National Science Foundation in Nuclear Theory (2018-).
Invited panelist of the "2016 Isaac Asimov Memorial Debate", hosted by Neil deGrasse Tyson at the American Museum of Natural History, NYC, NY, April 2016. Invited scientist and lesson writer of a TED-Ed project featuring the topic of simulating laws of nature, released in 2019.

Honors and Awards

Alfred P. Sloan Fellow, 2019
DOE Early Career Award, 2019
Kenneth Wilson Award in Lattice Gauge Theory, 2018
Sebastian Karrer Prize in Excellence in Graduate Studies in Physics, U of Washington, 2011

Collaborators (*past 5 years including name and current institution*)

Andrade, Barbara (ICFO, Barcelona), Alexandru, Andrei (George Washington University), Baroni, Alessandro (Los Alamos National Laboratory), Beane, Silas (U of Washington), Bennink, Ryan (Oak Ridge National Laboratory), Bhattacharya, Tanmoy (Los Alamos National Laboratory), Briceno, Raul (Jefferson Lab/Old Dominion University), Chang, Emmanuel (N/A), Cirigliano, Vincenzo (Los Alamos National Laboratory), Detmold, William (MIT), Dumitrescu, Eugene (Oak Ridge National Lab), Ekstrom, Andreas (Chalmers University of Technology, Sweden), Gambhir, Arjun (LLNL, Livermore/LBNL, Berkeley), Grass, Tobias (ICFO, Barcelona), Hansen, Maxwell (CERN), Harrison, James (N/A), Holt, Jason (TRIUMF, Canada), Illa, Marc (University of Barcelona), Izubuchi, Taku (Brookhaven National Laboratory), Juttner, Andreas (University of Southampton), Lamm, Henry (Fermilab), Lynn, Joel (Technische Universitat Darmstadt), Monroe, Christopher (Duke U), Murphy, David (MIT), Orginos, Kostas (Jefferson Lab/College of W&M), Pagano, Guido (Rice U), Parreno, Assumpta (University of Barcelona), Pochinsky, Andrew (MIT), Portelli, Antonin (University of Edinburgh), Savage, Martin (U of Washington, IQuS), Schindler, Matthias (University of South Carolina), Seif, Alireza (U of Chicago), Shanahan, Phiala (MIT), Syritsyn, Sergey (Stony Brook University), Tews, Ingo (Los Alamos National Laboratory), Brian, Tiburzi (The City College of New York), Wagman, Michael (Fermilab), Winter, Frank (Jefferson Lab).

Curriculum Vitae
WILLIAM DETMOLD

Contact Information

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email: wdetmold@mit.edu

Professional Preparation

Ph. D., Physics, University of Adelaide, 2002 (Advisor: Anthony W. Thomas)
B. Sc. (Hons), Mathematical Physics, University of Adelaide, 1997

Appointments

2017-present, Massachusetts Institute of Technology, Associate Professor
2012-17, Massachusetts Institute of Technology, Assistant Professor
2009-12, College of William & Mary, Assistant Professor
2004-8, University of Washington, Research Assistant Professor
2002-4, University of Washington, Research Associate

Five Publications Most Relevant to This Proposal

1. W. Detmold, W. Melnitchouk, J. W. Negele, D. B. Renner and A. W. Thomas, "Chiral extrapolation of lattice moments of proton quark distributions," Phys. Rev. Lett. **87**, 172001 (2001) [arXiv:hep-lat/0103006 [hep-lat]].

2. J. W. Chen, W. Detmold, J. E. Lynn and A. Schwenk, "Short Range Correlations and the EMC Effect in Effective Field Theory," Phys. Rev. Lett. **119**, no.26, 262502 (2017) [arXiv:1607.03065 [hep-ph]].

3. J. W. Chen and W. Detmold, "Universality of the EMC effect," Phys. Lett. B **625**, 165-170 (2005) 5doi:10.1016/j.physletb.2005.08.041 [arXiv:hep-ph/0412119 [hep-ph]].

4. S. R. Beane *et al.* [NPLQCD Collaboration], "Magnetic moments of light nuclei from lattice quantum chromodynamics," Phys. Rev. Lett. **113**, no. 25, 252001 (2014) [arXiv:1409.3556 [hep-lat]].

5. W. Detmold and K. Orginos, "Nuclear correlation functions in lattice QCD," Phys. Rev. D **87**, no. 11, 114512 (2013) [arXiv:1207.1452 [hep-lat]].

