2023 INCITE Proposal Submission
Proposal

Title: Precision calculations of matrix elements for Novel CP Violation Experiments

Principal Investigator: Rajan Gupta

Organization: Los Alamos National Lab

Date/Time Generated: 6/17/2022 7:11:04 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.

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Section 2: Project Information

Question #1

Select the category that best describes your project.

Research Category

Physics: High Energy 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

The observed universe has an almost total absence of antimatter, whose dynamical generation requires much larger violation of charge-conjugation-parity (CP) symmetry than exists in established theory. The proposed results increase the reach of experiments searching for novel CP violation in the neutrino sector and in neutron electric dipole moment.

Section 3: Early Career Track

Question #1

Early Career

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

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

How to Apply:

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

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

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

- *What is the Early Career Track?*
  - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
  - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*
- *What do I need to do to be considered on the Early Career Track?*
  - *In the application process, select ‘Yes’ at ‘If you are within 10 years of your PhD, would you like to be considered in the Early Career Track?’ You will need to write a paragraph*

about how the INCITE proposal fits into your 5-year research and career goals.

- *What review criteria will be used for the Early Career Track?*
    - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

Early Career Track

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

No

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

N/A

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

N/A

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

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Node Hours

205000

Storage (TB)

200

Off-Line Storage (TB)

1000

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Node Hours

505000

Storage (TB)

100

Off-Line Storage (TB)

1000

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Node Hours

625000

Storage (TB)

100

Off-Line Storage (TB)

2000

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 HEP

Grant Number

KA2401012

Funding Source

DOE HEP

Grant Number

KA2401032

Funding Source

Los Alamos National Laboratory

Grant Number

LDRD-20210041DR

Question #13

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

Other High Performance Computing Resource Allocations

Resource

ERCAP at NERSC

Allocation Agency

DOE HEP

Allocation

200K CPU and 17K GPU node hours

Allocation Year

2022

Resource

ERCAP at NERSC

Allocation Agency

DOR NP

Allocation

90K CPU and 20K GPU node hours

Allocation Year

2022

Resource

USQCD

Allocation Agency

DOE HEP and NP

Allocation

24 + 23 M KNL core hours

Allocation Year

2022-2023

Resource

INCITE

Allocation Agency

DOE

Allocation

440K node hours on Summiut

Allocation Year

2022

Section 5: Project Narrative and Supplemental Materials

Question #1

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

Concatenate all materials below into a single PDF file.

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

INCITE_proposal__Gupta_2023.pdf
The attachment is on the following page.

I PROJECT EXECUTIVE SUMMARY

Title: Precision calculations of matrix elements for Novel CP Violation Experiments
PI: Rajan Gupta, **Co-PIs:** Tanmoy Bhattacharya and Vincenzo Cirigliano
Applying Institution/Organization: Los Alamos National Laboratory
Node Hours Requested: 205K (Summit), 505K (Frontier) in CY2023 and CY2024
Amount of Archival Storage Requested: 2000TB (CY2023) and 2000TB (CY2024)

The goal of this project is to calculate matrix elements (ME) within nucleon ground state that are needed to quantify CP violation ($\not{CP}$) in two sectors: neutrino mixing matrix and neutron electric dipole moment (nEDM). These ME will allow us to probe beyond the standard model (BSM) physics in two different ways: In the first case, precision results for the axial form factors enter in the calculation of the neutrino-nucleus scattering cross-section and the neutrino flux that are needed for reaching the design precision of experiments such as SBN and DUNE at Fermilab. In the second, combined with the experimental bound [or result] for the nEDM, they put constraints on novel CP violating interactions at the TeV scale, and impact the analysis of whether baryogenesis is a credible mechanism for explaining the matter-antimatter asymmetry in the observed universe.

Our existing results on nucleon charges dominate the world averages for 2019 and 2021 compiled by the community effort (called Flavor Lattice Averaging Group (FLAG)) that are used by phenomenologists/experimentalists [1, 2]. Our ongoing and proposed simulations consist of five broad tasks: (i) generation of 2+1-flavor ensembles with the Wilson-clover lattice action; (ii) the analysis of isovector axial form factors that enter in the calculation of neutrino-nucleus scattering cross-section; (iii) calculation of the matrix elements of the leading $\not{CP}$ operators that arise in both the standard model (SM) and BSM that are determined using the tools of effective field theory; and (iv) theoretical developments needed for these calculations, and (v) optimization of the software for the Summit and Frontier leadership class computers.

Our recently published results on isovector axial form factors using seven 2+1-flavor clover ensembles [3], plus matrix elements of quark EDM [4–6] and Theta $\not{CP}$ [7] operators, and the pion-nucleon sigma term [8] also contain several theoretical and algorithmic developments to address systematics and reduce errors to the level needed for experimental/phenomenology goals. The team has a dedicated effort to improve code performance on both Summit and Frontier machines.

We have essentially already reached the goals proposed for INCITE 2021-2022 in each of the five areas. By the end of 2022, we will finish generating and analyzing 2000+ configurations on all 13 ensembles, including the one physical pion mass ensemble, $a070m130$. The improvement in axial and electromagnetic form factors and nucleon charges seen in the preliminary analysis of these 13 ensembles over the analysis from 7 of these clover ensembles [3] is significant. However, our work has also exposed large contributions from multihadron excited states in many nucleon matrix elements that impact the extraction of results in the physical limit needed by experimentalists. These artifacts are pion mass dependent, and necessitate further simulations closer to the physical value of the pion mass, $M_\pi = 135$ MeV, to demonstrate reliable control at the percent level.

We request allocation for the generation and analysis of two additional large volume ensembles at a fine lattice spacing, $a \sim 0.055$ fm, and at pion masses of 170 and 135 MeV. Such large volume, small pion mass ensembles can only be simulated using leadership-class resources such as at OLCF.

The team represents a balance in expertise between lattice QCD, phenomenology of $\not{CP}$, high performance computing, and code development and optimization (on Summit and Frontier). Three postdocs trained and mentored by us in all aspects of these calculations moved to new positions but are continuing to work on this project. One new postdoc, Jun-sik Yoo, joined us in May 2022.

II SIGNIFICANCE OF RESEARCH

The standard model (SM) of elementary particles, including the recent understanding of neutrino masses and mixing, is extremely successful in describing all phenomena up to the TeV scale probed at the Large Hadron Collider (LHC) in Geneva. At the same time new, and as yet unknown, physics is required to explain three profound mysteries: the observed matter-antimatter asymmetry of the universe, dark matter and dark energy. The proposed calculations address the first. Also, while the nature of dark matter is unknown, lattice QCD (LQCD) provides the low energy effective couplings with nucleons of possible scalar, pseudoscalar, axial, and tensor mediators.

The observed universe has $6.1^{+0.3}_{-0.2} \times 10^{-10}$ baryons for every black body photon [9], whereas in a baryon symmetric universe, we expect no more than about 10^{-20} baryons for every photon [10]. It is difficult to include such a large excess of baryons as an initial condition in an inflationary cosmological scenario [11]. The way out of the impasse lies in generating the baryon excess dynamically. In addition to non-equilibrium dynamics in the evolution of the universe and baryon number violation, dynamical generation requires additional charge-conjugation-parity (CP) violation that is $10^3 - 10^5$ times larger than exists in the SM [12].

