2023 INCITE Proposal Submission
Proposal

Title: Hadron physics from first principles
Principal Investigator: Konstantinos Orginos
Organization: William and Mary University
Date/Time Generated: 6/17/2022 5:49:07 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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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

We perform calculations of the properties of Hadrons (particles that interact strongly) from first principles using the fundamental theory of strong interactions know as Quantum ChromoDynamics (QCD). Our project utilizes modern computational methods in order to obtain information about the internal structure, the interactions and the spectrum of Hadrons.

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

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Node Hours

1,250,0000

Storage (TB)

101

Off-Line Storage (TB)

100

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Question #4

OLCF Frontier (Cray Shasta) Resource Request – 2025

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

DOE - Nuclear Theory

Grant Number

DE-FG02-04ER41302

Funding Source

DOE - Nuclear Theory

Grant Number

DE-AC05-06OR23177

Funding Source

DOE - Nuclear Theory

Grant Number

DE-FG02-97ER41028

Funding Source

DOE (ORNL contract)

Grant Number

DESC0018416

Question #13

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

Other High Performance Computing Resource Allocations

Resource

SUMMIT OLCF

Allocation Agency

ALCC

Allocation

600,000

Allocation Year

2022-2023

Resource

JLab MI100-GPU cluster

Allocation Agency

USQCD

Allocation

90,0000 GPU-hours

Allocation Year

2022-2023

Resource

JLab KNL cluster

Allocation Agency

USQCD

Allocation

13,000,000 KNL-core-hours

Allocation Year

2022-2023

Resource

JLab RTX2080-GPU cluster

Allocation Agency

USQCD

Allocation

538,000 GPU hours

Allocation Year

2022-2023

Resource

NERSC

Allocation Agency

DOE

Allocation

450,000 node-hours (CPU Perlmuter)

Allocation Year

2022-2023

Resource

Frontera (TACC)

Allocation Agency

LRAC

Allocation

750,000 node-hours

Allocation Year

2022-2023

Resource

CINECA MARCONI

Allocation Agency

PRACE

Allocation

400,000 node-hours

Allocation Year

2022-2023

Resource

Jean Zay (IDRIS)

Allocation Agency

Genci (French national call)

Allocation

600,000 node-hours

Allocation Year

2022-2023

Resource

Meluxina

Allocation Agency

EuroHPC

Allocation

127,000 node-hours

Allocation Year

2022-2023

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.

INCITE2023.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title: Hadron physics from first principles

PI: Kostas Orginos (William & Mary)
co-PIs: Robert Edwards (JLab), Colin Egerer (JLab), Bálint Joó (ORNL), Christopher Monahan (W&M), Jianwei Qiu (JLab), Anatoly Radyushkin (ODU), David Richards (JLab), Eloy Romero (JLab), Raza Sufian (JLab), Frank Winter (JLab), Savvas Zafeiropoulos (CNRS/Marseille, FR)

Applying Institution/Organization: William & Mary

Resource Name(s) and Number of Node Hours Requested: **1.25 M Frontier node-hours** on OLCF's Frontier system

Amount of Storage Requested: **101 TB** of scratch storage and **100 TB** of archival storage at OLCF

Executive Summary:

We request one year allocation on the Oak Ridge Leadership Computing Facility's (OLCF) OLCF Cray Shasta machine, Frontier, to compute the structure and spectrum of strongly-coupled hadronic states directly from quantum chromodynamics (QCD). These calculations will provide essential theoretical support to the experimental program of the Thomas Jefferson National Accelerator Facility (Jefferson Lab) and to the future Electron Ion Collider (EIC) at Brookhaven National Laboratory. We will generate resources of direct benefit to others working in the computational nuclear physics community that will broaden the impact of this proposal, from complementary aspects of proton structure to form factors relevant to upcoming long-baseline neutrino science at Fermilab and the Deep Underground Neutrino Experiment.

We have two main goals. First, to compute the x-dependent, isovector light-quark generalized parton distributions (GPDs) of the nucleon, in the continuum and physical quark-mass limits of lattice QCD. Second, to provide a lattice determination of the flavor decomposition of the proton sea through isoscalar GPDs. Leadership class computing is critical for our goals, which will provide the ab initio answers to a question "*essential for understanding the nature of visible matter*" [1] and central to the Department of Energy's experimental nuclear physics program: how do quarks and gluons form the wide range of hadronic bound states we observe in experiment?

PROJECT NARRATIVE

1 SIGNIFICANCE OF RESEARCH

The Standard Model of particle physics unites the electromagnetic, strong and weak nuclear forces, and underpins our understanding of the visible Universe at the smallest scales. The strong nuclear force binds quarks and gluons into hadronic states, from the protons and neutrons that form the basic building blocks of nuclei and the vast majority of the mass of the visible Universe, to exotic states recently discovered at the Large Hadron Collider (LHC). All three forces are important in the physics of these hadronic states, but the strong nuclear force, mathematically described by the theory of Quantum Chromodynamics (QCD), plays the central role. After decades of research and development, lattice QCD, the numerical approach to studying QCD, now enables calculations of the simplest properties of hadrons, such as their masses and interactions with the electromagnetic and weak forces, with precision. Understanding the detailed three-dimensional structure of hadrons and the nature of exotic states, however, lies at the frontier of the current computational capabilities of lattice QCD.

We propose a computational program that will drive significant new research in nuclear physics by addressing the structure and spectra of strongly-coupled states directly from QCD. The results of this project will provide immediate and critical theoretical support to the experimental program at Thomas Jefferson National Accelerator Facility (Jefferson Lab), while shaping the future potential of the planned Electron Ion Collider (EIC) at Brookhaven National Laboratory. This support was recognized as central to the research goals of the Office of Science of the Department of Energy (DOE) in the 2015 Nuclear Science Advisory Committee's (NSAC) Long Range Plan for Nuclear Science [1]:

> *Advances in theory underpin the goal that we truly understand how nuclei and strongly interacting matter in all its forms behave and can predict their behavior in new settings. To meet the challenges and realize the full scientific potential of current and future experiments, we require new investments in theoretical and computational nuclear physics. We recommend new investments in computational nuclear theory that exploit the U.S. leadership in high-performance computing.*

Petascale computers, such as Theta and Summit, have transformed our field, enabling lattice calculations with unprecedented precision in nuclear physics. Forntier will open the new horizons of the Exascale era and will allow us to answer questions that are for the first time accessible. Without the Exascale capability and capacity of leadership class facilities, computing the detailed three-dimensional images of the internal structure of hadrons or extracting precise determinations of the bound state properties of QCD would be impossible. Members of our team play leading roles in the Exascale project of USQCD and have developed algorithms and community codes that have made these advances possible. This projects seeks to build on the achievements achievements of the Exascale project and utilize the algorithmic and code advances to achieve unprecedented understanding of the properties of hadrons.

1.1 Generalized parton distributions

Efforts to unravel the structure of hadrons chart the story of QCD itself: from the first indications of the existence of partons in Hofstadter's elastic scattering experiments [2], through the development of the eightfold way [3], to the precision measurements of collinear structure in the LHC era [4]. Hadrons are strongly-coupled, many-body dynamical systems, with a correspondingly rich suite of theoretical quantities that capture different aspects of their structure. Our knowledge of these quantities has been both driven by and limited by the experimental data available. Until recently, generating systematic, rigorous theoretical predictions of many aspects of hadron structure directly from QCD has not been possible. New developments in lattice QCD, in which QCD is formulated on a discrete hypercubic Euclidean spacetime, now make calculations of the three-dimensional structure of hadrons feasible.

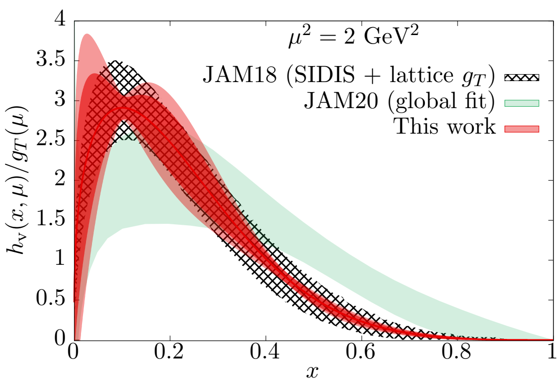
This structure is encapsulated in Generalized Parton Distributions (GPDs) [5, 6], which capture the correlations between longitudinal momentum and transverse impact-parameter space, and Transverse-Momentum-Dependent Distributions (TMDs), which correlate the longitudinal and transverse momenta of the proton's constituents. Parton Distribution Functions (PDFs) provide a collinear, one-dimensional description of the proton, and can be obtained from GPDs in the forward limit. GPDs and TMDs map out our conceptual picture of the proton, but the limited availability of experimental data clouds our ability to image the proton in its entirety.

In quantum field theory, GPDs and PDFs are defined in terms of quantum mechanical correlation functions of fields at light-like separations and cannot be accessed directly in Euclidean spacetime. This difficulty can be circumvented by direct calculation of correlation functions of space-like separated fields [7–10], which can be related to the corresponding GPDs by factorization [10–13]. Numerical calculations of PDFs show promise [10, 14–16] and the era of precision calculations of PDFs hovers on the horizon.

GPDs, however, lie at the frontier of what is possible with current computational techniques, and at the heart of the DOE's nuclear physics program. The measurement and extraction of GPDs are one of the prime objectives of the 12 GeV upgrade at Jefferson Lab. Using the CLAS12 detector of Hall B, a suite of experiments has been approved, and is underway, to extract GPDs from deeply virtual Compton scattering (DVCS), in which a highly virtual photon interacts with a single parton within a proton or neutron. GPDs are explored through the complementary processes of time-like Compton scattering in experiments E12-10-006A and E12-12-001 in Halls A and B respectively, of Deep Exclusive Meson Electro-Production in experiment E12-10-006C of Hall A, and in Deeply Virtual Meson Production (DVMP) in E12-06-108 of Hall B and through DVCS in E12-06-114 of Hall C. The experimental signatures of DVCS cannot be easily disentangled from the Bethe-Heitler process and the interference between these processes must be examined to extract GPDs from experimental data, whilst their extraction from DVMP relies on the applicability of factorization. Moreover, GPDs need to be experimentally measured for both up and down quarks, which requires measurement of DVCS not only from the proton, but also from the neutron. There are no free neutron targets available, so the signal for DVCS from the neutron must be extracted from experiments with nuclear targets, which introduces poorly-understood nuclear effects.

The connection between experimental data extracted in DVCS and DVMP and three-dimensional GPDs are Generalized Form Factors (GFFs), two-dimensional distributions that are convolutions of GPDs with complex kernels. These GFFs contain important insight, such as access to the gravitational form factors, but deconvoluting them to obtain the GPDs is a formidable inverse problem that experimental data alone cannot solve. In contrast, the lattice computations we propose will yield three-dimensional distributions in the kinematic variables (x, ξ, t) at specific values of x, the momentum transfer t and skewness ξ. Thus lattice computations are key to extracting the reliable three-dimensional pictures of hadrons that are encapsulated in GPDs. With the wealth of data emerging from the JLab 12 GeV program, and in anticipation of the physics program at the EIC, the development of a reliable analysis framework encompassing first principles lattice computation is urgent and timely, reflected in the establishment of the Center for Nuclear Femtography.

As a key step in this direction, we propose a series of calculations that will culminate in the first lattice QCD determination of isovector and isoscalar GPDs in the continuum limit, at physical pion masses, to unravel the three-dimensional structure of the nucleon and determine the flavor decomposition of the nucleon sea.