Research Interests and Expertise I am interested in the application of lattice QCD to particle and nuclear physics phenomenology and experiments. I focus on trying to understand the emergence of the complex structures of hadronic and nuclear physics from the underlying simplicity of the Standard Model. Most recently, I have been attempting to determine the structure and interactions of nuclei from QCD degrees of freedom. In addition, I have worked to understand the hadronic physics of bottom baryon decays at the LHC, enabling constraint of the parameters of the Standard Model and searches for physics beyond it.

Synergistic Activities

Member, USQCD Collaboration Executive Committee, 2016-present
PI of SciDAC4 project "Computing the Properties of Matter with Leadership Computing Resources" , 2018-present
Co-spokesperson, Topical Collaboration in Nuclear Theory for the Coordinated Theoretical Approach to Transverse Momentum Dependent Hadron Structure in QCD, 2016-present
Member, National Advisory Committee for National Institute for Nuclear Theory, 2017-19
Member-at-large, Executive Committee of American Physical Society Topical Group on Few Body Physics

Chair, Organizing Committee of National Nuclear Physics Summer School, 2016
Co-chair, Organizing Committee of the 38th International Symposium on Lattice Gauge Theory, Cambridge, USA, 2021
Member, International Advisory Committee for the International Symposium on Lattice Field Theory, 2012, 2013, 2016-19
Member, Computational Nuclear Physics Whitepaper Writing Committee, 2015

Honors and Awards

Adelaide University Medal, 1997
Harold Woolhouse Prize, University of Adelaide, 2002
Outstanding Junior Investigator Award, Department of Energy Office of Nuclear Physics, 2009
Early Career Research Award, Department of Energy, 2013
Fellow, American Physical Society, 2017

Collaborators (*past 5 years including name and current institution*)

Beane, Silas (University of Washington), Brower, Richard (Boston University), Carlson, Joseph (LANL), Chang, Emmanuel (Barcelona), Chen, Jiunn-Wei (National Taiwan University), Christ, Norman (Columbia), Cirigliano, Vincenzo (LANL), Davoudi, Zohreh (UMD), Dudek, Jo (JLab), Edwards, Robert (JLab), Endres, Micheal (Harvard), Engelhardt, Michael (New Mexico State) Flynn, Micheal (MIT), Gandolfi, Stefano (LANL), Gupta, Rajan (LANL), Horsley, Roger (Edinburgh), Illa Subina, Marc (Barcelona), Jafry, Murtaza (Washignton), Kanamori, Issaku (Hiroshima), Kanwar, Gurtej (MIT), Kronfeld, Andreas (FNAL), Joò, Balint (JLab) Jung, Chulwoo (BNL), Lamm, Henry (FNAL), Lehner, Christoph (Brookhaven), Lin, C.-J. David (National Chiao-Tung University), Lin, Huey-Wen (Michigan State), Liu, Keh-Fei (Kentucky), Lonardoni, Diego (Michigan State)m Lynn, Joel (Darmstadt) Meinel, Stefan (MIT), Meyer, Aaron (BNL), Mondal, Santanu (LANL), Murphy, David (MIT), Nakamura, Yooshifumi (RIKEN), Nicholson, Amy (LBNL), Orginos, Konstantinos (College of William and Mary), Parreño, Assumpta (Barcelona), Perfkou, Dimitra (MIT), Perlt, Holger (Leipzig), Pochinsky, Andrew (MIT), Rackow, Paul (Liverpool) Richards, David (JLab) Savage, Martin (University of Washington), Schierholz, Gerrit (DESY) Schwenk, Achim (Darmstadt), Shanahan, Phiala (MIT), Stüben, Hinnerk (Hamburg) Sufian, Raza (JLab), Syritsyn, Sergey (Stonybrook), Tiburzi, Brian (City College of New York), Trewartha, Daniel (Berkeley), Wagman, Michael (FNAL), Warrington, Neil (Washington), Wilhem, Johannes (Giessen), Winter, Frank (Jefferson Lab), Young, Ross (Adelaide), Zanotti, Jimbo (Adelaide), Zhao, Yong (BNL)

Curriculum Vitae
ASSUMPTA PARREÑO

Contact Information

Departament de Física Quàntica i Astrofísica
Institut de Ciències del Cosmos. U of Barcelona phone: +34 934039195
Martí i Franquès, 1 email: assum@fqa.ub.edu
Barcelona - 08028 (Spain)