In the SM, CP violation ($\not{CP}$) is accounted for by a complex phase in the Cabibbo-Kobayashi-Maskawa (CKM) matrix that relates the mass eigenstates of quarks (the quark states that are produced in strong interactions) and the linear combination of these states that couple to $W^\pm$ bosons, the carriers of the weak force. This $\not{CP}$ is, perhaps, the most subtle feature of the SM, and is about a thousand times weaker than weak interactions that are responsible, for example, for the decay of a free neutron. This tiny phase explains all the observed $\not{CP}$ in the kaon, charm and bottom mesons. However, it is too small to explain the almost complete absence of antimatter. Baryogenesis mechanisms require new and larger sources of $\not{CP}$ in couplings to quarks and gluons and their validation (and/or interpretation) require the accurate LQCD calculations of the nucleon matrix elements, which are the goal of this proposal.

For weak scale baryogenesis to be a viable mechanism, new sources of $\not{CP}$ are needed in Beyond the Standard Model (BSM) theories. At the TeV scale, many mechanisms for $\not{CP}$ can be designed. Each new $\not{CP}$ interaction that involves quarks and gluons automatically makes a contribution to the neutron electric dipole moment (nEDM), whose discovery is being pursued by a number of experiments worldwide [13]. At the hadronic scale (≤ 2 GeV), one can write down the leading interactions in terms of quark and gluon fields and organize them by importance using the tools of effective field theory [14–16]. Such analyses show that there are five leading types of operators that need to be considered for a complete analysis, of which we are in the process of calculating the matrix elements of four (quark EDM, Θ-term, Weinberg and quark chromo-EDM operators) as discussed in Sec. V C. The lattice methodology for the fifth, the 4-fermion operators, is not yet developed enough to get results using current HPC resources.

The structure of their contributions to the nEDM, d_n, is as follows: If the low-energy effective $\not{CP}$ Hamiltonian is written as $\mathcal{H}_{\not{CP}} = \sum_i d_i O_i$, where d_i and O_i are the $\not{CP}$ couplings and operators, then their contributions to the nEDM are $d_n = \sum_i d_i g_i$ where g_i are the matrix elements of the operators within the neutron state, $g_i \propto \langle N|O_i|N\rangle$. The role of lattice QCD is to calculate the g_i. Then, given a measurement of (or bound on) the d_n and knowing g_i, one can invert the relation $d_n = \sum_i d_i g_i$ to bound the d_i, and thereby the space of possible $\not{CP}$ couplings that can arise at the TeV scale. Current phenomenological estimates of the g_i are based on models and have $O(100\%)$ uncertainties in some cases [17–20]. Such large uncertainties make it very hard to disentangle models of BSM physics, to falsify EW baryogenesis scenarios, and to quantitatively compare constraints on $\not{CP}$ operators from EDMs and high-energy colliders. Based on current work, reducing the uncertainty in the 4 proposed $\not{CP}$ operators to the 2–20% level (except possibly quark chromo-EDM) is within the reach of our lattice calculations. This can have a dramatic impact, e.g. improving the bounds on $\not{C}\not{P}$ scenarios in which $\not{C}\not{P}$ appears in the top-Higgs sector by 1–2 orders of magnitudes [21].

So far, robust LQCD estimates ($\lesssim 5\%$ uncertainty [1, 2, 4–6]) exist for only the contributions of the quark EDM to the nEDM. This is because they are given by the flavor diagonal tensor charges, i.e., $g_T^{u,d,s,c}$. Reducing uncertainties in the remaining matrix elements will allow phenomenologists to use new nEDM limits of 10^{-27} e cm expected soon [13] to constrain $\not{C}\not{P}$ Higgs couplings significantly beyond what is accessible at the colliders [22]. This makes the proposed calculations timely.

A second popular mechanism that could account for the matter-antimatter asymmetry is leptogenesis, which requires $\not{C}\not{P}$ in the lepton sector, in particular in the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) neutrino mixing matrix [23] that is being probed by the Tokai-to-Kamioka (T2K) experiment in Japan [24] and is the motivation for the DUNE experiment at Fermilab [25]. The precision required for establishing $\not{C}\not{P}$ depends on knowing the neutrino-nucleus cross-section over a range of momentum transfers at the $\sim 2\%$ or better level [26]. First evidence that this larger $\not{C}\not{P}$ could arise due to a maximal phase, $\pi/2$, in the mixing matrix between the 3 flavors of neutrinos has recently been presented by the T2K experiment [24].

To reach the precision goals of DUNE, axial, electric and magnetic form factors of nucleons are needed to describe the interaction of neutrinos, electrons and muons scattering off nuclear targets. Of these, the axial form factor, $G_A(Q^2)$ that gives the Q^2 dependent coupling of a nucleon to the weak $W^\pm$ boson, is a key unmeasured input needed to calculate the differential cross section for all neutrino-nucleus scattering experiments [27, 28]. To fully describe interactions of neutrinos (or electrons or dark matter) with heavy nuclei that are used as targets, one also needs to include nuclear corrections due to the binding/interactions of nucleons within nuclei that make up the targets. LQCD Calculations of matrix elements between nuclei and transition matrix elements such as $\langle N|A_\mu|N\pi\rangle$ are still in exploratory stages. Joseph Carlson at LANL, and his collaborators are pursuing these using nuclear many-body methods.

Also entering in this analysis are electric and magnetic form factors, for which precise experimental data exist from electron and muon scattering off various nuclear targets. So, lattice results will be compared to these for validation of the lattice methodology. In short, the proposed calculations address the needs of the long baseline neutrino experiment at Fermilab (DUNE), the electron scattering experiments at JLab and at the future electron-ion collider (EIC) at Brookhaven in the US. As these experiments are already in the pipeline, the calculation of these quantities is timely.

Operationally, the extraction of the matrix elements of the proposed Θ and Weinberg gluonic $\not{C}\not{P}$ operators involve the calculation of the 3-point functions $C^{\rm 3pt}_{A_\mu} \equiv \langle\Omega|\mathcal{N}(\tau)A_\mu(t)\overline{\mathcal{N}}(0)|\Omega\rangle$ and $C^{\rm 3pt}_{V_\mu} \equiv \langle\Omega|\mathcal{N}(\tau)V_\mu(t)\overline{\mathcal{N}}(0)|\Omega\rangle$ with isovector axial ($A_\mu = \overline{u}\gamma_\mu\gamma_5 d$) or vector ($V_\mu = \overline{u}\gamma_\mu d$) currents inserted at time t as illustrated in Fig. 1 and discussed in Sections V B and V C. Here u and d are the up and down quarks and $\mathcal{N}$ is a nucleon interpolating operator that creates the nucleon state at time zero from the QCD vacuum $|\Omega\rangle$ and also annihilates it at time τ. One then constructs the correlation of these 3-point functions with the Θ and the Weinberg gluonic operators as shown in Eqs. 6 and 7. In short, 95% of the cost of the proposed calculation is the same as that for the standard calculation of axial, electric and magnetic form factors.

Explaining the matter-antimatter asymmetry is a strong motivation to look for additional $\not{C}\not{P}$, however, the EDM experiments are very difficult. On the theory side, as described in this proposal, the two synergistic calculations, one aimed at the neutrino experiments to enable them to reach their desired precision, and the other that provides the matrix elements of novel CP violating operators within the neutron's ground state, are challenging. Having developed some of the theoretical and computational methods for each, and carried out first calculations on seven ensembles [3], we are confident that with the requested 2023 and 2024 INCITE resources, we can obtain estimates from 15 ensembles, thereby improving chiral-continuum-finite-volume (CCFV) fits to obtain continuum results with few percent uncertainty and impact phenomenological analyses.