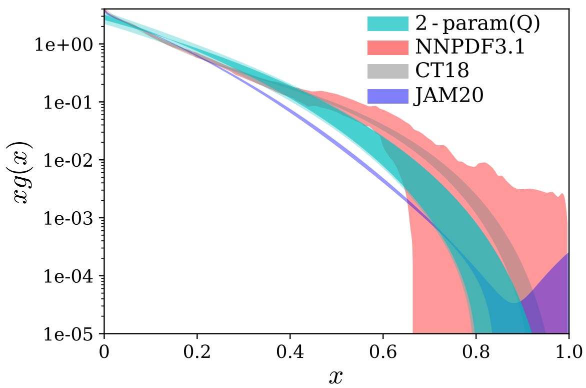


Figure 1. (Left panel) Our recent computation of the isovector transversity distribution of the nucleon [22] in comparison with phenomenological extractions. (Right panel) Our recent computation of the gluon unpolarized distribution in the nucleon [23]

1.2 Results from previous INCITE allocations

The 2018 INCITE allocation (PI Kostas Orginos, ID NP122) had several components related to PDFs of the pion and the nucleon. First, we explored the underlying framework adopted here, the pseudo-PDF approach, by calculating the isovector valence quark PDF of the pion [3, 4], a hadron that is computationally considerably less demanding than the proton. Our previous award enabled us to develop two distinct aspects of our analysis methods [2, 19]: renormalization and matching; and the inverse problem. We developed a procedure to renormalize the Wilson-line operators, and to obtain the continuum Ioffe time distributions. We also investigated effective methods to tackle the inverse problem that relates the Ioffe-time distributions, for which we have a limited, discrete set of data, to their Fourier transforms, the PDFs extracted from experimental data. So far we had several highly cited publications on lattice QCD computations of x-dependent parton densities [1–4, 19, 21–28, 30–37]. In these works, we developed new methods and new algorithms and pointed out the importance of our calculations to phenomenology collaborating with colleagues work on global fit analysis of experimental data. In Figure 1 we present our most recent results of the nucleon transversity and gluon PDFs at heavier than physical quark masses. This proposal will address the systematic error associated with the quark mass as calculations at physical quark masses will be performed.

The current proposal capitalizes on our essential methodological and algorithmic developments by extending the pseudo-PDF framework to the three-dimensional imaging of hadrons via GPDs, and by including flavor-singlet hadron structure through the computation of disconnected quark contributions. Furthermore, multi-hadron interpolating fields will be used for the first time in order to achieve firm control of excited state contamination which becomes more significant at high momentum and physical quark masses.

In addition to the work directly associated with this proposal, members of our team have contributed to significant advances using INCITE resources across a broad range of topics in lattice QCD, including precision calculations of the nucleon charges, and the gluonic structure of light nuclei.

2 RESEARCH OBJECTIVES AND MILESTONES

We have two milestones. First, to compute isovector quark GPDs at physical pion masses in the continuum limit. Second, to determine the flavor dependence of the proton sea through isoscalar GPDs. Leadership class computing is critical for our goals, which will provide the ab initio answers to a question "*essential* *for understanding the nature of visible matter*" [1] and central to the DOE's experimental nuclear physics program: how do quarks and gluons form the bound states of QCD that we observe in the world around us?

2.1 Formalism

2.1.1 Generalized parton distribution functions

Generalized parton distribution functions can be extracted from correlation functions of quantum fields at light-like or space-like separations. In the case of unpolarized quark GPDs of the nucleon, the basic building blocks are the matrix elements

$$\mathcal{M}^\alpha(z, p_1, p_2) \equiv \langle p_1|\bar{\psi}(0)\,\gamma^\alpha\, W(0, z; A)\psi(z)|p_2\rangle\,, \tag{1}$$

where $W(0, z; A_\mu)$ is the $0 \to z$ straight "Wilson line" gauge link (formed by the gauge field A_μ) in the quark (fundamental) representation. The external nucleon states $|p\rangle$ carry momentum p. In continuum QCD, GPDs are defined with quark and antiquark fields at light-like separations, $z^2 = 0$. On the lattice, GPDs can be extracted from space-like separated fields, and we choose the on-axis separation $z^\mu = (0, 0, 0, z^3)$, the Dirac structure $\alpha = 0$, and momenta p_1 and p_2 such that $P^\mu = (p_1^\mu + p_2^\mu)/2 = (P^0, 0, 0, P^3)$.

In the continuum limit, the resulting on-shell matrix element is Lorentz invariant and therefore a function of Lorentz-invariants: the Ioffe-time $\nu = P\cdot z$; the skewness, $\xi = (\nu_1 - \nu_2)/(\nu_1 + \nu_2)$, where $\nu_i = p_i \cdot z$; and the Mandelstam variable $t = (p_1 - p_2)^2$. GPDs can be directly extracted from the regularization-independent "reduced matrix element"

$$\mathfrak{M}(\nu, \xi, t, z^2) \equiv \frac{\mathcal{M}^0(p_1, p_2, z)}{\mathcal{M}^0(0, 0, z)}\,, \tag{2}$$

which is finite in the continuum limit [10, 13]. This reduced matrix element is an example of one class of factorizable matrix elements [38, 39], which are quantities that are computable directly in lattice QCD and factorizable into GPDs with calculable coefficients, in the same manner as experimentally-measurable hadronic cross sections.

The factorization formula

$$\mathfrak{M}(\nu, \xi, t, z^2) = \int_0^1 d\alpha\, C(\alpha, \xi, z^2\mu^2, \alpha_s(\mu))Q(\alpha\nu, \xi, t, \mu) + \sum_{k=1}^{\infty} \mathcal{B}_k(\nu, \xi, t)(z^2)^k\,, \tag{3}$$

relates the twist-2 Ioffe-time GPD, $Q(\nu, \xi, t, \mu)$, to the reduced matrix element in the continuum limit [10, 40, 41]. The Ioffe-time GPD is the Fourier transform in Ioffe time of the x-dependent GPD $H(x, \xi, t, \mu)$. The terms $O((z^2)^k)$ correspond to higher twist effects that can be eliminated in the limit of $z^2 \to 0$. The coefficient function $C(\alpha, \xi, z^2\mu^2, \alpha_s(\mu))$ can be computed in perturbation theory and is known to $O(a_s)$ [11–13].

Determining GPDs from the reduced matrix element proffers two significant computational advantages. First, the ultraviolet behavior of both the numerator and the denominator is identical, so that divergences cancel in the ratio in Eq. 2. This ratio can therefore be extrapolated to the continuum limit without additional renormalization, removing the need for additional high performance computing resources for obtaining renormalization constants. Second, there are statistical correlations between the numerator and denominator, which are both evaluated via Monte-Carlo sampling, that are largely removed in the ratio. This enables precise evaluations of the reduced matrix element, even though both the numerator and the denominator become exponentially small at large Ioffe times, ν. Thus, the ratio method simultaneously removes the need for the additional computational cost of renormalization constants and significantly improves the signal-to-noise ratio of the renormalized matrix elements.

Task	β	L/a_s	T/a_t	a_s (fm)	L (fm)
I1	6.3	64	128	0.093	5.95
I2	6.5	72	192	0.072	5.18
I3	6.7	96	256	0.055	5.28

Table 1. Parameters for the physical limit ensembles of configurations relevant to this proposal. The three lattices have an isotropic formulation of the gauge and fermion action. Column two gives the bare coupling β, columns three and four the spatial and temporal extents, in spatial and temporal lattice units, respectively. We give the approximate spatial lattice spacing, a_s and spatial lattice extent, L, in columns five and six, in physical units (1 fm = 10^{-15} m).

2.2 Milestone summary

Milestone 1: Generalized parton distributions We will calculate the x-dependent isovector Ioffe-time GPDs of the nucleon at the physical light-quark masses, and at three values of the lattice spacing using the ensembles I1 − I3 catalogued in Table 1. We have chosen the ensemble parameters such that they have a spatial extent $L \simeq 5$ GeV to provide small finite-volume effects [42], while working at sufficiently fine lattice spacings to control both higher twist contamination and momentum-dependent discretization effects, and to enable a controlled continuum extrapolation.

To achieve this, we will compute the perambulators, quark propagators projected onto a "distillation" basis, and generalized propagators (genprops), quark propagators projected on the distillation basis that contain an insertion of an appropriate operator at a particular time slice, for the proposed three ensembles I1, I2, and I3. These genprops and perambulators are the primary data products of our work, and can be re-used in multiple lattice calculations for a variety of physics applications. In our project, these building blocks are combined into the reduced Ioffe-time isovector GPDs at three lattice spacings from which we obtain the isovector GPDs in the continuum limit.

We will calculate the nucleon correlation functions with isospin $I = \frac{1}{2}$ quantum numbers. This will include roughly 10 local nucleon qqq quark operators as well as nonlocal nucleon-meson operators, if allowed by the quantum numbers at rest and at non-zero finite-volume momenta of the system. We have demonstrated that these non-local nucleon-pion operators are essential to obtain an accurate determination of the excited state spectrum within the nucleon channels. We obtain the finite-volume spectra for these channels and momenta by solving the Generalized Eigenvalue Problem (GEVP) [43] from the relevant correlation functions.

The determination of the spectrum in finite-volume, including these local nucleon and multi-body nucleon-meson operators, will allow for the accurate extraction of the lowest energy nucleon state at non-zero momentum with significantly reduced excited state contamination.

We already have existing ensembles I1 and I2, each of which contains at least Hybrid Monte Carlo (HMC) 10,000 trajectories. To perform the extrapolation of our results to the continuum limit, we require a third, finer ensemble, I3, and this comprises the remaining task. In particular, we will generate 10,000 HMC trajectories for the I3 ensemble. The I3 ensemble will be available for use by other groups within USQCD undertaking lattice calculations relevant to a wide range of nuclear physics applications, from nucleon form factors relevant to long-baseline neutrino experiments to the gluonic content of light nuclei, and will significantly reduce discretization effects in those calculations.

Milestone 2: Flavor decomposition of the proton sea We will calculate the x-dependent isoscalar, Ioffe-time GPDs on three ensembles I1, I2, and I3. To achieve this milestone we need to compute the so-called *disconnected* contributions to hadronic matrix elements, which involve traces of a matrix known implicitly in terms of the inverse of the Dirac matrix, and must be estimated stochastically. We detail the algorithmic improvements that enable our calculation of these disconnected contributions in the next Section. In addition to the disconnected contributions, we must also determine the perambulators, which are the building blocks for constructing the nucleon two point function and have already been computed in Milestone 1.

The building blocks we generate, together with those of Milestone 1 and the gluonic building blocks, generated at a negligible computational cost, will allow us to determine the isoscalar GPDs of the nucleon.

Both these milestones require the same building blocks, namely the same perambulators and generalized perambulators. The extraction of matrix elements in systems with non-local operator constructions as already been demonstrated at heavier quark masses, demonstrating that the technology for the generation of the correlation functions and the subsequent analysis is robust.

We first determine the two-point correlations of the $\pi\pi$ system, then construct linear combinations of operators that maximally couple to a generically-labeled n^{th} nucleon state with momentum $\mathbf{P}$, $\Omega_{N\pi,n}(\mathbf{P})$. We require three-point functions, coupling the initial and final $N\pi$ state via current insertion,

$$\langle 0|\Omega_{\pi\pi,n'}(\mathbf{P}_f, t_f)\mathcal{J}^{\mu}(t_c)\Omega_{\pi\pi,n}(\mathbf{P}_i, t_i)|0\rangle_L \propto \langle n', \mathbf{P}_f|\mathcal{J}^{\mu}(0)|n, \mathbf{P}_i\rangle_L + \cdots , \tag{4}$$

where the ellipses denote contributions that vanish when the optimal operators are exact. Note, in the proportionality we neglect terms that are determined from the two-point functions.