Professional Preparation

Master Degree on Environmental Control and Quality, Institut Català de Tecnologia, 2003
Pedagogical Aptitude Certification, Universitat Politècnica de Catalunya, 1997
Ph. D. Physics, U of Barcelona, 1997 (Advisors: C. Bennhold and A. Ramos)
B. Sc. Physics, U of Barcelona, 1992

Appointments

2018- , Univ. Barcelona, Deputy Director of the Institute of Cosmos Sciences
2007- , Univ. Barcelona, Associate Professor of Physics
2003-2007, Univ. Barcelona, Ramón y Cajal Researcher
2001-2003, Univ. Barcelona, Postdoctoral Research Associate
10/1998-01/2001, Institute for Nuclear Theory, Seattle, Research Associate

Five Publications Most Relevant to This Proposal

1.- A. Parreño *et al.* [NPLQCD Collab], “The axial charge of the triton from lattice QCD", Phys. Rev. D **103**, 074511 (2021)
2.- M. Illa *et al.* [NPLQCD Collab], “Low-energy scattering and effective interaction of two baryons at m(pion) 450 MeV from lattice quantum chromodynamics", Phys. Rev. D **103**, 054508 (2021)
3.- A. Parreño *et al.* [NPLQCD Collab], “Octet baryon magnetic moments from lattice QCD: Approaching experiment from a three-flavor symmetric point", Phys. Rev. D **95**, 114513 (2017)
4.- W. Detmold *et al.* [NPLQCD Collab], “Unitary Limit of Two-Nucleon Interactions in Strong Magnetic Fields", Phys. Rev. Lett. **116**, no. 13, 112301 (2016)
5.- S. R. Beane *et al.* [NPLQCD Collab], “Ab initio Calculation of the $np \to d\gamma$ Radiative Capture Process", Phys. Rev. Lett. **115**, no. 13, 132001 (2015)

Research Interests and Expertise

Baryon-baryon interactions at low energies
Hypernuclear physics: understanding the structure and decay of hypernuclei using both, meson-exchange models and effective field theories
Lattice QCD: study of the structure of hadrons and nuclear systems, including hypernuclei and other exotic systems, from the fundamental degrees of freedom of QCD, as well as hadronic and nuclear reactions of astrophysical interest

Synergistic activities for the last five years

- PI of the FI-2022-1-0040 project "Variational study of the baryon-baryon system in the strange sector", BSC, Red Española de Supercomputación, March-June 2022
- PI of the PID2020-118758GB-I00 project "Understanding matter governed by the strong force: quarks, hadrons, nuclei and neutron stars" , Spanish Science, Innovation and Universities Office, 2021 - 2024
- PI of the NPLQCD PRACE project No. 2020235570 'Nuclear Physics from the Standard Model", 01/04/2021-31/03/2022
- Member of the National Advisory Committee for the Institute for Nuclear Theory, Seattle, 2020 - 2022
- co-PI of the "Spanish network of Lattice Gauge Theory" (Barcelona node) Spanish Science, Innovation and Universities Office, 2020 - 2021
- PI of the project "Nuclear states emerging from quantum chromodynamics", BSC, Red Española de Supercomputación, 01/07/2019 - 9/02/2020
- "Hadron resonances, form factors, LECs, fundamental parameters of QCD and light nuclei spectroscopy" task co-ordinator, WP 25, STRONG-2020, UE H2020-INFRAIA-2018-1, grant No. 824093, 2019 - 2023
- Chair of the Diversity, Equity and Inclusion Commission of the ICCUB, 2018 - present
- Member of the FIS2017-87534-P project: "Challenges in many-body physics: hadrons, nuclei and atoms", MCOC, 2018-2021
- Member of the 2017SGR533 project: "Theoretical nuclear physics and physics of systems with many interacting particles", AGAUR, 2017 - 2020
- Co-organizer of the 35th International Symposium on Lattice Field Theory (Lattice 2017), Granada, Spain, June 18-24, 2017
- Serving on the Agency for Quality Assurance in the Galician University System, Spain, 2017 - present
- Member of the Scientific Board of the ICCUB, 2016 - present
- Serving on the Agencia Nacional de Evaluación y Prospectiva, 2015 - present
- Co-PI of the Maria de Maeztu MDM-2014-0369 project, "Institut de Ciències del Cosmos, U of Barcelona", MCOC, 2015 - 2019

Outreach to the General Public:

- 15a Festa de la Ciència, Ajuntament de Barcelona, 28/05/2022,
- VIII Festa de la Ciència de la UB, 27/05/2022.
- Biennal Ciutat i Ciència, 13/06/2021,
- Quarks: the bricks of matter
- International Day of Women and Girls in Science, ACCIONA