III OVERVIEW OF THE CALCULATIONS AND THE GOALS

Results from the proposed 13 ensembles will be published towards the end of 2022. Here we provide the status of our analyses with respect to the four overall physics goals:

- Generation of ensembles with 2+1-flavors of Wilson-clover fermions. Sufficient number of lattices (2000+) for the thirteen ensembles described in Table I have already been generated. For 2023–2024, we propose to generate two more large volume ensembles, $a055m170$ and $a055m135$, which will complete the current project. With these 15 ensembles, we expect to control the uncertainty in the CCFV extrapolation to within few percent, and excited-state contributions (ESC) that are a major systematic in the extraction of ground state matrix elements. These lattices are stored at Oak Ridge and we have already made available 1000 lattices from each ensemble to the US lattice QCD community for other calculations.

- Isovector axial vector form factors of the neutron for the analysis of charged current neutrino-nucleus interactions (DUNE, T2K). The robustness of the results first presented in Ref. [3] has improved very significantly as shown in Figs. 3, 5 and 6. The same calculation also gives
  - Axial, scalar and tensor charges, $g_{A,S,T}^{u-d}$, of the nucleons. The g_S^{u-d} and g_T^{u-d} charges, combined with neutron decay distribution parameters b and b_1, provide constraints on novel scalar and tensor interactions at the TeV scale [5, 29].
  - Electric and magnetic form factors, $G_E(Q^2)$ and $G_M(Q^2)$ [3].
  - The momentum fraction, helicity and transversity moments. These are the first moments of the associated parton distribution functions [30].

- Flavor diagonal charges of the nucleons. These require additional calculations of disconnected quark-loop diagrams. Calculations on 7 ensembles, each with 1000 configurations, will be completed by the end of 2022.
  - The axial charges, $g_A^{u,d,s}$, give the contribution of $\{u\,,d\,,s\}$ quarks to proton spin [31, 32].
  - The scalar charges, $g_S^{u,d,s}$, give the strength of spin independent interaction of dark matter with nucleons. They also give the pion-nucleon sigma term and strangeness content of the nucleons that quantify the amount of nucleon mass arising due to quarks having finite mass [8].
  - The tensor charges, $g_T^{u,d,s}$, give the contribution of the quark EDM operators to the neutron EDM [5, 32].

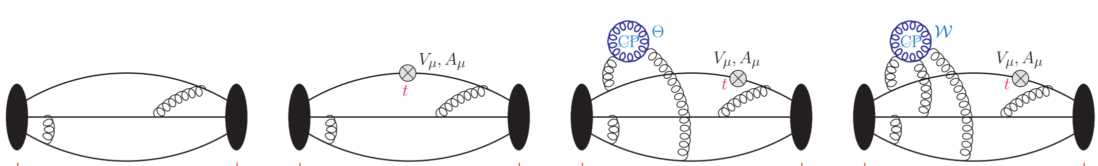

FIG. 1: Illustration of the correlation functions, 2-point (left), 3-point for form factors (second), $\not{CP}$ Θ-term (third) and $\not{CP}$ Weinberg operator (right) being calculated (qcEDM not shown). The source-sink separation is τ, with the operator (axial or vector current) inserted at Euclidean time t. The contribution of $\not{CP}$ operators to the nEDM is given by their correlation with 3-point functions as shown in the right 2 panels.

- The contributions of the Θ-term [7], Weinberg three-gluon operator and the quark chromo-EDM operator to the nucleon EDM.

IV CORRELATION FUNCTIONS CALCULATED

We calculate expectation values of 2- and 3-point nucleon correlation functions, $C^{2\text{pt}} \equiv \langle\Omega|\mathcal{N}(\tau)\overline{\mathcal{N}}(0)|\Omega\rangle$ and $C_O^{3\text{pt}} \equiv \langle\Omega|\mathcal{N}(\tau)O(t)\overline{\mathcal{N}}(0)|\Omega\rangle$ with $O = \{A_\mu, V_\mu, S, T, P\}$, using numerical simulations of lattice QCD. The $C^{2\text{pt}}$, illustrated in the first panel in Fig. 1, represents the propagation of the nucleon for Euclidean time τ. It has the spectral decomposition

$$C^{2\text{pt}} = \sum_i |A_i|^2 e^{-E_i\tau}\,, \tag{1}$$

where A_i is the amplitude for the creation of state $|i\rangle$ by the nucleon interpolating operator $\mathcal{N}$, and E_i is its energy. The sum is over all possible intermediate states with the same quantum numbers as the nucleon. Thus, a fit to infinitely precise data for $C^{2\text{pt}}$ (on an ensemble with $a \approx 0$, L large and $M_\pi = 135$ MeV), using Eq. (1) would give the complete spectrum of QCD with nucleon quantum numbers in a finite box for all states that couple to $\mathcal{N}$, i.e., for which $A_i \neq 0$.

Charges and form factors are obtained from 3-point functions $C^{3\text{pt}}_{A_\mu,V_\mu}$ with operator O injecting momentum $\boldsymbol{q} = \boldsymbol{p}-\boldsymbol{p}'$ at time t as shown in the second panel of Fig. 1. Its spectral decomposition is

$$C_O^{3\text{pt}}(t;\tau;\boldsymbol{p}',\boldsymbol{p}) = \sum_{i,j}\ \mathcal{A}_i'\mathcal{A}_j\langle i'|\mathcal{O}|j\rangle e^{-E_it-M_j(\tau-t)} \tag{2}$$

where the sum is again over all intermediate states. In all our calculations of 3-point functions, the momentum $\boldsymbol{p}$ at the sink is fixed to zero while state $|i'\rangle$ has nonzero momentum $\boldsymbol{p}' = -\boldsymbol{q}$.

The goal is to extract the ME $\langle 0'|O|0\rangle$ for various operators O within the nucleon ground state $|0\rangle$ from fits to Eqs. (1) and (2). The ideal situation for extracting $\langle 0'|\mathcal{O}|0\rangle$ is when A_0, A_0', M_i and E_i can be taken from fits to the 2-point function. Then the dependence on the remaining unwanted unknowns involving excited states, $\mathcal{A}_i'\mathcal{A}_j\langle i'|\mathcal{O}|j\rangle$ with $(i,j>0)$, is simple. Unfortunately, for axial form factors, we have shown that this expectation fails [33]. This is because multihadron excited states such as $N\pi$ and $N\pi\pi$ give large contribution in many $C_O^{3\text{pt}}$ that needs to be removed, however, their A_i and E_i are not given by current fits to $C^{2\text{pt}}$. We return to this issue in Sec. VI.

V PROJECT ACHIEVEMENTS AND METHODOLOGY

In this section, we briefly summarize the achievements and methods. New technical developments are discussed, while details that are standard and given in our published works are referenced.

A A suite of 2+1-flavor ensembles with the Wilson-Clover Action

The calculations of matrix elements within the nucleon state are most expedient with Wilson like fermions as they preserve the spin and flavor structure of continuum Dirac fermions. Such a suite of Wilson-clover ensembles did not exist for the US community, so we had to undertake their generation as an essential part of our project. Most of the lattices and ensembles are summarized in Table I have been generated by us with this and previous ALCC and INCITE allocations.