The technology for evaluating the contractions of the three-point functions has been already developed, including multi-body operator constructions [44, 45]. The generalized perambulators used in this proposal will be computed at distinct values of the insertion momentum $\mathbf{P_f} - \mathbf{P_i}$. These objects are reused for calculations of three-point functions in Eq. 4 at fixed momentum insertion but with initial and final state operator constructions, whether they are single-body are multi-body operator constructions.

Our milestones will provide key contributions to Nuclear Physics. We will compute the first continuum results for the three-dimensional structure of the nucleon, encoded in Ioffe-time isovector GPDs, and the first-ever lattice calculation of sea-quark isoscalar GPDs of the nucleon in the continuum limit. Moreover, the data generated as part of our proposal–perambulators, genprops and the gauge configuration I3–are important resources for a community-wide effort to understand the fundamental properties of the bound states of QCD.

3 COMPUTATIONAL READINESS

To guide and confront the JLab 12GeV experimental program requires a dedicated effort in lattice QCD computational techniques utilizing capability and capacity resources. Software and algorithm development for our program has been supported by DOE SciDAC projects and the Exascale Computing Project. These efforts tackle the main computational challenges in our workflow and progress towards accelerating these computations on Summit, Frontier, and Aurora, constitute the key performance indicator for the project's success. Our project is in an ideal position to efficiently utilize the capabilities of these new systems with development efforts carried out on Summit and early Exascale test systems.

The generation of gauge field ensembles requires leadership resources. Our project will exploit recent tremendous advances in algorithms and software for sparse linear system solvers using multigrid and improved Markov chain Monte Carlo methods. Compounding correlation functions of single and multi-hadron quark and glue constructions is a combinatoric challenge. Under the SciDAC and Exascale programs, we have developed new methods to tackle these computations. A technique called "distillation" allows us to compute, with high precision, the unprecedentedly large number of correlation functions required to determine hadronic amplitudes. The distillation method allows us to simplify and factorize the calculations further into computations of many propagators and generalized propagators, quantities that support the computation of matrix elements. These data products of our computations are highly reusable and feature in single and multi-hadron systems. Their computation requires the capacity resources that can only be provided in a timely fashion by Frontier and the new Exascale systems for which the codes and workflow have been highly optimized.

Here we discuss our computational approach, including our algorithms, workflow, and code, focusing on recent advances geared specifically toward Frontier that make our proposal possible. We then give a detailed account of our computational resource request, including timings and resource needs for our Milestones, based on the performance of our software on Summit and Frontier test systems.

3.1 Use of Resources Requested

We request time on OLCF Frontier for this single-year project. We have carried out extensive work on our codebase to optimize for the most recent NVIDIA and AMD GPU systems. We have tested our code on Crusher, an early-access testbed for Frontier. And we are in a good position to operate on the facility. And Frontier brings us the first opportunity to carry out simulations with ensembles as large as I2 and I3 affordably on a US facility.

In the following, we detailed the requested resources for gauge generation and the computations that support the calculation matrix elements (propagators, generalized propagators, and disconnected components).

Gauge generation We already have access to configurations for the ensembles I1 and I2. For that reason, in this campaign we propose to generate HMC trajectories for the I3 ensemble. We estimate our computational requirements by timing a single HMC trajectory for a lattice with volume $96^3 \times 192$, and scaling the timings for a fourth-order integrator, $r_V^{9/8} \approx 1.38$ where r_V is the quotient between the $96^3 \times 192$ volume and the I1 lattice volume, $96^3 \times 256$. A single HMC trajectory on an $96^3 \times 192$ lattice took 1871 seconds on 64 Crusher nodes, resulting in an estimation of 46 node-hours per trajectory for the I3 ensemble. Sixty four Crusher nodes are the minimum number of nodes to fit all the required memory on GPU devices. HMC computations have low computational intensity, and having good strong scalability is challenging, as we explain in a following section. However, we can run various HMC instances in parallel (usually referred to as *streams*), which is sufficient to increase the consumption rate without increasing the number of nodes running for each HMC instance.

We plan to compute 10,000 trajectories, which should be sufficient for having 500 decorrelated enough configurations. Each HMC instance will run on 64 nodes, and four HMC instances will run simultaneously. A new configuration will be written every a few trajectories and has all the information to reset the running from that point, making the computation very resilient. We ask 100 TB of archive storage for storing I3 ensembles configurations, each of them having a size of 135GB.

We currently have a few thermalized lattices from the I3 ensemble, so we do not budget for additional initial thermalization time. We summarize our production of the I3 ensemble in Tab. 2.

Propagators, generalized propagators, and disconnected diagrams Most of the time expended by computing propagators and disconnected diagrams is in the solution of the Dirac equation, as for HMC. For the generalized propagators, approximately half of the time is expended in the solution of the Dirac equation

Ensemble	Trajectory cost (n-h)	Number of traj.	Total (n-h)
I3	46	10K	440 K

Table 2. Resources for gauge generation in Frontier node-hours. Only new I3 ensembles required. For further details see the accompanying text.

and the other half in contracting lattice fields. We took the times for the solution of the Dirac equation from the HMC runnings on Crusher (and scale up with the volume for estimating I3). The contracting fields time are estimated from an I1 run on Perlmutter, and scale up with the lattice volume for I2 and I3. We expect that contracting fields will have a similar performance on Crusher than on Perlmutter. Nevertheless the total cost in contracting fields will amount around 10% of the total allocation.

From the HMC runs on Crusher we took that solution of the Dirac equation C_{inv} is 19.2, 140, and 187 node-seconds for the ensembles I1, I2, and I3, respectively. From the running of a generalized propagator for I1, we got a cost of $C_{\mathrm{mat}} = 30$ node-seconds on Perlmutter for doing all lattice fields contractions for $N_v = 128$ distillation vectors for a single momentum and displacement. The values for C_{mat} for the lattices I2 and I3 in Table 3 are scaled with the lattice volume.

Our program Chroma carries away the computation of propagators, generalized propagators, and disconnected diagrams. All three computations have no dependency, and each configuration from each ensemble can be executed independently. Therefore we have thousands of independent tasks to run, each running on 64, 144, and 432 Frontier nodes for I1, I2, and I3 configurations, respectively, and each less than 8 hours. We will submit jobs bundling many independent tasks of the same type that will run simultaneously to fill around 1000 nodes. We expect a constant burn rate throughout the year. We have scripts that automatize the creation of the tasks, bundle jobs, track the state, and mark the failed tasks to be resubmitted.

The three ensembles have the same physical volume, so we will use the same number of distillation vectors N_v for computing the propagators and the generalized propagators. We will use 128 distillation vectors, which have given us good results in previous analyses for this physical volume. We will compute time-slice propagators that will be used to compute correlation functions over a 16 time-slice window for single particle nucleon operators as well as multi-particle nucleon-meson operators. Multi-particle nucleon-meson operators will allow us for the first time to study the effect of multi-particle states in the extraction of single nucleon matrix elements. At physical quark masses, as well as at high momentum, excited state contamination effects become more important and careful treatment is needed in order to achieve the required control of this systematic.

For each one of these ensembles, we compute a single generalized propagator for all the active time-slices between the source and the sink, using source-sink separations that range from roughly 0.5 fm to 1.2 fm. We use $N_z = 17$ different displacements in the z direction and $N_{mom} = 20$ momentum transfer combinations to evaluate the GPDs at many different kinematic points of skewness and total momentum transfer.

We will compute disconnected diagrams that allow us to access flavor singlet distributions. This computation requires a trace estimation for which we will use the "probing" technique coupled with multi-grid deflation [25, 31]. As shown in our recent paper [25], 250 probing vectors, together with spin-color dilution, are effective in computing disconnected diagrams of displaced and non-displaced quark bi-linears with good accuracy. Therefore, the runs solve $N_{\mathrm{inv,d}} = 250 \cdot 12 = 3000$ Dirac equations per configuration. The time for computing the deflation space is negligible compared to the inversion cost.

In summary, we request 810 K node-hours on Frontier for doing propagators, generalized propagators, and disconnected diagrams. Table 3 details the costs.

Factor	Value	Description
C_{inv}		Single inversion cost
C_{mat}		Tensor contraction cost per momentum and displacement
N_{cfg}		Number of configurations
N_v	128	Rank of the distillation basis
s	4	Number of spins
$N_{\text{s,prop}}$	$16 \cdot s$	Number inversions per distillation vector for propagators
$N_{\text{s,gprop}}$	$7 \cdot s$	Number inversions per distillation vector for gen. propagators
N_{mom}	20	Number of momenta
N_z	17	Number of Wilson-line lengths
$N_{\text{inv},d}$	3000	Number of probing vectors (incl. spin-color dilution)

$$C_{\text{prop}} = C_{\text{inv}} \cdot N_v \cdot N_{\text{s,prop}} \cdot N_{\text{cfg}}$$
$$C_{\text{gprop}} = (C_{\text{inv}} \cdot N_v \cdot N_{\text{s,gprop}} + C_{\text{mat}} \cdot N_z \cdot N_{\text{mom}}) \cdot N_{\text{cfg}}$$
$$C_{\text{disco}} = C_{\text{inv}} \cdot N_{\text{inv,d}} \cdot N_{\text{cfg}}$$

Ensemble	N_{cfg}	C_{inv} (n-s)	C_{mat} (n-s)	C_{prop} (n-h)	C_{gprop} (n-h)	C_{disco} (n-h)
I1	500	19.2	30	22 K	–	–
I2	500	140	64	159 K	98 K	58 K
I3	500	187	203	213 K	182 K	78 K
			Subtotal:	394 K	280 K	136 K
			Total:	810 K		

Table 3. Resources in Frontier node-hours for computing the propagators C_{prop}, the generalized propagators C_{gprop}, and the disconnected components C_{disco} for ensembles I1, I2, and I3. For more details see the accompanying text.

The scratch space is estimated to hold around 100 configurations and all the data generated (propagators, generalized propagators, and disconnected diagram). We will bring a batch of configurations for ensembles I1 and I2 from JLab (I3 configurations will be on the facility). After the computations are done for all configurations in the batch, the propagators, disconnected diagrams, and the computed correlation functions generated are transferred back to JLab. The scratch space is cleaned to hold another batch of configurations. The size of each configuration is 20GB, 43GB, and 135GB for I1, I2, and I3, respectively. And the amount transferred back is up to 40 GB per configuration.

3.2 Computational approach

Gauge field ensemble generation: The state-of-the-art algorithm for gauge field generation is Hybrid Monte Carlo (HMC) [46, 47], a hybrid molecular-dynamics Markov chain Monte Carlo algorithm. The majority ($\sim$ 95%) of the cost lies in computing the molecular dynamics forces, and likewise, the majority of those computations (roughly 60%-80% of the total run-time) are in the solution of the Dirac equation, called at each step of the algorithm.