Mentoring:

- Undergraduate mentoring at the Physics degree of the University of Barcelona, 2021 - present
- Erasmus+ Summer School "Diversity in the Cultures of Physics", 2018

Collaborators (*past 5 years including name and recent affiliation*)

Beane, S. and Savage, M (U of Washington), Chang, E. (Taiwan), Cohen, S. (NDIVIA), Davoudi, Z. (Maryland), Entem, D. R. (Salamanca), Illa, M., Juliá-Díaz, B, Maneu, J., Pérez-Obiol, A. and Ramos, A. (Barcelona) Lin, H.-W. (Michigan State U.), Murphy, D.J., Detmold, W. and Shanahan, P. (MIT), Orginos, K. (William and Mary), Tiburzi, B. (City College of New York), Wagman, M. (Fermilab), Wilhelm, J. (Giessen), Winter, F. (JLab)

Curriculum Vitae
MICHAEL WAGMAN

Contact Information

Fermilab phone: (630) 840-3000
PO Box 500 fax: (630) 840-4343
Batavia, IL 60510-5011 email: mwagman@fnal.gov

Professional Preparation

Ph. D., Physics, University of Washington, 2017 (Advisor: Martin J. Savage)
B. Sc. (Hons), Mathematical Physics, Brown University, 2012

Appointments

2019-present, Fermi National Accelerator Laboratory, Associate Scientist
2017-2019, Massachusetts Institute of Technology, Pappalardo Fellow

Five Publications Most Relevant to This Proposal

1. W. Detmold, M. Illa, D. J. Murphy, P. Oare, K. Orginos, P. E. Shanahan, M. L. Wagman, F. Winter, "Lattice QCD Constraints on the Parton Distribution Functions of ^{3}He," Phys. Rev. Lett. **126**, no.20, 202001 (2021) doi:10.1103/PhysRevLett.126.202001 [arXiv:2009.05522 [hep-lat]].

2. P. Shanahan, M. L. Wagman and Y. Zhao, "Collins-Soper kernel for TMD evolution from lattice QCD," Phys. Rev. D **102**, no.1, 014511 (2020) doi:10.1103/PhysRevD.102.014511 [arXiv:2003.06063 [hep-lat]].

3. E. Chang, Z. Davoudi, W. Detmold, A. S. Gamhbir, K. Orginos, M. J. Savage, P. E. Shanahan, M. L. Wagman, and F. Winter [NPLQCD Collaboration], "Scalar, Axial, and Tensor Interactions of Light Nuclei from Lattice QCD," Phys. Rev. Lett. **120**, no.15, 152002 (2018) [arXiv:1712.03221 [hep-lat]].

4. F. Winter, W. Detmold, A. S. Gambhir, K. Orginos, M. J. Savage, P. E. Shanahan and M. L. Wagman [NPLQCD Collaboration], "First lattice QCD study of the gluonic structure of light nuclei," Phys. Rev. D **96**, no.9, 094512 (2017) [arXiv:1709.00395 [hep-lat]].

5. M. L. Wagman and M. J. Savage, "Statistics of baryon correlation functions in lattice QCD," Phys. Rev. D **96**, no.11, 114508 (2017) [arXiv:1611.07643 [hep-lat]].

Research Interests and Expertise

I am interested in using lattice QCD to improve the ability of particle and nuclear physics experiments to search for new physics, as well as to improve our understanding of how the complexity of hadron and nuclear structure emerges from the interactions of quarks and gluons in QCD. Recently, I have worked on pioneering lattice QCD calculations of nuclear matrix elements as well as techniques for constraining aspects of light-front structure functions relevant to experiments at Jefferson Lab and a future Electron Ion Collider. I have also worked on lattice QCD calculations enabling new physics constraints to be extracted from intensity frontier experiments searching for fundamental symmetry violation and other new physics signatures using nucleons and nuclei as targets.