This suite of ensembles should have large statistics since there is an exponential decay in signal with source-sink separation τ for all nucleon correlation functions. These ensembles have to be generated at sufficient number of values of $\{a, M_\pi\}$ with $M_\pi L > 4$ to control, at the desired accuracy, systematics associated with the chiral-continuum-finite-volume extrapolations of lattice

ID	β	a (fm)	M_π (MeV)	L^3	T	$M_\pi L$	Lattices	$N_{\rm HP}$	$N_{\rm LP}$	τ
$a127m285$	6.1	0.127	285(5)	32^3	96	5.85	2002/2002	8,008	256,256	{8, 10, 12, 14}
$a094m270$	6.3	0.094	269(3)	32^3	64	4.1	2469/2469	7,407	237,024	{10, 12, 14, 16}
$a094m270L$	6.3	0.094	269(3)	48^3	128	6.16	4510/4510	18,040	577,280	{8, 10, 12, 14, 16, 18}
$a091m170$	6.3	0.091	169(2)	48^3	96	3.7	4012/4012	16,048	513,536	{8, 10, 12, 14, 16}
$a091m170L$	6.3	0.091	170(2)	64^3	128	5.1	3000/5000	12,000	480,000	{8, 10, 12, 14, 16}
$a073m270$	6.5	0.073	272(3)	48^3	128	4.18	4720/4720	18,880	604,160	{11, 13, 15, 17, 19}
$a071m170$	6.5	0.071	166(2)	72^3	192	4.4	2500/5000	12,600	201,600	{13, 15, 17, 19, 21}
$a093m220X$	6.3	0.093	220	48^3	128	5.0	2006/2500	8,024	124,764	{10, 12, 14, 16, 18}
$a093m220$	6.3	0.093	220	48^3	128	5.0	2000/4500	8,000	124,000	{10, 12, 14, 16, 18}
$a072m220$	6.5	0.072	220	64^3	192	5.2	2000/3000	9,144	146,304	{13, 15, 17, 19, 21}
$a070m130$	6.5	0.070	128	96^3	192	4.4	850*/2500	2,600	105,400	{13, 15, 17, 19, 21}
$a056m280$	6.7	0.056	279(2)	64^3	192	4.8	2700/5000	10,800	259,200	{15, 18, 21, 24, 27}
$a056m220$	6.7	0.056	220	72^3	192	4.5	1000*/2500	4,000	124,000	{18, 21, 24, 27, 30}
$a055m170$	6.7	0.056	170	96^3	192	4.5				Proposed for
$a055m135$	6.7	0.055	170	128^3	256	4.8				2023-2024 INCITE

TABLE I: Parameters of the isotropic 2+1-flavor clover ensembles being generated by the JLab/W&M/LANL/MIT collaborations using the highly tuned CHROMA code [34]. Column 7 labeled "Lattices" gives the number of configurations already analyzed/generated for charges and form factors. The $N_{\rm HP}$ ($N_{\rm LP}$) give the number of high precision (low precision), measurements of isovector quantities already completed. The values of source-sink separation τ simulated to remove ESC are given in columns 9–11. Results from ensembles 1-7 have already been published in Ref. [3]. The analysis of ensembles 8-13 will be completed by the end of 2022. The 2023-24 INCITE proposal is to generate and analyze the $a055m170$ and $a055m135$ ensembles.

results to the physical point, $\{a = 0, M_\pi = 135\text{MeV}\}$. Furthermore, we have shown that quantities for which $N\pi$ and $N\pi\pi$ ESC are significant, for example axial form factors [3], Θ-term [7] and the pion-nucleon sigma term [8], one needs simulations near the physical pion mass because their effects increase rapidly as $M_\pi \to 135$ and $\boldsymbol{q} \to 0$. Our ensembles with $M_\pi \approx 170$ and 135 MeV are, therefore, crucial to control artifacts due to $N\pi$ and $N\pi\pi$ excited states.

Subsequent to results presented in Ref. [3], we have, in 2021–2022, added six ensembles: four ($a093m220$, $a093m220X$, $a072m220$ and $a056m220$) at $M_\pi \approx 220$ MeV, one, $a056m280$, at $M_\pi \approx 280$ MeV, and one at the physical pion mass, $a071m130$. Statistics have been increased on the $a091m170L$ and $a071m170$ ensembles. The two ensembles $a093m220$ and $a093m220X$ have different strange quark mass to quantify dependence of observables with respect to it in CCFV fits. The four $M_\pi \approx 220$ MeV ensembles have improved control over the chiral part of the fit with respect to both M_π and M_K, and $a056m280$ has improved the continuum extrapolation. The $a071m130$ ensemble is critical in obtaining results at the physical pion mass. The current errors in $a056m220$ and $a071m130$ data, illustrated in Figs. 2–6, are still large, so the remaining 2022 allocation (about 50%) will be devoted to increasing their statistics. Results from these 13 ensembles will be presented at Lattice 2022 in August and published by the end of 2022.

To validate the trends observed and further control the systematics, we propose to generate and analyze the $a055m170$ and $a055m135$ lattices with the INCITE 2023–2024 award. We will also continue to opportunistically increase statistics on the $a091m170L$, $a071m170$ and $a070m130$ ensembles. This set of 15 ensembles will then include three at $M_\pi \approx 170$ MeV and two at $M_\pi \approx 135$ MeV. With these, we anticipate reducing the CCFV uncertainty to a few percent level and clarifying the ESC, including those from $N\pi$ and $N\pi\pi$ states, to various quantities.

The generation and analysis of these 15 ensembles will complete this project. We consider these ensembles a resource for the US lattice community. We have already made available 1000 lattices from each of the 13 ensembles already generated and will open up the rest at the end of 2022.

B Axial Vector Form Factors for Neutrino-Nucleus Scattering

Current and future charged-current neutrino-scattering experiments cover a large range of momentum transfer Q^2. The short and medium baseline (US SBN neutrino program at Fermilab and T2K in Japan) covers the region 0.2–1 GeV, while the long baseline (DUNE) experiment at Fermilab covers 0.2–5 GeV. Three different physical phenomena have to be addressed over this range: quasi-elastic (< 1 GeV), resonant (1–2 GeV) and deep-inelastic scattering (> 2 GeV) that are not easy to model [27]. Experimentally, the axial form factors for nucleons are unlikely to be measured directly due to safety concerns posed by the needed liquid hydrogen targets. (The Minerva experiment with a CH target aims to extract them.) Large-scale simulations of LQCD is the current best approach for first-principle results. Our first goal is to calculate these for the challenging quasi-elastic region (0.1–1 GeV) and later extend these up to 2 GeV to include the resonant region. To calculate cross-sections of neutrino scattering off ^{40}Ar target requires including nuclear corrections for which many-body nuclear theory is being used [28].