Our code, Chroma [48], utilizes sophisticated multiple time-scale, higher-order MD time-steppers [49–53], advanced linear solvers such as adaptive aggregation multi-grid (AAMG) [54–57] provided by interfacing to NVIDIA's QUDA library, and sophisticated determinant break-up schemes to construct the pseudo-fermion action [47, 58, 59]. Gauge generation is a strong scaling challenge because a single Markov chain is sequential, and one can exploit only the data parallelism of the lattice. In the strong scaling limit, one faces the twin challenges of a small amount of work-per-compute-element and the constraining effect of latency and bandwidth of the communication fabrics between the computing elements.

One can overcome some of these challenges by running several Markov chains (streams) simultaneously, but care must be taken to ensure that the streams have become fully independent before computing correlation functions to avoid unwanted correlation effects in the final analyses.

The AAMG solver can provide nearly an order-of-magnitude speed-up compared to the standard BiCGStab [60] for the linear solves needed for computing the MD forces. We have also implemented several other optimizations, such as a force-gradient time-stepper [52, 53] in the MD.

Correlation functions through distillation. Within the last few years, our group has pioneered the use of a new technique for the construction of correlation functions called *distillation*, Ref. [61]. This technique has enabled the major progress made in our spectroscopy studies and is at the heart of our hadron structure project. The method allows us to unify our our research efforts within one set of algorithm and code infrastructure that supports constructing reusable data components, suitable for computing correlation functions of two-point and three-point functions, in single hadron as well as multi-particle and nuclear systems.

Distillation is a quark-smearing method designed to increase overlap onto low modes relevant for low-lying hadronic states. We define a smearing operator on a time-slice, using the lowest N eigenvectors of the three-dimensional gauge-covariant Laplacian, $\{\xi_n\}$, with $n = 1 \dots N$. The quark fields that appear in two-point correlation functions are smeared by application of this operator, thus the combination of eigenvectors and the Dirac matrix inverse, M^{-1}, called a 'perambulator', $\xi_n^\dagger(t')M^{-1}(t',t)\xi_m(t) \equiv \tau_{nm}(t',t)$ will appear in any propagation. Thus, the basic numerical problem to be solved is inversion of the Dirac matrix on sources, $\{\xi_n\}_{n=1\dots N}$, which is a vastly smaller vector space than that of the full lattice.

Topologies can appear in correlation functions which require light-quark and strange quark perambulators between fixed $t_{\rm src}$ and varying t, requiring inversion of the Dirac matrix from a source on $t_{\rm src}$. However, depending on isospin, there can be topologies involving propagation from $t_{\rm t}$ to $t_{\rm t}$ which require inversions from sources at every t. Such $\tau(t,t)$ perambulators are referred to as "annihilation" lines since they feature in the annihilation of quarks between operators on a single time-slice. Obtaining these quantities is a major goal of this project. They form the data products that can be used in subsequent analyses.

The factorization of the quark lines allows for the computation of generalized propagators ("genprops"), for current insertions, formed from the inner product of two sets of solution vectors taking the form

$$J(t_f, t, t_i; \vec{p}) = \xi_n^\dagger(t_f)M^{-1}(t_f, t)\mathbf{\Gamma}_A(\vec{p}, t)M^{-1}(t, t_i)\xi_m(t_i), \tag{5}$$

with $\mathbf{\Gamma}$ some operator acting in coordinate, color and spin space, and projected onto a definite three-dimensional momentum, $\vec{p}$ and time-slice, t. There will be several different types of these genprops indicated by the subscript, A. Thanks to the nice factorization properties of distillation, these nodes can be reused in the calculation of ground state or transition amplitudes, including those featuring many particle scattering states. The computation of these genprops is a major goal of the project.

For the genprop computations, the calculation of the sink, $\xi_n^\dagger(t_f)M^{-1}(t_f, t)$ and source, $M^{-1}(t, t_i)\xi_m(t_i)$, tensors involves M^{-1} that uses a four-dimensional space-time layout and runs in capacity mode utilizing all compute nodes within the job. The correlation length t varies only over a sub-domain of the full time-extent of the lattice, so we are interested in computing the contraction of the sink and the source on this sub-domain only. However, because of how the data is arranged, only a small portion of the computing nodes will participate in the computation, dramatically impacting the overall performance. The new code reduces by an

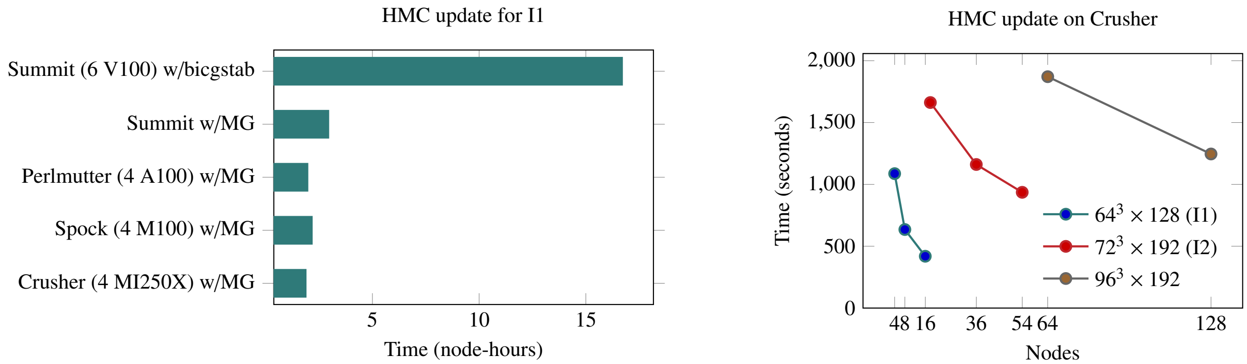


Figure 2. On the left, times in node-hours for I1 lattice, with $64^3 \times 128$ sites, comparing performance for a single HMC trajectory on different facilities and remarking the improvement with multi-grid over bicgstab as the the Dirac equation iterative solver. On the right, strong scaling of HMC for three different lattices.

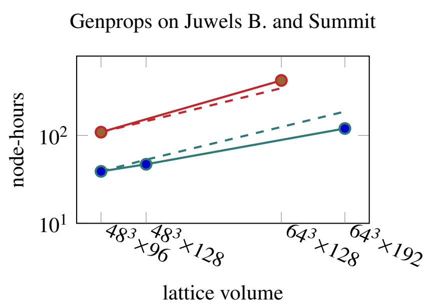


Figure 3. Weak scaling comparison (including IO) on the lattice volume for generating generalized propagators for a single gauge configuration on Juwels Booster in blue (4 A100 GPUs on a node) and Summit in red. The ideal times (dashed lines) assume perfect linear scaling with respect to the lattice volume based on the timings for the lattice $48^3 \times 96$.

order of magnitude the time expended in contractions by redistributing the data to balance the computation among the nodes and rearranging the contractions as dense matrix-matrix multiplications, which are done with batched GEMM kernels available on cuBLAS/hipBLAS.

Disconnected diagrams. We compute the quark-disconnected diagrams using a stochastic estimator of a trace of a matrix given implicitly in terms of the inverse of the Dirac matrix. We have recently developed [62] methodologies that rely on AAMG deflation as well state-of-the-art probing methods [25, 63] to reduce by orders-of-magnitude the variance of the stochastic estimator. We implement these methods on GPU-based machines using QUDA and PRIMME.

Programming languages, libraries and other software: Chroma, QDP-JIT, QIO, and QUDA are written primarily in C++, CUDA/HIP, and C. For node-parallelism, we use OpenMP threading on the CPU side and CUDA/HIP on the GPU side. Some GPU kernels are generated with LLVM. They utilize *standard* libraries such as `cuBLAS/hipBLAS`, `cuFFT/hipFFT`, `CUB/hipCUB`, and `cuRand/hipRand`. For inter-node parallelism, we use MPI.

3.3 Parallel Performance

Most of the requested allocation is dedicated to gauge field generation and calculation of propagators, generalized propagators, and disconnected diagrams. Because the total number of independent tasks ascends to thousands, we rely on executing many tasks simultaneously (batching several in a single script job if necessary or using SLURM job array support) to take full advantage of the resource. Therefore, strong scalability is not a relevant performance metric for our computation.

As mentioned above, the dominant operation in HMC for generating gauge fields is the solution of the Dirac equation with the AAMG inverter. Figure 2 (left) shows the performance of an HMC trajectory for the I1 lattice across three relevant facilities. It supports the claim that the speedups achieved using multigrid over a simpler iterative solver such as Bicgstab and the accumulative effect of the recent optimizations to take advantage of the recent hardware capabilities. In Fig. 2 (right), we show the strong scaling over an HMC trajectory to prove the performance of AAMG inverter. The performance degrades eventually, but it is sufficient for our runs. A gauge field is written every few trajectories and takes a negligible amount of time.

The profiling time for generating propagators and disconnected diagrams is similar to gauge-field generation: the AAMG inverter is the dominant time, other times are negligible, and the jobs run on a small number of nodes sufficient to hold the Dirac operator on the GPUs' memory. On the other hand, the computation of generalized propagators is more challenging, as described above. Roughly half of the time is spent in the solution of the Dirac equation and the other half in the contraction of the sink and source fields resulting from the solution of the Dirac equation contracted with several other operators. These dense tensor contractions are carried out efficiently by batched GEMM kernels and involve a small amount of communications that have almost no impact on performance. Benchmarks on Summit and Juwels Booster show almost perfect weak scalability for the lattice volume, see Fig. 3.

3.4 Developmental Work

Members of our team are active participants in the lattice QCD Application Development component of the DOE Exascale Computing Project (ECP). One of the ECP's milestones for this year is devoted to exploiting new opportunities for parallelism in the simultaneous solution of multiple linear systems with the same operator, which may improve the performance of computing propagators, generalized propagators, and disconnected diagrams.

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PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

PERSONNEL JUSTIFICATION

- Kostas Orginos (William & Mary, PI) 20 years. Expert on partonic structure and lattice QCD algorithms for fermion traces.
- Robert Edwards (JLab) 25 years. Lead author of the Chroma software suite used in this proposal. PI on SciDAC-4 project "Computing the properties of matter", co-PI on Exascale Computing Project in lattice QCD.
- Colin Egerer (JLab) 4 years. Expert in hadron structure calculations with specialization to GPDs and PDFs.
- Christopher Monahan (William & Mary) 10 years. Expert in formal aspects of hadron structure calculations and analysis of lattice QCD calculations relevant to the LHC.
- Bálint Joó (ORNL) 20 years. Developer of chroma software suite and underlying libraries. Developer of QPhiX library and expert in integration of QUDA into the USQCD software stack. Co-PI On SciDAC-4 project "Computing the properties of matter".
- Joseph Karpie (Columbia) 3 years. Expert in hadron structure calculations.
- Jianwei Qiu (JLab) 30 years. Expert in formal aspects of hadron structure calculations.
- Anatoly Radyushkin (Old Dominion University) 30 years. Expert in formal aspects of hadron structure calculations.
- David Richards (JLab) 25 years. Expert in hadron structure calculations.
- Eloy Romero (JLab) 7 years. Developer of GPU-optimized codes for hadron structure.
- Raza Sufian (William & Mary) 6 years. Expert in hadron structure calculations and light-front QCD.
- Frank Winter (JLab) 10 years. Developer of QDP-JIT just-in-time compilation version of the QDP++ data parallel software library.
- Savvas Zafeiropoulos (CNRS/Marseille, FR) 9 years. Expert in hadron structure calculations and sign problems in QFT.

MANAGEMENT PLAN

4.1 Personnel management

As members of the JLab HadStruc and HadSpec collaborations, the PI and co-PIs meet weekly (with occasional exceptions) to discuss the planning, status and execution of the project. In particular, we work to ensure that computer resources are distributed according to plan, and this INCITE project will be central to these discussions. Once a sufficient set of correlator data is available, we will divide into working groups, devoted to the analysis of specific sets of data.