Synergistic Activities

Member, Snowmass Early Career Leadership Committee, 2020-present
Member, USQCD Collaboration, 2017-present

Honors and Awards

Brown University Mary Widgoff Prize, 2012

University of Washington Sebastian Karrer Prize in Physics, 2014
University of Washington Graduate Medalist in the Natural Sciences, 2017

Collaborators (*past 5 years including name and current institution*)

Beane, Silas (University of Washington), Bi, Zhen (MIT), Buchoff, Michael (Lawrence Livermore National Lab), Cherman, Aleksey (Minnesota University), Chang, Emmanuel, Davoudi, Zohreh (University of Maryland), Gambhir, Arjun (Lawrence Livermore National Lab), Grebe, Anthony (MIT), Horsley, Roger (Edinburgh University), Illa, Marc (Barcelona), Jafry, Murtaza (University of Washington), Kanwar, Gurtej (MIT), Lamm, Henry (FNAL), Ledwith, Patrick (MIT), Miller, Gerlad (University of Washington), Murphy, David (MIT), Orginos, Konstantinos (College of William and Mary), Nakamura, Yoshifumi (RIKEN Kobe), Perlt, Holger (Leipzig University), Pochinsky, Andrew (MIT), Rakow, Paul (University of Liverpool), Rinaldi, Enrico (RIKEN), Savage, Martin (University of Washington), Sen, Srimoyee (Iowa State University), Schierholz, Gerrit (DESY), Schroeder, Chris (Lawrence Livermore National Lab), Shanahan, Phiala (MIT), Stüben, Hinnerk (Hamburg University), Syritsyn, Sergey (Stony Brook), Tiburzi, Brian (City College of New York), Ünsal, Mithat (North Carolina State University), Warrington, Neill (University of Washington), Wasem, Joseph (Lawrence Livermore National Lab), Winter, Frank (Jefferson Lab), Yaffe, Laurence (University of Washington), Young, Ross (Adelaide University), Zanotti, James (Adelaide University), Zhao, Yong (Brookhaven National Lab)

Curriculum Vitae
FRANK WINTER
Contact Information

Professional Preparation

PhD in Physics, University Regensburg, 2011
Dipl.-Phys. , Freie University, 2006

Appointments

2013–present, Staff Scientist, Jefferson Lab
2011–2013, Postdoc, University of Edinburgh

Five Publications Most Relevant to This Proposal

1. S. R. Beane, et. al. “Charged multi-hadron systems in lattice QCD+QED”, submitted to PRL
2. Colin Egerer, et al. “Controlling Excited-State Contributions with Distillation in Lattice QCD Calculations of Nucleon Isovector Charges g_S^{u-d}”, Phys. Rev. D 99, 034506 (2019)
3. Emmanuel Chang, et. al. “Nuclear modification of scalar, axial and tensor charges from lattice QCD”, Phys. Rev. Lett. 120, 152002 (2018)
4. Michael L. Wagman, et. al. “Baryon-Baryon Interactions and Spin-Flavor Symmetry from Lattice Quantum Chromodynamics”, Phys. Rev. D 96, 114510 (2017)
5. Brian C. Tiburzi, et. al. “Double-β Decay Matrix Elements from Lattice Quantum Chromodynamics”, Phys. Rev. D 96, 054505 (2017)

Research Interests and Expertise

High performance computing. Author and maintainer of QDP-JIT/LLVM.

Synergistic Activities

1. Member of Program Committee of The Fifth Workshop on the LLVM Compiler Infrastructure in HPC (multiple years)

Collaborators (*past 5 years including name and current institution*)

B. Joo, Thomas Jefferson National Accelerator Facility
B. C. Tiburzi, The City College of New York
C. Egerer, William and Mary
D. Richards,Thomas Jefferson National Accelerator Facility
D. J. Murphy, Massachusetts Institute of Technology
E. Chang, University of Maryland
G. Schierholz, Deutsches Elektronen-Synchrotron DESY
H. Perlt, Universitaet Leipzig
H. Stueben, Universitaet Hamburg
J. M. Zanotti, University of Adelaide
K. Orginos, William and Mary
M. J. Savage, University of Washington
M. L. Wagman, University of California
M. Illa, Universitat de Barcelona
M. Jafry, University of Washington
P. E. L. Rakow, University of Liverpool
P. E. Shanahan, Massachusetts Institute of Technology
R. D. Young, University of Adelaide
R. Horsley, University of Edinburgh
R. Edwards, Thomas Jefferson National Accelerator Facility

S. R. Beane, University of Washington
W. Detmold, Massachusetts Institute of Technology
Y. Nakamura, RIKEN Center for Computational Science
Z. Davoudi, University of Maryland

Section 6: Software Applications and Packages

Question #1

Please list any software packages used by the project, and indicate if they are on open source or export controlled.

Application Packages

Package Name

Chroma

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

Quda

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

Qdp-jit

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

Tiramisu

Indicate whether Open Source or Export Controlled.