To get the axial vector form factors for nucleons, we start by calculating the 3-point function, $C^{3\text{pt}}_{A_\mu}$ where $A_\mu = \overline{u}\gamma_\mu\gamma_5 d$ is the isovector axial current. After removing the contributions of all the excited states using Eq. (2), the decomposition of the ground state matrix elements, in the isospin limit and generalized to include $\cancel{CP}$ interactions, give the axial, G_A, the induced pseudoscalar, $\tilde{G}_P$, and the $\cancel{CP}$ scalar, $\overline{G}^0_S$, form factors:

$$\langle N(\boldsymbol{p'})|A_\mu(\boldsymbol{q})|N(\boldsymbol{p})\rangle = \overline{u}_N(\boldsymbol{p'})\left(G_A(q^2)\gamma_5\gamma_\mu + \frac{q_\mu}{2M_N}[\gamma_5\tilde{G}_P(Q^2) + i\overline{G}^0_S(Q^2)]\right)u_N(\boldsymbol{p}), \qquad (3)$$

where $u_N(\boldsymbol{p})$ is the free neutron spinor with momentum $\boldsymbol{p}$ that obeys $(\not{p} - M_N)u_N = 0$, and $Q^\mu = p'^\mu - p^\mu$ is the 4-momentum carried by the axial current. The axial charge of the nucleon is given by $g_A \equiv G_A(Q^2 = 0)$. The quantity $\overline{G}^0_S(0)$ provides the contribution of the $\cancel{CP}$ interaction to the pion-nucleon coupling $g_{\pi NN}$, which gives the dominant contribution to the EDM of nuclei. Similarly, the nucleon matrix element of the electromagnetic current $J^{\text{EM}}_\mu \equiv eV_\mu = e\sum_q \bar{q}\gamma_\mu q$ can be parameterized in terms of the Dirac and Pauli form factors F_1 and F_2 as

$$\langle N|J^{\text{EM}}_\mu(q)|N\rangle \;=\; \overline{u}_N(p')\left[\gamma_\mu\, F_1(q^2) + i\frac{[\gamma_\mu,\gamma_\nu]}{2}q^\nu\,\frac{F_2(q^2)}{2M_N} - \frac{[\gamma_\mu,\gamma_\nu]}{2}q^\nu\gamma_5\,\frac{F_3(q^2)}{2M_N}\right]u_N(p). \qquad (4)$$

From these, the Sachs electric, $G_E = F_1 - (q^2/4M^2)F_2$, and magnetic form factors, $G_M = F_1 + F_2$, are obtained. We have included the electric dipole form factor F_3, which violates parity P and time reversal T invariances (also $\cancel{CP}$ if CPT is a good symmetry). Thus, the real and imaginary components of $\langle N|V_\mu(Q)|N\rangle$ give the form factors and the charges (the electric charge is $G_E(0) = F_1(0)$, the (anomalous) magnetic dipole moment is $F_2(0)/2M_N$). And, for each $\cancel{CP}$ operator included in the analysis, $F_3(0)/2M_N = d_n$ is its contribution to the nEDM as discussed in Sec. V C.

The valence quark-line diagram of both $C^{3\text{pt}}_{A_\mu}$ and $C^{3\text{pt}}_{V_\mu}$ is illustrated by the second panel in Fig. 1. The basic building block of all these calculations is the Feynman quark propagator shown as solid lines. The only difference between operators $O = \{A_\mu, V_\mu, S, T, P\}$ in $C^{3\text{pt}}_{A_\mu}$ is in the gamma matrix structure. For the $\cancel{CP}$ Θ and Weinberg operators, we have to calculate the correlation of $C^{3\text{pt}}_{A_\mu,V_\mu}$ with the gluonic operators as shown in the third and fourth panels of Fig. 1. The cost of calculating the gluonic part is small. In practice, we calculate $C^{3\text{pt}}$ for all sixteen Dirac matrices since the overall cost of doing the additional spin contractions is tiny. The lattice methodology for all these 3-point functions is mature and a good signal versus τ is obtained up to 1.5 fm as shown in Ref. [3]. Calculating all Dirac structures simultaneously gives the following iso-vector quantities: axial, scalar and tensor charges, axial and vector form factors, moments of momentum, helicity and transversity distributions. The first results for all these quantities from ensembles 1–7 have been presented in Refs. [3, 30]. The highlights are that axial, electric and magnetic form factors show very little dependence on M_π and lattice spacing a. Current data show this behavior persists in the analysis of ensembles 1–13, so we expect to reduce the uncertainties by a factor of about two.

However, challenges remain. In the calculation of all nucleon ME, as discussed in Ref. [3], the ESC are still large at $\tau \approx 1.5$ fm. For the calculation of $\cancel{CP}$ operators, there are the additional issues that the statistical signal in their contribution to nEDM (the signal in the from factor $F_3(Q)$) is small as discussed in Ref. [7] for the Θ-term. Furthermore, operator mixing and renormalization for the qcEDM and Weinberg operators [35] require additional calculations and theoretical developments. The proposed calculations (increasing statistics, adding 2 ensembles and renormalization of $\cancel{CP}$ operators discussed in Sec. V C) are geared to address these.

In Ref. [36], we showed that, in spite of using state-of-the-art methods, the relation imposed on the axial form factors by the partially conserved axial current (PCAC) relation, $\partial_\mu A_\mu = 2mP$, was violated in all previous lattice calculations by almost a factor of two. Here $P = \overline{u}\gamma_5 d$ is the pseudoscalar operator and $m = (m_u + m_d)/2$ is the average of the two light quark masses. Since PCAC is an operator identity that has to be satisfied up to discretization errors, and because the original axial and pseudoscalar correlation functions, $C^{3\text{pt}}_{A_\mu}$ and $C^{3\text{pt}}_P$ satisfy it, the problem is introduced while extracting the ground state matrix elements. In Ref. [33], we showed that the reason is that the energy gap, $a\Delta M_1$ and $a\Delta E_1$, on the two sides of A_μ in $C^{3\text{pt}}_{A_\mu}$ correspond to $N(\boldsymbol{p})\pi(-\boldsymbol{p})$ and $N(\boldsymbol{0})\pi(\boldsymbol{p})$ excited states for momentum transfer $\boldsymbol{q} = -\boldsymbol{p}$, and these energy gaps are much smaller than those obtained from straightforward fits to $C^{2\text{pt}}$, especially for small $\boldsymbol{q}$ and as $M_\pi \to 135$ MeV. Theoretical corroboration that these excited states should give the leading contribution in the axial channel is provided by chiral perturbation theory [37, 38]. In Refs. [3, 33], we developed strategies to take these into account. In Fig. 6, we show the improvement in how well the form factors satisfy the PCAC relation between the standard strategy (called $\{4, 3^*\}$) and the one including the $N\pi$ as the lowest excited state (strategy called $\{4^{N\pi}, 2^{\text{sim}}\}$). In general, determining all the states that contribute significantly to a given $C^{3\text{pt}}_O$ remains a challenge.