- K. Orginos [*kostas@wm.edu*] will coordinate the project and provide the point of contact for updates.
- R. Edwards will coordinate code optimization and development, leading our development team: B. Joó, K. Orginos, E. Romero, and F. Winter.
- C. Monahan will coordinate work on the theoretical aspects of our GPD calculations, with J. Karpie, K. Orginos, J. Qiu, A. Radyushkin, R. Sufian, and S. Zafeiropoulos.
- D. Richards will coordinate the analysis of our correlator data by C. Egerer, J. Karpie, C. Monahan, R. Sufian, and S. Zafeiropoulos.

4.2 Data management

The primary data products of our work are the perambulators, genprops, and gauge field configurations. We estimate that we need about 101 TB of scratch storage at OLCF to stage gauge configuration generation as well as quark loop, perambulator and genprop generation. We will retain these data sets at off-site storage, beyond the end of this project, and we will generate a Document Object Indicator (DOI) for each of the saved datasets, which we will publish on OSTI. We will need 100 Tb of long-term storage to keep important data such as gauge field configurations for the duration of the project. Scientific results will be published in refereed journal publications, conference presentations, seminars and colloquia. In addition, we will inform DOE sponsors in ASCR and the Office of Nuclear Physics, as well as the public of major achievements via Scientific Highlights generated as usual through the Public Affairs offices of Jefferson Lab and OLCF.

MILESTONE TABLES

Proposal Title: Hadron physics from first principles

Year 1		**Total number of node-hours for Year 1:** 1,250 K
Milestone:	**Details (as appropriate):**	**Dates:**
M1: Generalized Parton Distribution	**Resource:** OLCF Frontier **Node-hours:** 1,114 K **Filesystem storage (TB and dates):** 100 TB, entire year **Archival storage (TB and dates):** 50 TB **Software Application:** Chroma **Tasks:** Gauge generation for I3 and compute propagators and genprops for I1, I2 and I3 **Dependencies:** None	01/01/23 - 12/31/23
M2: Flavor decomposition	**Resource:** OLCF Frontier **Node-hours:** 136 K **Filesystem storage (TB and dates):** 1 TB, entire year **Archival storage (TB and dates):** None **Software Application:** Chroma **Tasks:** Disconnected diagrams for I2 and I3 **Dependencies:** I3 gauge generation from GDP	01/01/23 - 12/31/23

PUBLICATIONS RESULTING FROM PRIOR INCITE AWARDS

C. Egerer *et al.* [HadStruc], Phys. Rev. D **105**, no.3, 034507 (2022) doi:10.1103/PhysRevD.105.034507 [arXiv:2111.01808 [hep-lat]].

C. Egerer, R. G. Edwards, K. Orginos and D. G. Richards, Phys. Rev. D **103**, no.3, 034502 (2021) doi:10.1103/PhysRevD.103.034502 [arXiv:2009.10691 [hep-lat]].

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A. J. Woss *et al.* [Hadron Spectrum], Phys. Rev. D **103**, no.5, 054502 (2021) doi:10.1103/PhysRevD.103.054502 [arXiv:2009.10034 [hep-lat]].

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B. Joó, J. Karpie, K. Orginos, A. V. Radyushkin, D. G. Richards and S. Zafeiropoulos, Phys. Rev. Lett. **125**, no.23, 232003 (2020) doi:10.1103/PhysRevLett.125.232003 [arXiv:2004.01687 [hep-lat]].

R. S. Sufian, C. Egerer, J. Karpie, R. G. Edwards, B. Joó, Y. Q. Ma, K. Orginos, J. W. Qiu and D. G. Richards, Phys. Rev. D **102**, no.5, 054508 (2020) doi:10.1103/PhysRevD.102.054508 [arXiv:2001.04960 [hep-lat]].

E. Romero, A. Stathopoulos and K. Orginos, J. Comput. Phys. **409**, 109356 (2020) doi:10.1016/j.jcp.2020.109356 [arXiv:1909.12234 [math.NA]].

B. Joó, J. Karpie, K. Orginos, A. V. Radyushkin, D. G. Richards, R. S. Sufian and S. Zafeiropoulos, Phys. Rev. D **100**, no.11, 114512 (2019) doi:10.1103/PhysRevD.100.114512 [arXiv:1909.08517 [hep-lat]].

B. Joó, J. Karpie, K. Orginos, A. Radyushkin, D. Richards and S. Zafeiropoulos, JHEP **12**, 081 (2019) doi:10.1007/JHEP12(2019)081 [arXiv:1908.09771 [hep-lat]].

A. J. Woss, C. E. Thomas, J. J. Dudek, R. G. Edwards and D. J. Wilson, Phys. Rev. D **100**, no.5, 054506 (2019) doi:10.1103/PhysRevD.100.054506 [arXiv:1904.04136 [hep-lat]].

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A. Woss, C. E. Thomas, J. J. Dudek, R. G. Edwards and D. J. Wilson, JHEP **07**, 043 (2018) doi:10.1007/JHEP07(2018)043 [arXiv:1802.05580 [hep-lat]].

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Z. S. Brown, W. Detmold, S. Meinel and K. Orginos, Phys. Rev. D **90**, no.9, 094507 (2014) doi:10.1103/PhysRevD.90.094507 [arXiv:1409.0497 [hep-lat]].

J. J. Dudek *et al.* [Hadron Spectrum], Phys. Rev. Lett. **113**, no.18, 182001 (2014) doi:10.1103/PhysRevLett.113.182001 [arXiv:1406.4158 [hep-ph]].

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M. Padmanath, R. G. Edwards, N. Mathur and M. Peardon, Phys. Rev. D **90**, no.7, 074504 (2014) doi:10.1103/PhysRevD.90.074504 [arXiv:1307.7022 [hep-lat]].

R. G. Edwards *et al.* [Hadron Spectrum], Phys. Rev. D **87**, no.5, 054506 (2013) doi:10.1103/PhysRevD.87.054506 [arXiv:1212.5236 [hep-ph]].

J. J. Dudek *et al.* [Hadron Spectrum], Phys. Rev. D **87**, no.3, 034505 (2013) [erratum: Phys. Rev. D **90**, no.9, 099902 (2014)] doi:10.1103/PhysRevD.87.034505 [arXiv:1212.0830 [hep-ph]].

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L. Liu *et al.* [Hadron Spectrum], JHEP **07**, 126 (2012) doi:10.1007/JHEP07(2012)126 [arXiv:1204.5425] [hep-ph]].

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J. J. Dudek and R. G. Edwards, Phys. Rev. D **85**, 054016 (2012) doi:10.1103/PhysRevD.85.054016 [arXiv:1201.2349 [hep-ph]].

C. E. Thomas, R. G. Edwards and J. J. Dudek, Phys. Rev. D **85**, 014507 (2012) doi:10.1103/PhysRevD.85.014507 [arXiv:1107.1930 [hep-lat]].

R. G. Edwards, J. J. Dudek, D. G. Richards and S. J. Wallace, Phys. Rev. D **84**, 074508 (2011) doi:10.1103/PhysRevD.84.074508 [arXiv:1104.5152 [hep-ph]].

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J. J. Dudek, R. G. Edwards, M. J. Peardon, D. G. Richards and C. E. Thomas, Phys. Rev. Lett. **103**, 262001 (2009) doi:10.1103/PhysRevLett.103.262001 [arXiv:0909.0200 [hep-ph]].

M. Peardon *et al.* [Hadron Spectrum], Phys. Rev. D **80**, 054506 (2009) doi:10.1103/PhysRevD.80.054506 [arXiv:0905.2160 [hep-lat]].

BIOGRAPHICAL SKETCHES

Curriculum Vitae
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Professional Preparation

Ph.D. (Theoretical Physics), Brown University, 1997
B.Sc. (Physics) University of Patras, Greece, 1991

Appointments

2017–present, Professor, William & Mary
2011–2017, Associate Professor, William & Mary
2005–2011, Assistant Professor, William & Mary
2003–2005, Research Scientist, MIT
2000–2003, Postdoctoral Associate, RIKEN/BNL Research Center
1997–2000, Postdoctoral Associate, University of Arizona

Five Publications Most Relevant to This Proposal

1. B. Joó, J. Karpie, K. Orginos, A. V. Radyushkin, D. G. Richards and S. Zafeiropoulos, *"Parton Distribution Functions from Ioffe Time Pseudodistributions from Lattice Calculations: Approaching the Physical Point,"* Phys. Rev. Lett. **125**, no.23, 232003 (2020) doi:10.1103/PhysRevLett.125.232003.
2. B. Joó, J. Karpie, K. Orginos, A. V. Radyushkin, D. G. Richards, R. S. Sufian and S. Zafeiropoulos, *Pion valence structure from Ioffe-time parton pseudodistribution functions,* Phys. Rev. D **100** (2019) no.11, 114512.
3. K. Orginos, A. Radyushkin, J. Karpie and S. Zafeiropoulos, *Lattice QCD exploration of pseudo-PDFs*, Phys. Rev. D 96 (2017) 094503.
4. C. C. Chang *et al.*, *A per-cent-level determination of the nucleon axial coupling from quantum chromodynamics*, Nature 558 (2018) 91.
5. R. G. Edwards, G. T. Fleming, Ph. Hagler, J. W. Negele, K. Orginos, B. Musch, A. Pochinsky, D. B. Renner, D. G. Richards, W. Schroers, *Nucleon Generalized Parton Distributions from Full Lattice QCD*, Phys. Rev. D 77 (2008) 094502.

Research Interests and Expertise

Nonperturbative properties of hadrons and nuclei from Lattice QCD. Large-scale computations and algorithm development.

Synergistic Activities

1. USQCD Executive Committee, 2014–present
2. USQCD Scientific Program Committee, 2014–2016
3. Advisory committee of the RIKEN/BNL Research Center, 2014–present

4. 2010 Nuclear Physics decadal review committee of the National Academies
5. Chairman of the local organizing committee of the International conference LATTICE 2008, Williamsburg, VA, 2008
6. Co-organizer of the summer school on “Lattice QCD and its applications", INT, 2007
7. Co-organizer of the 3rd Topical Workshop on Lattice Hadron Physics (LHP06), Jlab, 2006
8. International Advisory Committee for LATTICE 2020,2019, 2018, 2013, 2012, 2011 and 2007

Collaborators

Silas Beane, University of Washington
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Professional Preparation

Ph.D. (Physics), New York University, 1989
M.S. (Physics), New York University, 1986
B.S. (Mathematics), University of Texas at Austin, 1984
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Appointments

2017–present, Deputy Associate Director for Theoretical and Computation Physics
1999–2016, Senior Staff Scientist, Jefferson Lab, USA
1997–1999, Associate Research Scientist, S.C.R.I., Florida State University,
1992–1997, Associate Research Scientist, S.C.R.I., Florida State University

Five Publications Most Relevant to This Proposal

1. R.A. Briceño, J. J. Dudek, R. G. Edwards, C.J. Shultz, C. E. Thomas, D. J. Wilson, *The resonant $\pi^+\gamma \to \pi^+\pi^0$ amplitude from Quantum Chromodynamics*, Phys. Rev. Lett. 115 (2015) 242001.
2. M.J. Peardon, J. Bulava, J. Foley, C. Morningstar, J.J. Dudek, R.G. Edwards, B. Joo, H.-W. Lin, D.G. Richards, K.J. Juge, *A Novel Quark Field Creation Operator Construction for Hadronic Physics in Lattice QCD*, Phys. Rev. D80 (2009) 054506.
3. H.-W. Lin, S.D. Cohen, J. Dudek, R.G. Edwards, B. Joo, D.G. Richards, J. Bulava, J. Foley, C. Morningstar, E. Engelson, S. Wallace, K.J. Juge, N. Mathur, M.J. Peardon, S.M. Ryan, *First results from 2+1 dynamical quark flavors on an anisotropic lattice: Light-hadron spectroscopy and setting the strange-quark mass*, Phys. Rev. D79 (2009) 034502.
4. P. Hagler, W. Schroers, J. Bratt, J.W. Negele, A.V. Pochinsky, R.G. Edwards, D.G. Richards, M. Engelhardt, G.T. Fleming, K. Orginos, D.B. Renner, *Nucleon Generalized Parton Distributions from Full Lattice QCD*, Phys. Rev. D77 (2008) 094502.
5. R.G. Edwards, B. Joó, *The Chroma Software System for Lattice QCD*s, Nucl. Phys. Proc. Suppl. 140 (2005) 832.