Open Source

Section 7: Wrap-Up Questions

Question #1

National Security Decision Directive (NSDD) 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information obtainable free of charge (other than minor shipping or copying fees) and without restriction, which is available via the internet, journal publications, textbooks, articles, newspapers, magazines, etc.

The INCITE program distinguishes between the generation of proprietary information (deemed a proprietary project) and the use of proprietary information as input. In the latter, the project may be considered as Fundamental Research or nonproprietary under the terms of the nonproprietary user agreement. Proprietary information, including computer codes and data, brought into the LCF for use by the project - but not for generation of new intellectual property, etc., using the facility resources - may be protected under a nonproprietary user agreement.

Proprietary Information

Are the proposed project and its intended outcome considered Fundamental Research or Publicly Available Information?

No

Will the proposed project use proprietary information, intellectual property, or licensing?

No

Will the proposed project generate proprietary information, intellectual property, or licensing as the result of the work being proposed?

If the response is Yes, please contact the INCITE manager, INCITE@doeleadershipcomputing.org, prior to submittal to discuss the INCITE policy on proprietary work.

No

Question #2

The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate - but not substitute for - any export control review required for this proposal.

PIs are responsible for knowing whether their project uses or generates sensitive or restricted information. Department of Energy systems contain only data related to scientific research and do not contain personally identifiable information. Therefore, you should answer "Yes" if your project uses or generates data that fall under the Privacy Act of 1974 U.S.C. 552a. Use of high-performance computing resources to store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI); naval nuclear propulsion information (NNPI); and the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585, 202-586-9211.

Export Control

Does this project use or generate sensitive or restricted information?

No

Does the proposed project involve any of the following areas?

i. Military, space craft, satellites, missiles, and associated hardware, software or technical data

ii. Nuclear reactors and components, nuclear material enrichment equipment, components (Trigger List) and associated hardware, software or technical data

iii. Encryption above 128 bit software (source and object code)

iv. Weapons of mass destruction or their precursors (nuclear, chemical and biological)

No

Does the proposed project involve International Traffic in Arms Regulations (ITAR)?

No

Question #3

The following questions deal with health data. PIs are responsible for knowing if their project uses any health data and if that data is protected. Note that certain health data may fall both within these questions as well as be considered sensitive as per question #2. Questions regarding these answers to these questions should be directed to the centers or program manager prior to submission.

Health Data

Will this project use health data?

No

Will this project use human health data?

No

Will this project use Protected Health Information (PHI)?

No

Question #4

The PI and designated Project Manager agree to the following:

Monitor Agreement

I certify that the information provided herein contains no proprietary or export control material and is correct to the best of my knowledge.

Yes

I agree to provide periodic updates of research accomplishments and to acknowledge INCITE and the LCF in publications resulting from an INCITE award.

Yes

I agree to monitor the usage associated with an INCITE award to ensure that usage is only for the project being described herein and that all U. S. Export Controls are complied with.

Yes

I understand that the INCITE program reserves the right to periodically redistribute allocations from underutilized projects.

Yes

Section 8: Outreach and Suggested Reviewers

Question #1

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Outreach

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Email notices

Question #2

Suggested Reviewers

Suggest names of individuals who would be particularly suited to assess the proposed research.

Ubirajara Van Kolck (vankolck@arizona.edu)

Section 9: Testbed Resources

Question #1

The ALCF and OLCF have test bed resources for new technologies, details below. If you would like access to these resources to support the work in this proposal, please provide the information below. (1 Page Limit)

The OLCF Quantum Computing User Program is designed to enable research by providing a broad spectrum of user access to the best available quantum computing systems, evaluate technology by monitoring the breadth and performance of early quantum computing applications, and Engage the quantum computing community and support the growth of the quantum information science ecosystems. More information can be found here: https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation.

The ALCF AI Testbed provides access to next-generation of AI-accelerator machines to enable evaluation of both hardware and workflows. Current hardware available includes Cerebras C-2, Graphcore MK1, Groq, Habana Gaudi, and SambaNova Dataflow. New hardware is regularly acquired as it becomes available. Up to date information can be found here: https://www.alcf.anl.gov/alcf-ai-testbed.

Describe the experiments you would be interested in performing, resources required, and their relationship to the current proposal. Please note, these are smaller experimental resources and a large amount of resources are not available. Instead, these resources are to explore the possibilities for these technologies might innovate future work. This request does not contribute to the 15-page proposal limit.

testbed.pdf
The attachment is on the following page.

N/A