C Matrix Elements of Leading $\cancel{CP}$ Operators and their Contributions to nEDM

Our near-term goal is to calculate the matrix elements of the Θ-term, which may be present in the SM, and of the quark EDM (qEDM), the quark chromo-EDM (qcEDM), and the Weinberg dimension six 3-gluon ($\mathcal{W}$) operators that encapsulate $\cancel{CP}$ interactions arising in BSM. At the hadronic scale, the QCD Lagrangian in the presence of these $\cancel{CP}$ operators is

$$\mathcal{L}_{\text{QCD}} \longrightarrow \mathcal{L}_{\text{QCD}}^{\cancel{CP}} = \mathcal{L}_{\text{QCD}} - \frac{i}{32\pi^2}\Theta G_{\mu\nu}\tilde{G}_{\mu\nu} \; - \frac{i}{2}\sum_q d_q \; \bar{q}\sigma^{\mu\nu}\tilde{F}_{\mu\nu}q - \frac{i}{2}\sum_q \; \tilde{d}_q \; \bar{q}\sigma^{\mu\nu}\gamma_5 G_{\mu\nu}q \\ + d_{\mathcal{W}} \; f^{abc} G^a_{\mu\nu}\tilde{G}^{\nu\beta,b}G^{\mu,c}_{\beta} \tag{5}$$

where $F_{\mu\nu}$ and $G_{\mu\nu}$ are the electromagnetic and chromo field strength tensors, $\tilde{G}^{\mu\nu} = \epsilon^{\mu\nu\alpha\beta}G_{\alpha\beta}/2$, and $\sigma_{\mu\nu} = (i/2)[\gamma_\mu, \gamma_\nu]$. The first, Θ-term, is part of the SM, but is usually neglected under the assumption that some form of Peccei-Quinn mechanism relaxes $\Theta \to 0$ [39]. (We work in the basis in which the $\cancel{CP}$ isoscalar pseudoscalar mass term $im_*(\Theta)\; \bar{q}\gamma_5 q$ has been rotated into the Θ-term through a chiral transformation [40].) If a BSM $\cancel{CP}$ operator generates the Θ-term due to mixing under renormalization, or due to contributions to the Peccei-Quinn potential, then Θ gets an additional amount proportional to their d_i. For a non-zero cumulative Θ (and similarly for the Weinberg operator ($\mathcal{W}$) [41]), the contribution to the nEDM is obtained by calculating the correlation of these operators with the vector current,

$$\langle\Omega|\mathcal{N}(\tau)V_\mu(t)\mathcal{N}(0)|\Omega\rangle|^{\Theta}_{\not{C}\mathrm{P}} = \left\langle \mathcal{N}(\tau)\ \Big(V_\mu\ \int d^4x\ \Theta\ G^{\mu\nu}\tilde{G}^{\mu\nu}\Big)(t)\ \mathcal{N}(0)\right\rangle , \tag{6}$$

$$\langle\Omega|\mathcal{N}(\tau)V_\mu(t)\mathcal{N}(0)|\Omega\rangle|^{\mathcal{W}}_{\not{C}\mathrm{P}} = \left\langle \mathcal{N}(\tau)\ \Big(V_\mu\ \ \int d^4x\ d_{\mathcal{W}}\ f^{abc}G^a_{\mu\nu}\tilde{G}^{\nu\beta,b}G^{\mu,c}_{\beta}\Big)(t)\ \mathcal{N}(0)\right\rangle , \tag{7}$$

as shown by the right two diagrams in Fig. 1. From these, to get the ground state ME in the left hand side of Eq. (4), and from it the $\not{C}\not{P}$ form factor $F_3 = 2M_N d_n$, we need to remove ESC. We also need to determine the P-violating phase α_O characterizing the state, $\langle\Omega|\overline{\mathcal{N}}|N\rangle \propto e^{(i\alpha_O\gamma_5)}$, for each $\not{C}\not{P}$ operator O. This is obtained from the two-point function [6, 42].

We have recently presented an analysis of the Θ-term contribution to nEDM in Ref. [7] using the clover-on-HISQ formulation. This work also addressed two theoretical issues, the presence of an $O(m_q^0)$ term in CCFV fits with clover fermions and the contributions of $N\pi$ excited states in chiral perturbation theory. The final result is, unfortunately, consistent with zero at the 1σ level and showed large variation depending on whether the $N\pi$ excited state is included in the analysis. We propose to address both issues with the much higher statistics clover-on-clover analysis. Some recent theoretical analyses for the Weinberg operator ($\mathcal{W}$) [41] can be found in Refs. [43, 44] and the numerical calculations are underway with the status given in Table II. We anticipate publishing the first results for both the Θ-term and Weinberg operator from the clover ensembles by the end of 2022.

The second and third terms in Eq. (5) are the qEDM and the qcEDM operators with the sum over all the quark flavors, $q \in \{u, d, s, c, b, t\}$. Operationally, the leading contribution of the qEDM comes from an additional $\not{C}\not{P}$ term in the vector current itself that is proportional to the tensor bilinear operator. Thus, the contribution of the qEDM operator is given by the flavor diagonal tensor charges. For the clover ensembles, the status of the calculation of the 2-point and the connected 3-point functions is the same as the isovector calculation described in Sec. V B and is summarized in Table I. The status of the calculations for light and strange disconnected quark loops is shown in Table II. Our methodology for these calculations has been developed over the last six years using the clover-on-HISQ formulation as discussed in Refs. [4, 5]. These references also contain results for qEDM and the constraints on the split SUSY model in which the qEDM are the dominant novel CP violating operators. The qcEDM operator requires additional theoretical analysis of renormalization and mixing that is almost complete and a paper describing our methods using the clover-on-HISQ formulation should be published by September 2022 [45]. We will start the calculation on the clover ensembles once these issues are under full control, which we anticipate will be in 2023.

In short, the presence of $\not{C}\not{P}$ operators changes the coupling of the vector current to the neutron by a tiny amount. The contribution to the nEDM from the gluonic operators (Θ or $\mathcal{W}$) and of qcEDM, is given by their correlation with the vector 3-point function as in Eqs. (6) and (7). Similarly, the $\not{C}\not{P}$ modification of $g_{\pi NN}$, $\overline{g}^0_S$, is obtained by a similar calculation with V_μ replaced by A_μ in Eqs. (6)and (7). The contribution of qEDM is given by the flavor diagonal tensor charges.

VI Challenges to precision nucleon matrix elements and way forward

In spite of very considerable progress, there still remain four challenges to obtaining precision results for nucleon matrix elements and physical observables from them. This section gives a brief enumeration of these and how these are being addressed and the methods in hand today. The requested 2023–2024 allocations will add two ensembles with $a \approx 0.055$ fm and $M_\pi \approx 170$ and 135 MeV. Their parameters have been selected to have a small lattice spacing and to clarify the chiral behavior near the physical pion mass. These will improve the CCFV fits and resolve ESC.

Ensemble ID	Disconnected Light	Disconnected Strange	Θ and Weinberg	Ensemble ID	Disconnected Light	Disconnected Strange	Θ and Weinberg
$a127m285$	1002	1002	1000	$a073m270$	1132	1377	2166
$a094m270$	1197	1197		$a071m170$			1000
$a094m270L$	1000	1000	1800	$a056m280$			1000
$a093m220$	985	726	1800				
$a091m170$	1170	1170	1170				

TABLE II: The number of 2+1-flavor clover lattices already analyzed for the calculation of (i) disconnected contributions of light and strange quarks, and (ii) of the Θ and Weinberg operators.

High Statistics are needed to address the exponential, $e^{-(M_N-1.5M_\pi)\tau}$, degradation of signal in nucleon correlation functions with near-future novel algorithms and formulations of the calculations (see Fig. 2). Precision in calculations at a given value of $\{a, M_\pi, M_\pi L\}$ is needed to first address systematics associated with removing ESC, and later in making reliable CCFV fits to get physical results. To improve the statistical signal, our mid-term goal is to make $O(5\times10^5)$ measurements on $O(5000)$ configurations. Making $O(100)$ measurements from randomly selected points on each configuration is the observed sweet spot with respect to increasing statistics.