Research Interests and Expertise

Nuclear and high energy physics, hadron spectroscopy, software and hardware architecture.

Synergistic Activities

1. Deputy Spokesperson and Executive Committee Deputy Chair, USQCD Collaboration
2. Panel, DOE/ASCR/NP Computational Requirements for NERSC, NSF/OCI Tier 1 and Tier 2 computational facilities
3. Fellow of the American Physical Society, 2011

Collaborators

R.A. Briceño, ODU/JLab
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Professional Preparation

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B.S. (Physics & Mathematics), University of Wisconsin - La Crosse, 2015

Appointments

September 2021 - present: Post-doctoral Fellow, Jefferson Lab

Five Publications Most Relevant to This Proposal

1. C. Egerer, R. Edwards, C. Kallidonis, K. Orginos, A. Radyushkin, D. G. Richards, E. Romero, S. Zafeiropoulos, *Towards high-precision parton distributions from lattice QCD via distillation*, JHEP 11 (2021) 148.
2. C. Egerer, R. Edwards, K. Orginos, D. Richards, *Distillation at High-Momentum*, Phys. Rev. D 103 (2021) 3, 034502.
3. R. S. Sufian, C. Egerer, J. Karpie, R. Edwards, B. Joó, Y. Q. Ma, K. Orginos, J. W. Qiu and D. G. Richards, *Pion Valence Quark Distribution from Current-Current Correlation in Lattice QCD*, Phys. Rev. D 102 (2020) 5, 054508.
4. R. S. Sufian, J. Karpie, C. Egerer, K. Orginos, J. W. Qiu and D. G. Richards, *Pion Valence Quark Distribution from Matrix Element Calculated in Lattice QCD*, Phys. Rev. D 99 (2019) 7, 074507.
5. C. Egerer, D. G. Richards, F. Winter, *Controlling excited-state contributions with distillation in lattice QCD calculations of nucleon isovector charges* g_S^{u-d}, g_A^{u-d}, g_T^{u-d}, Phys. Rev. D 99 (2019) 3, 034506.

Research Interests and Expertise

First-principles determinations of parton distribution functions and generalized parton distributions, especially software development in support of these scientific goals. Regularization of ill-posed inverse problems through parametric or non-parametric means.

Collaborators

Kostas Orginos, William & Mary and Jefferson Lab
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Oak Ridge Leadership Computing Facility
Oak Ridge National Laboratory
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Professional Preparation
Ph.D. (Physics), University of Edinburgh, UK, 2000
B.Sc.(Hons.) (Computer Science and Physics), University of Edinburgh, UK, 1996

Appointments
Group Leader (Advanced Computing for Nuclear, Astro and Particle Physics), Oak Ridge National Laboratory, Oct, 2020 - present
Sr. Staff Computational Scientist, Oak Ridge National Laboratory, July 2020 - Sep 2020
2005–2020, Staff Computer Scientist, Jefferson Lab
2002–2005, Postdoctoral Research Associate, University of Edinburgh,
2000-2002, Postdoctoral Research Associate, University of Edinburgh (at Columbia University),
2000, Postdoctoral Research Associate, University of Kentucky

Five Publications Most Relevant to This Proposal

1. R.G. Edwards, B. Joó, *The Chroma Software System for Lattice QCD*, Nucl. Phys. Proc. Suppl. 140 (2005) 832.
2. B. Joó, T. Kurth, M. A. Clark, J. Kim, C. R. Trott, D. Ibanez, D. Sunderland, J. Deslippe, *Performance portability of a Wilson Dslash Stencil Operator Mini-App using Kokkos and SYCL*, 2019 International Workshop on Performance, Portability and Productivity in HPC (P3HPC 2019), at SC'19: The International Conference for High Performance Computing, Networking, Storage, and Analysis, Denver, CO, Nov. 22, 2019
3. M. A. Clark, B. Joó, A. Strelchenko, M. Cheng, A. Gambhir, R Brower, *Accelerating Lattice QCD Multigrid on GPUs Using Fine-Grained Parallelization*, proceedings of SC16, The International Conference for High Performance Computing, Networking, Storage and Analysis (2016)
4. F. T. Winter, M. A. Clark, R. G. Edwards, B. Joó, *A Framework for Lattice QCD Calculations on GPUs*, proceedings of 2014 IEEE 28th International Parallel and Distributed Processing Symposium (2014)
5. R. Babich, M. A. Clark, B. Joó, G. Shi, R. C. Brower, S. Gottlieb *Scaling Lattice QCD beyond 100 GPUs*, proceedings of SC11, The International Conference for High Performance Computing, Networking, Storage and Analysis (2011)

Research Interests and Expertise
Lattice QCD Algorithms: Linear Solvers, Multi-Grid, Molecular Dynamics Monte Carlo algorithms
Software: Chroma/QDP++ (co-author), QPhiX library & MG_Proto (author), QUDA (contributor)
Recent Architectures: NVIDIA GPUs, Intel Gen-9 HD Graphics, AMD MI60, Intel Xeon Phi
Performance Portability: Kokkos, DPC++
Programming: C++,C, Fortran, Python, SYCL, Nim, MPI, OpenMP, Kokkos, CUDA, HIP
Systems Experience: QCDSP, QCDOC, BlueGene, Cray Systems since 2016 (T3D, T3E, XE, XK, XC)

Synergistic Activities

1. SC20 Program committee, 2020
2. Co-PI of SciDAC-4 Project: Computing the Properties of Matter with Leadership Computing
3. Vice Chair of NERSC User Group Executive, 2019
4. Panel Chair: ALCF Theta Acceptance Review, 2016
5. Panel Member: OLCF-4 Acceptance Test Review and NERSC-9 Technical Design Review, 2018; NERSC Operational Assessment Review, 2016; OLCF Operational Assessment Review, 2015
6. Reviewer for DOE/ASCR SciDAC 2017, 2016, 2014
7. Lecturer: INT Summer School on Lattice QCD for Nuclear Physics, 2012; INT Summer School on Lattice QCD and its Applications, 2007; HackLatt Summer School, 2008,2009,2012
8. Co-designer of QCDOC supercomputer (2000-2002)

Collaborators

Robert Edwards, JLab
Anatoly Radyushkin, Old Dominion University/JLab
Raza Sufian, JLab
David Richards, JLab
Savvas Zafeiropoulos, CNRS/Marseille (France)
Joe Karpie, Columbia University
Tanmoy Bhattacharya, Los Alamos National Laboratory
Rajan Gupta, Los Alamos National Laboratory
Yong-Chull Jang, Brookhaven National Laboratory
Huey-Wen Lin, Michigan State University
Boram Yoon, Los Alamos National Laboratory
Chia Cheng Chang, Lawrence Berkeley National Laboratory
Ben Hörz, Lawrence Berkeley National Laboratory
Enrico Rinaldi, RIKEN
Dean Howarth, Boston University
Evan Berkowitz, University of Maryland
David A. Brantley,
Arjun Singh Gambhir, Lawrence Livermore National Laboratory
Christopher Körber, Lawrence Berkeley National Laboratory
Christopher Monahan, William & Mary
Henry Monge-Camacho, UNC-Chapel Hill
M. A. Clark, NVIDIA
Thorsten Kurth, NVIDIA
Amy Nicholson, UNC-Chapel Hill
Kostas Orginos, William & Mary/JLab
Pavlos Vranas, Lawrence Livermore National Laboratory
André Walker-Loud, Lawrence Berkeley National Laboratory

Curriculum Vitae
Christopher J. Monahan

Contact Information

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Williamsburg, VA 23185
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Email: cjmonahan@wm.edu

Professional Preparation

Ph.D. (Theoretical Physics), University of Cambridge, UK, 2012
M.Phys. (Physics), University of Edinburgh, UK, 2007

Appointments

Assistant Professor, William & Mary, 2019-present
Postdoctoral Research Associate, Institute for Nuclear Theory, 2017-2019
Postdoctoral Research Associate, Rutgers, The State University of New Jersey, 2015-2017
Postdoctoral Research Associate, University of Utah, 2014-2015
Postdoctoral Research Associate, William & Mary, 2011-2014

Five Publications Most Relevant to This Proposal

1. T. Khan, R. S. Sufian, J. M. Karpie, C. J. Monahan, C. Egerer, B. Joó, W. Morris, K. Orginos, A. Radyushkin, D. G. Richards, E. Romero, S. Zafeiropoulos, *Unpolarized gluon distribution in the nucleon from lattice quantum chromodynamics*, PRD 104 (2021) 094516
2. L. Del Debbio, T. Giani and C. J. Monahan, *Notes on lattice observables for parton distributions: nongauge theories*, JHEP 09 (2020) 021.
3. Ch. Ch. Chang, A. Nicholson, E. Rinaldi, E. Berkowitz, N. Garron, D. A. Brantley, H. Monge-Camacho, C. J. Monahan, C. M. Bouchard, M. A. Clark, B. Joó, T. Kurth, K. Orginos, P. Vranas, A. Walker-Loud, *A percent-level determination of the nucleon axial coupling from Quantum Chromodynamics*, Nature 558 (2018) 91.
4. R. A. Briceño, M. T. Hansen, and C. J. Monahan, *The role of the Euclidean signature in lattice calculations of quasi-distributions and other non-local matrix elements*, Phys. Rev. D 96 (2017) 014502.
5. C. J. Monahan and K. Orginos, *Quasi parton distributions and the gradient flow*, JHEP 03 (2017) 116

Research Interests and Expertise

Nonperturbative approaches to nucleon structure, particularly the gluonic structure of nucleons and light nuclei. Heavy quark flavor physics and nonperturbative inputs into searches for new physics and tests of CKM unitarity. Hydrodynamics.