Excited states: The number of possible multihadron excited states, $N\pi$, $N\pi\pi$, $\ldots$, that could contribute to Eqs. (1) and (2) increase as $\mathbf{q}\to 0$ and $M_\pi \to 135$ MeV. Their mass gaps are small compared to the nucleon mass and these towers of states start at ~ 1200 MeV, i.e., much lower than the radial excitation $N(1440)$. Thus their contributions can be large at source-sink separations possible with current statistics (see Fig. 3). In fact, we have shown that these contaminations are large in axial form factors Refs. [3, 33], in the contribution of the Θ-term to the nEDM Refs. [7], and in the pion-nucleon sigma term [8]. Our overall strategy to reduce ESC is: (i) use the Wuppertal smeared source method [46] with radius ≈ 0.72 fm that is seen to suppress excited states. (ii) use chiral perturbation theory (χPT) to understand if multihadron, $N\pi$ and $N\pi\pi$, states are expected to make large contributions, for example as done for the axial form factors [37, 47], in the Θ-term [7] and in the nucleon sigma term [8]. (iii) Carry out multiple analyses using different plausible estimates of the first excited state mass guided by χPT analyses and the data to quantify the variation in the results. This variation is included as an additional systematic uncertainty. One known technology to further remove ESC is to include the multihadron states in a variational basis [48]. This method is under investigation, but has not yet been developed and demonstrated. The reasons are: (i) the set of states required for a given observable are still being determined, (ii) even for the axial form factors, the leading excited states, $N(\boldsymbol{p})\pi(-\boldsymbol{p})$ and $N(\boldsymbol{0})\pi(\boldsymbol{p})$, are different for each momentum transfer $\boldsymbol{q}$, and (iii) the technology for including multi-hadron initial and final states composed of nucleons and pions in 3-point functions is under development. While these methods are being developed, our work shows that the residual systematic can be 1–10% depending on the observable.

Operator mixing and renormalization: The renormalization factor provides the relationship between the operator used on the lattice and what a phenomenologist uses to connect theory to experiment. In QCD, this factor gets quantum corrections that can be large at $Q \lesssim 2$ GeV and can have energy scale dependence. Renormalization under scale change and discretization effects also introduce mixing with other operators with the same symmetry. When operators mix with those with lower dimensions, the coefficients often diverge as $O(1/a^n)$, for example, the $\not{CP}$ Weinberg and the qcEDM operators have a divergent mixing with lower dimensional Θ and pseudoscalar, $\bar{q}\gamma_5 q$, operators. As an illustration, consider the mixing between the Weinberg operator with the Θ-term, $\mathcal{W}^R = \mathcal{W} + \frac{b}{a^2}\Theta$. Any systematic error in the determination of b will lead to a divergent result for the matrix element $\langle N|V_\mu \mathcal{W}|N\rangle$ in the continuum limit $a\to 0$. Thus, to get results that are finite in the continuum limit, we need to calculate b and its scale dependence non-perturbatively.

The renormalization of all isovector quantities, flavor diagonal charges and moments of distributions has been carried out nonperturbatively using the RI-sMOM intermediate scheme [49, 50] on the lattice. This method gives results within 1–2% uncertainty. The renormalization of the Θ-term [7] and the Weinberg operator (including divergent mixing with the Θ-term) is being carried out using gradient flow (GF) scheme [51]. GF is an evolution of the quark and gluon fields in a fictitious dimension denoted by the *flow-time* $\tau^{\rm GF}$ towards stationary points of the QCD action. In this method, the gluonic and quark fields are smeared in space and time (using $N_\tau^{\rm GF}$ small "time" steps, $\delta\tau^{\rm GF}$) along the gradient of an action, to a fixed physical size $\tau^{\rm GF} = N_\tau^{\rm GF} \times \delta\tau^{\rm GF}$, before evaluating the operators. This fixed smearing size now sets the ultraviolet cutoff of the theory that respects the gauge and chiral symmetries of the continuum action as the lattice spacing is taken to zero without encountering any singularity except for one *universal* logarithmic multiplicative factor for the quark fields [52], which cancels in appropriately constructed ratios.

The connection to the $\overline{\rm MS}$ scheme, the most common in the phenomenology community, requires a simpler perturbative calculation in the continuum, which is underway for the Weinberg operator. A check of the overall calculation is the demonstration that the final results for the contribution of $\mathcal{W}$ to the nEDM are independent of $\tau^{\rm GF}$. The Θ-term does not mix and its renormalization in GF scheme is scale independent. For the qcEDM operator, we are developing the theoretical framework for determining the divergent mixing with the pseudoscalar operator using the axial Ward identity [6, 45]. We expect to present results demonstrating these methods at Lattice 2023.

The chiral-continuum-finite-volume extrapolation is needed to get physical results for all quantities calculated using lattice QCD. The uncertainty depends on the size of the effect and the range covered by the simulations in the three variables, $\{M_\pi, a, M_\pi L\}$. There are four ways to improve it: (i) use improved action (our tadpole improved clover action with stout smearing is very close to $O(a)$ improved) to reduce discretization errors, (ii) have precise data at the physical pion mass $M_\pi = 135$ MeV, (iii) use large volumes ($M_\pi L > 4$) so that the leading finite-volume correction term is sufficient, and (iv) simulate at a large number of values of $\{a, M_\pi, M_\pi L\}$ to constrain simultaneous fits in the three variables. Compared to our first publication [3] (see updated Fig. 4), our final results with 2021–2022 INCITE allocation will have (i) data on six additional ensembles (see Table I), (ii) higher statistics, (iii) all but one ensemble satisfy $M_\pi L > 4$, (iv) data at finer lattice spacing $a \approx 0.055$ fm, and (v) one physical mass ensemble at $M_\pi = 130$ MeV. With these improvements, and because the variation with $\{a, M_\pi\}$ is observed to be small, we anticipate the final uncertainty, including that due to the CCFV fits, will be reduced by about a factor of two.

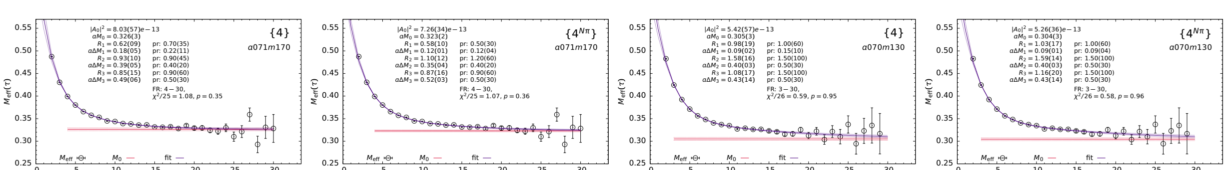

FIG. 2: Comparison of the standard 4-state fit $\{4\}$, (wide priors used only to stabilize fits) and $\{4^{N\pi}\}$ (narrow prior for aM_1 corresponding to the $N\pi$ state) to $\boldsymbol{p} = 0$ nucleon 2-point data from $a071m170$ (left 2 panels) and $a070m130$ (right 2 panels). The augmented χ^2/dof does not distinguished the fits, and in fact, is equally good for a large area of parameter space. Surprisingly, the $a\Delta M_1$ are different for $a071m170$ (and all other ensembles) but almost the same and low ($\sim N\pi$ state) in the still low statistics $a070m130$ data.

VII Illustration of Results and Issues

Figure 2 illustrates the $e^{(M_N - 1.5M_\pi)\tau}$ growth in the errors in 2-point function data and fits using Eq. (1) with two very different estimates of the first excited-state mass. The two fits (actually a whole region of parameter space) give different ground state mass aM_0 and amplitude $|A_0|^2$ but are not distinguished on the basis of χ^2/dof. Figure 3 illustrates that different estimates of excited-state mass give significantly different g_A, and this difference grows as $M_\pi \to 135$ MeV.