Synergistic Activities

1. Lecturer: "2022 CFNS Summer School on the Physics of the Electron-Ion Collider", Stony Brook University, 2022.
2. Lecturer: "Advanced Cyberinfrastructure Training for Modeling Physical Systems", RPI, 2020, 2021.
3. Co-organizer: "QCD real-time dynamics and inverse problems", ACFI, 2020

Collaborators

Raúl Briceño, Old Dominion University
Jiunn-Wei Chen, National Taiwan University (Taiwan)
Christine Davies, Glasgow University
Rachel Dowdall, University of Cambridge (UK)
Elvira Gámiz, Universidad de Granada (Spain)
Maxwell Hansen, CERN (France/Switzerland)
Judd Harrison, University of Cambridge (UK)
Ron Horgan, University of Cambridge (UK)
Ciaran Hughes, Fermilab
G. Peter Lepage, Cornell University
Heechang Na, Ohio Supercomputer Center
Junko Shigemitsu, The Ohio State University
Andrea Shindler, Michigan State University
Matthew Wingate, University of Cambridge (UK)
Jiahui Zhang, Regensburg (Germany)
Chia Cheng Chang, Lawrence Berkeley National Laboratory
Ben Hörz, Lawrence Berkeley National Laboratory
Enrico Rinaldi, RIKEN
Dean Howarth, Boston University
Evan Berkowitz, University of Maryland
David A. Brantley,
Arjun Singh Gambhir, Lawrence Livermore National Laboratory
Christopher Körber, Lawrence Berkeley National Laboratory
Henry Monge-Camacho, UNC-Chapel Hill
M. A. Clark, NVIDIA
Thorsten Kurth, NVIDIA
Amy Nicholson, UNC-Chapel Hill
Kostas Orginos, William & Mary/JLab
Pavlos Vranas, Lawrence Livermore National Laboratory
André Walker-Loud, Lawrence Berkeley National Laboratory

Curriculum Vitae
JIANWEI QIU

Contact Information

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Professional Preparation

Ph.D. (Physics), Columbia University in the New York City, 1987
M.Ph. (Physics), Columbia University in the New York City, 1984
M.A. (Physics), Columbia University in the New York City, 1983

Appointments

2017 - present, Governor's Distinguished CEBAF Professor, The College of William & Mary
2016 - present, Associate Director for Theoretical and Computational Physics, and Theory Center Director, Jefferson Lab
2010 - 2016, Physicist, Senior Physicist, Brookhaven National Lab
2010 - 2016, Brookhaven Professor, Stony Brook University
1991 -2012, Assistant Professor, Associate Professor, Professor, Iowa State University
1989 - 1991, Postdoctoral Research Associate, YITP, Stony Brook University
1987 - 1989, Postdoctoral Research Associate, HEP Division, Argonne National Laboratory

Five Publications Most Relevant to This Proposal

1. R. Sufian, C. Egerer, J. Karpie, R.G. Edwards, B. Joó, Y.-Q. Ma, K. Orginos, J.-W. Qiu, D.G. Richards, *Pion Valence Quark Distribution at Large x from Current-Current Correlation in Lattice QCD*, Phys. Rev. D102 (2020) 054508
2. J. Bringewatt, N. Sato, W. Melnitchouk, J. W. Qiu, F. Steffens and M. Constantinou, *Confronting lattice parton distributions with global QCD analysis,* Phys. Rev. D103 (2021) 016003
3. Z. Y. Li, Y. Q. Ma and J. W. Qiu, *Extraction of Next-to-Next-to-Leading-Order Parton Distribution Functions from Lattice QCD Calculations,* Phys. Rev. Lett. 126 (2021) 072001.
4. Z.Y. Li, Y.Q. Ma and J.W. Qiu, *Multiplicative Renormalizability of Operators defining Quasiparton Distributions*, Phys. Rev. Lett. 122 (2019) 062002.
5. Y.Q. Ma and J.W. Qiu, *Exploring Partonic Structure of Hadrons Using ab initio Lattice QCD Calculations*, Phys. Rev. Lett. 120 (2018) 022003

Research Interests and Expertise

Perturbative QCD and QCD factorization; interplay between lattice QCD, QCD phenomenology and experimental data; hadron structure.

Synergistic Activities

1. Co-organizer: "Coordinated mini-lecture series on quantum computing and quantum information science for nuclear physics" (DOE-supported), Jefferson Lab, 2020
2. P.I. and Co-Spokesperson, The TMD Collaboration (Topical Collaboration in Nuclear Theory for the Coordinated Theoretical Approach to Transverse Momentum Dependent Hadron Structure in QCD), 2016–present
3. Member: Steering Committee for the new "Virginia Center for Nuclear Femtography", funded by Virginia Commonwealth
4. Co-Editor: community White Paper, "Electron-Ion Collider: The Next QCD Frontier – Understanding the glue that binds us all" [Eur. Phys. J. A52 (2016) 268].

Collaborators

Alberto Accardi, Hampton University	Mathias Burkardt, New Mexico State University
Martha Constantinou, Temple University	William Detmold, MIT
Abhay Deshpande, Stony Brook University	Robert Edwards, Jefferson Lab
Michael Engelhardt, New Mexico State University	Sean Fleming, University of Arizona
Leonard Gamberg, Penn State University at Berks	Manvir Grewal, Columbia University
Kawtar Hafidi, Argonne National Lab	Tomomi Ishikawa, Shanghai Jiaotong University
Xiangdong Ji, University of Maryland	Bálint Joó, JLab
Sylvester J. Joosten, Temple University	Zhong-Bo Kang, UCLA
Joseph Karpie, Columbia University	Christopher Lee, Los Alamos National Lab
Zheng-Yang Li, Peking University	Huey-Wen Lin, Michigan State University
Keh-Fei Liu, University of Kentucky	Simonetta Liuti, University of Virginia
Yan-Qing Ma, Peking University	Tom Mehen, Duke University
Andrea Metz, Temple University	Zein-Eddine Meziani, Argonne National Lab
Fred Olness, Southern Methodic University	Jen-Chieh Peng, UIUC
Alexei Prokudin, Penn State University at Berks	Felix Ringer, UC, Berkeley & LBNL, NSD
Ted Rogers, Old Dominion University	Marc Schlegel, New Mexico State University
Andrea Signori, Pavia University & INFN & Jefferson Lab	George Sterman, Stony Brook
Iain Stewart, MIT	Raza Sufian, Jefferson Lab
Raju Venugopalan, Brookhaven National Lab	Ivan Vitev, Los Alamos National Lab
Xiang-Peng Wang, Argonne National Lab	Xin-Nian Wang, UC, Berkeley & LBNL, NSD
Hongxi Xing, Southern China Normal University	Shinsuke Yoshida, SCNU
Zhite Yu, Michigan State University	Chieh-Peng Yuan, Michigan State University
Hong Zhang, Technische Universitaet Muenchen	Pia Zurita, University Regensburg, main)

Curriculum Vitae
ANATOLY RADYUSHKIN

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Professional Preparation

Habil. (Theoretical & Mathematical Physics), JINR-Dubna, Russia, 1987
Ph.D. (Theoretical & Mathematical Physics), Moscow University, Russia, 1978
M.S. (Physics), Moscow University, Russia, 1975

Appointments

1992 – present, Old Dominion University, Full Professor
1992 – present, Jefferson Lab, Senior Staff Scientist
1978 –1992, Junior, Senior and Leading Scientist at JINR-Dubna

Five Publications Most Relevant to This Proposal

1. A. V. Radyushkin, *Quasi-parton distribution functions, momentum distributions, and pseudo-parton distribution functions*, Phys. Rev. D 96 (2017) 034025.
2. A. V. Radyushkin, *Quark pseudodistributions at short distances*, Phys. Lett. B 781 (2018) 433.
3. A. V. Radyushkin, *Generalized parton distributions and pseudodistributions*, Phys .Rev. D 100 (2019) 116011.
4. I. Balitsky, W. Morris, A. Radyushkin, *Gluon Pseudo-Distributions at Short Distances: Forward Case*, Phys. Lett. B 808 (2020) 135621
5. A. V. Belitsky and A. V. Radyushkin, *Unraveling hadron structure with generalized parton distributions*, Phys. Rep. 418 (2005) 1.

Research Interests and Expertise

Theoretical basis of the lattice QCD extraction of PDFs and GPDs; hadron structure; perturbative QCD.

Synergistic Activities

1. Member of American Physical Society
2. Co-organizer: annual "QCD Evolution" workshops in 2011 – 2019, 2021, Editor of the Proceedings
3. Proposal reviewer: US Department of Energy and National Science Foundation

Collaborators

J. Karpie, Columbia University
K. Orginos, W&M
S. Zafeiropoulos, CPT Marseille (France)
B. Joó, JLab
D. Richards, JLab
R. S. Sufian, JLab
I. Balitsky, Old Dominion University
W. Morris, Old Dominion University

Curriculum Vitae
DAVID RICHARDS

Contact Information

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Newport News, VA 23606
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Email: dgr@jlab.org

Professional Preparation

PhD. (Theoretical Physics), University of Cambridge, UK, 1984
B.A. (Maths), University of Cambridge, UK, 1980

Appointments

2009-present, Senior Staff Scientist, JLab
2009-2010, Acting Associate Director for Theoretical and Computational Physics, JLab
2002-2009, Scientist II, III, JLab
1999-2002, Joint Assistant Professor, JLab/Old Dominion University
1993-1999, PPARC Advanced Fellow, University of Edinburgh
1988-1993, Postdoctoral Fellow/Physicist-programmer, University of Edinburgh
1986-1988, Postdoctoral Fellow, Argonne National Laboratory
1984-1986, Postdoctoral Fellow, Southampton University

Five Publications Most Relevant to This Proposal

1. C. Egerer, R. G. Edwards, K. Orginos and D. G. Richards, "Distillation at High-Momentum," Phys. Rev. D **103**, no.3, 034502 (2021)

2. B. Joó, J. Karpie, K. Orginos, A. V. Radyushkin, D. G. Richards and S. Zafeiropoulos, "Parton Distribution Functions from Ioffe Time Pseudodistributions from Lattice Calculations: Approaching the Physical Point," Phys. Rev. Lett. **125**, no.23, 232003 (2020)

3. R. S. Sufian, J. Karpie, C. Egerer, K. Orginos, J. W. Qiu and D. G. Richards, "Pion Valence Quark Distribution from Matrix Element Calculated in Lattice QCD," Phys. Rev. D **99**, no. 7, 074507 (2019)

4. B. Joó, J. Karpie, K. Orginos, A. V. Radyushkin, D. G. Richards, R. S. Sufian and S. Zafeiropoulos, "Pion valence structure from Ioffe-time parton pseudodistribution functions," Phys. Rev. D **100** (2019) no.11, 114512

5. J. D. Bratt, D. .G. Richards *et al.* [LHPC Collaboration], "Nucleon structure from mixed action calculations using 2+1 flavors of asqtad sea and domain wall valence fermions, Phys. Rev. D **82**, 094502 (2010).

Research Interests and Expertise

Nonperturbative computations of the internal structure of hadrons; spectrum of excited states of QCD.

Synergistic Activities

1. Steering-Committee Co-Chair: Center for Nuclear Femtography (CN), 2019–2020; Associate Director since 2020.

2. Chair: Topical Group for Hadronic Physics (GHP) of the APS, 2019.
3. Chair: USQCD Scientific Program Committee
4. Member: USQCD Executive Committee, 2004-2016; currently *ex officio*
5. Program Committee: GHP sessions at APS 2018 April Meeting
6. co-Chair: Program Committee, GHP Meeting 2019.
7. Co-organizer: INT Summer School on “Lattice QCD for Nuclear Physics”, 2012.

Collaborators T. Bhattacharya, LANL
C. Bouchard, University of Glasgow
C. Carlson, W&M
B. Chakraborty, University of Cambridge
C.C. Chang, LBNL
L. Chang, Nankai (China)
J. Dudek, JLAB/WM
R.G. Edwards, JLab
C. Egerer, WM
M. Engelhardt, New Mexico State University
A. Gambhir, Lawrence Livermore National Lab
J. Green, Mainz University
R. Gupta, Los Alamos National Lab
T. Horn, CUA
Y.C. Jang, Los Alamos National Lab
B. Joó, ORNL
J. Karpie, Columbia University
T. Khan, WM
K-F-Liu, University of Kentucky
Y-Q Ma, Beijing University
J.W. Negele, MIT
K. Orginos, JLab/W&M
M. Peardon, Trinity College Dublin
J-W Qiu, JLab
A. Radyushkin, JLab/Old Dominion University
C. Roberts, Nanjing (China) S. Ryan, Trinity College Dublin
R. Sufian, JLab
S. Syritsyn, Stony Brook University
F. Winter, JLab
S. Zafeiropoulos, CPT Marseille

Curriculum Vitae (*2-page limit*)
ELOY ROMERO

Contact Information
Computational Sciences & Technology Division
Jefferson Laboratory
Newport News, VA 23606 Email: eromero@jlab.org

Professional Preparation
Ph.D. (Comp. Sci.), Universitat Politecnica de Valencia, Spain, 2012
M.Sc. (Parallel and Distributed Computing), Universitat Politecnica de Valencia, Spain, 2008
B.S. (Comp. Sci.), Universitat Politecnica de Valencia, Spain, 2007

Appointments
2020–present, High-performance Computational Scientist, Computational Sciences & Technology Division
2019–2020, Postdoctoral Research Associate, Physics Department, William & Mary
2015–2019, Postdoctoral Research Associate, Computer Science Department, William & Mary
2012–2015, Postdoctoral Research Associate, Universitat Politecnica de Valencia

Five Publications Most Relevant to This Proposal

1. E. Romero, A. Stathopoulos, and K. Orginos, *Multigrid deflation for lattice QCD*, J. Comp. Phys. 409 (2020) 109356.
2. S. Goldenberg, A. Stathopoulos, and E. Romero, *A Golub–Kahan Davidson method for accurately computing a few singular triplets of large sparse matrices*, SIAM J. on Sci. Comp. 41 (2019) A2172
3. L. Wu, E. Romero, and A. Stathopoulos, *PRIMME_SVDS: A high-performance preconditioned SVD solver for accurate large-scale computations*, SIAM J. on Sci. Comp. 39 (2017) S248.
4. M. Caballer, C. de Alfonso, G. Moltó, E. Romero, I. Blanquer, and A. García, *Codecloud: A platform to enable execution of programming models on the clouds*, J. Systems and Software. 93 (2014) 187.
5. E. Romero, A. Tomás, A. Soriano, and I. Blanquer, *A fast sparse block circulant matrix vector product*, Euro-Par (2014)

Research Interests and Expertise High-performance methods for solving large linear systems and eigenvalue/singular value problems; cache-friendly methods for dense linear algebra, especially matrix multiplications and tensor contractions; best practices for developing efficient, maintainable, and portable software.

Synergistic Activities

1. Main developer: PRIMME software, 2015–present

Collaborators
Jose Miguel Alonso, Universitat Politecnica de Valencia (Spain)
Miguel Caballer, Universitat Politecnica de Valencia (Spain)
Amanda Calatrava, Universitat Politecnica de Valencia (Spain)
James McCombs, Indiana University (Principal Research Software Engineer)
Germán Moltó, Universitat Politecnica de Valencia (Spain)

Kostas Orginos, W&M
Jose E. Roman, Universitat Politecnica de Valencia (Spain)
Andreas Stathopoulos, W&M
Lingfei Wu, IBM AI Foundations Labs, Reasoning group at IBM T.J. Watson Research Center

Curriculum Vitae
RAZA SABBIR SUFIAN

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Professional Preparation
Ph.D. (Physics), University of Kentucky, 2017
M.S. (Physics), University of Kentucky, 2013
B.S. (Physics), University of Dhaka, Bangladesh, 2009

Appointments
2017–present: Postdoctoral Researcher, Jefferson Lab

Five Publications Most Relevant to This Proposal

1. R. S. Sufian, C. Egerer, J. Karpie, R. G. Edwards, B. Joó, Y. Q. Ma, K. Orginos, J. W. Qiu and D. G. Richards,*Pion Valence Quark Distribution from Current-Current Correlation in Lattice QCD*, Phys. Rev. D **102**, no.5, 054508 (2020).
2. R. S. Sufian, J. Karpie, C. Egerer, K. Orginos, J. W. Qiu and D. Richards, *Pion valence quark distribution from matrix element calculated in lattice QCD*, Phys. Rev. D 99 (2019) 074507.
3. T. Liu, R. S. Sufian, G. F. de Téramond, H. G. Dosch, S. J. Brodsky and A. Deur, *Unified Description of Polarized and Unpolarized Quark Distributions in the Proton*, Phys. Rev. Lett. 124 (2020) 082003.
4. G. de Téramond, T. Liu, R. S. Sufian, H. G. Dosch, S. Brodsky, A. Deur, *Universality of generalized parton distributions in light-front holographic QCD*, Phys. Rev. Lett. 120 (2018) 182001.
5. B. Joó, J. Karpie, K. Orginos, A. V. Radyushkin, D. G. Richards, R. S. Sufian and S. Zafeiropoulos, *Pion valence structure from Ioffe-time parton pseudo-distribution functions*, Phys. Rev. D 100 (2019) 114512.

Research Interests and Expertise
Lattice QCD methods for calculating parton distributions (GPDs, TMDs, PDFs); spin structure of the nucleon; holographic description of QCD.

Collaborators
Andrei Alexandru, George Washington University
Stanley J. Brodsky, SLAC National Accelerator Laboratory
Guy F. de Téramond, Universidad de Costa Rica (Costa Rica)
Hans Günter Dosch, Institut für Theoretische Physik der Universität (Germany)
Terrence Draper, University of Kentucky
Robert G. Edwards, JLab
Bálint Joó, JLab
Joseph Karpie, Columbia University
Keh-Fei Liu, University of Kentucky
Tianbo Liu, JLab
Yan-Qing Ma, Peking University (China)
Kostas Orginos, W&M
Jian-Wei Qiu, JLab

Anatoly Radyushkin, JLab
David Richards,JLab
Yi-Bo Yang, Institute of Theoretical Physics, Chinese Academy of Sciences (China)
Savvas Zafeiropoulos, CPT Marseille (France)

Curriculum Vitae (*2-page limit*)
FRANK WINTER

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Professional Preparation

Ph.D. (Theoretical Physics), University Regensburg, Germany, 2011
Dipl.-Phys. (M.Sc. Physics), Freie University Berlin, Germany, 2006

Appointments

2013–present, Staff Scientist, Jefferson Lab
2011–2013, Postdoctoral Research Associate, PPT (Particle Physics Theory), 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 Phys. Rev. Lett.
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 (2019) 034506.
3. Emmanuel Chang *et al.*, *Nuclear modification of scalar, axial and tensor charges from lattice QCD*, Phys. Rev. Lett. 120 (2018) 152002.
4. Michael L. Wagman *et al.*, *Baryon-Baryon Interactions and Spin-Flavor Symmetry from Lattice Quantum Chromodynamics*, Phys. Rev. D 96 (2017) 114510.
5. Brian C. Tiburzi *et al.*, *Double-β Decay Matrix Elements from Lattice Quantum Chromodynamics*, Phys. Rev. D 96 (2017) 054505.

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

A. S. Gambhir, Lawrence Berkeley National Laboratory
B. Joo, JLab
B. C. Tiburzi, The City College of New York
D. Richards, JLab
D. J. Murphy, MIT
E. Chang, University of Maryland
G. Schierholz, Deutsches Elektronen-Synchrotron DESY (Germany)
H. Perlt, Universitaet Leipzig (Germany)
H. Stueben, Universitaet Hamburg (Germany)
J. M. Zanotti, University of Adelaide (Australia)
K. Orginos, W&M

M. J. Savage, University of Washington
M. L. Wagman, Fermilab
M. Illa, Universitat de Barcelona (Spain)
M. Jafry, University of Washington
P. E. L. Rakow, University of Liverpool (UK)
P. E. Shanahan, MIT
R. D. Young, University of Adelaide (Australia)
R. Horsley, University of Edinburgh
R. Edwards, JLab
S. R. Beane, University of Washington
W. Detmold, MIT
Y. Nakamura, RIKEN Center for Computational Science
Z. Davoudi, University of Maryland

Curriculum Vitae (*2-page limit*)
SAVVAS ZAFEIROPOULOS

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13009 Marseille, France Phone:+3 (349) 126-9518

Professional Preparation

Ph.D. (Physics), Stony Brook University, 2013
B.Sc. (Physics), University of Athens, Greece, 2006

Appointments

2019–present, Permanent researcher, CPT Marseille, CNRS, France
2017–2019, Postdoctoral researcher, Universität Heidelberg, Germany
2016–2017, Postdoctoral researcher, William & Mary and JLab
2014–2016 Alexander von Humboldt fellow, Goethe University of Frankfurt, Germany
2013–2014, CNRS postdoctoral researcher, LPC Clermont-Ferrand, France

Five Publications Most Relevant to This Proposal

1. K. Orginos *et al.*, *Lattice QCD exploration of parton pseudo-distribution functions*, Phys. Rev. D 96 (2017) 094503.
2. J. Karpie *et al.*, *Moments of Ioffe time parton distribution functions from non-local matrix elements*, JHEP 11 (2018) 178.
3. J. Karpie *et al.*, *Reconstructing parton distribution functions from Ioffe time data: from Bayesian methods to Neural Networks*, JHEP 04 (2019) 057.
4. B. Joó *et al.*, *Parton Distribution Functions from Ioffe time pseudo-distributions*, JHEP 12 (2019) 081.
5. B. Joó *et al.*, *Pion valence structure from Ioffe-time parton pseudodistribution functions*, Phys. Rev. D 100 (2019) 114512.

Research Interests and Expertise

Nonperturbative determinations of x-dependent hadron structure; fundamental parameters of QCD; sign problems in QFT; systems of strongly correlated electrons (graphene and the Hubbard model).

Synergistic Activities

1. Co-organizer: 15$^{\text{th}}$ Workshop on Non-Perturbative Quantum Chromodynamics, Paris, France, 2018

Collaborators

Philippe Boucaud, LPT Orsay
Jose Rodriguez-Quintero, University of Huelva
Feliciano de Soto, University of Sevilla
Jorge Segovia, University of Sevilla
Jacobus Verbaarschot, Stony Brook University
Maksim Ulybyshev, Universität Würzburg
Christopher Winterowd, Kent University

Craig Roberts, Nanjing University
Joannis Papavassiliou University of Valencia
Daniele Binosi, ECT
Owe Philipsen, Goethe University Frankfurt
Alexander Rothkopf, Stavanger
Jacques Bloch, University of Regensburg
Karl Jansen, DESY
Carsten Urbach, Bonn University
Constantia Alexandrou, University of Cyprus
Martha Constantinou, Temple University
Kostas Orginos, College of William & Mary and JLAB
Joseph Karpie, Columbia University
B. Joo, ORNL
David Richards, JLAB Anatoly Radyushkin, Old Dominion University and JLAB

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++/QDP-JIT

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

CUDA

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

QIO

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

QMP

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

MPI

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

LAPACK, OpenBLAS, cuBLAS, and hipBLAS

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

PRIMME

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

LLVM-12

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

MAGMA

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?

Yes

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.

Colleagues from the USQCD collaboration

Question #2

Suggested Reviewers

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

Laurent Lellouch

CNRS Research Director

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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.

We do not need any testbed resources.