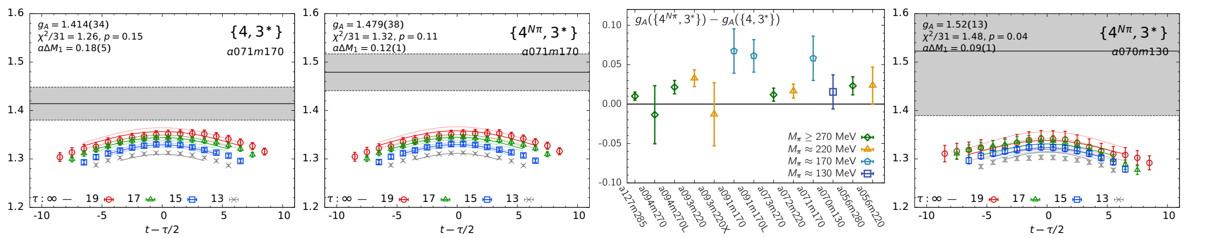

FIG. 3: The 2 left panels illustrate that $\{4,3^*\}$ versus $\{4^{N\pi},3^*\}$ fits to remove ESC give significantly different values for g_A. Panel 3 shows the systematic difference, $g_A(\{4^{N\pi},3^*\}) - g_A(\{4,3^*\})$, increases as $M_\pi \to 135$ MeV, except for $a070m130$, which surprisingly has almost the same $a\Delta M_1$ for the two strategies as shown in Fig.2. (This behavior to be confirmed by $a055m135$ calculation.) The need for higher statistics in this crucial physical pion mass ensemble for reliable excited-state fits is evident from the right panel.

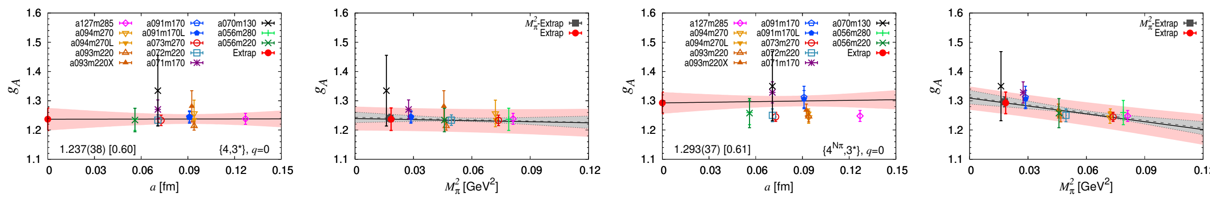

FIG. 4: Simultaneous CCFV fit to g_A from 13 ensembles with $\{4,3^*\}$ (left 2 panels) and $\{4^{N\pi},3^*\}$ (right 2 panels) strategies. The red star gives the physical result at $\{a = 0,\ M_\pi = 135, M_\pi L = \infty\}$ MeV. The main difference is in the slope versus M_π^2, which is larger for $\{4^{N\pi},3^*\}$, a consequence of smaller $a\Delta M_1$ in ESC fits. Our final CCFV analysis will also include the dependence on M_K, i.e., the strange quark mass.

Figure 4 shows the simultaneous CCFV fit to the axial charge g_A from the 13 ensembles. The main difference between the data with $\{4,3^*\}$ and $\{4^{N\pi},3^*\}$ strategies translates into different slopes with respect to M_π^2, and consequently a different final value. At present, our results for the nucleon charges, obtained using the clover-on-HISQ formulation and similar lattice methodology, dominate the averages in the 2019 and 2021 FLAG reports [1, 2], and we anticipate a similar impact in the FLAG Review 2023 from the ongoing clover-on-clover analysis.

Current data for the electric and magnetic form factors from 13 ensembles continue to agree with the Kelly parameterization of the experimental data and show no significant variation with a or M_π. In contrast to the axial channel, fits to get the ground state matrix elements in the vector channel are not sensitive to the excited-state mass gaps, and $\{4^{N\pi},2^{\rm sim}\}$ and $\{4,3^*\}$ strategies give consistent results [3]. We stress that this favorable behavior of electric and magnetic form factors observed in Ref. [3] persists under increases in statistics and the addition of 6 ensembles.

Figure 6 shows the axial form factors extracted with excited-state strategies $\{4,3^*\}$ (left) and $\{4^{N\pi},2^{\rm sim}\}$ (second) that are defined in Ref. [3] along with the test of how well the PCAC relation is satisfied. These data underscore the need to increase the statistics on the $a071m130$ ensemble.

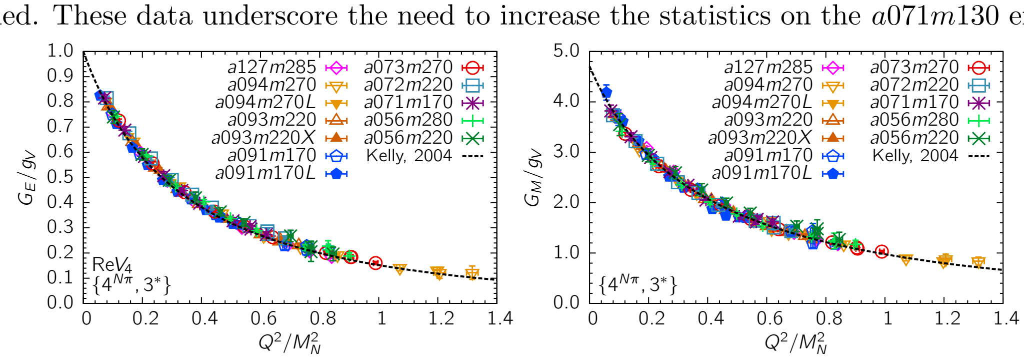

FIG. 5: Form factors $G_E(Q^2)$ (left) and $G_M(Q^2)$ (right) obtained with strategy $\{4^{N\pi},3^*\}$ continue to agree with Kelly parameterization of the experimental data and show no significant variation with a or M_π.

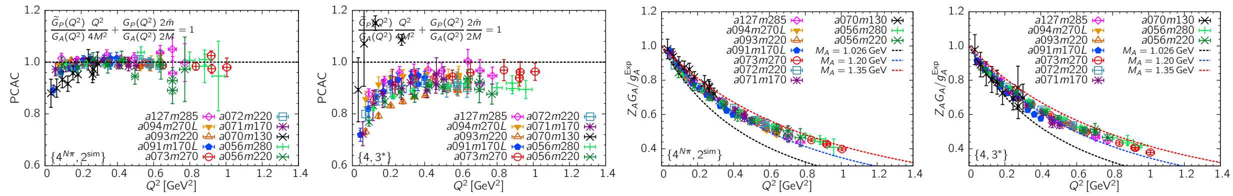

FIG. 6: The form factors $G_A(Q^2)$, $\widetilde{G}_P(Q^2)$, $G_P(Q^2)$ from strategy $\{4^{N\pi}, 3^*\}$ (left) much better satisfy the PCAC relation (result should be unity) than $\{4, 3^*\}$ (right). The axial form factors, $G_A(Q^2)$, from these two strategies are shown in the right two panels. The dipole ansatz (shown by the three curves with axial mass $M_A = 1.026$, 1.20, and 1.35 GeV drawn to guide the eye) does not describe the data. The statistics on the $a070m130$ ensemble are being increased.

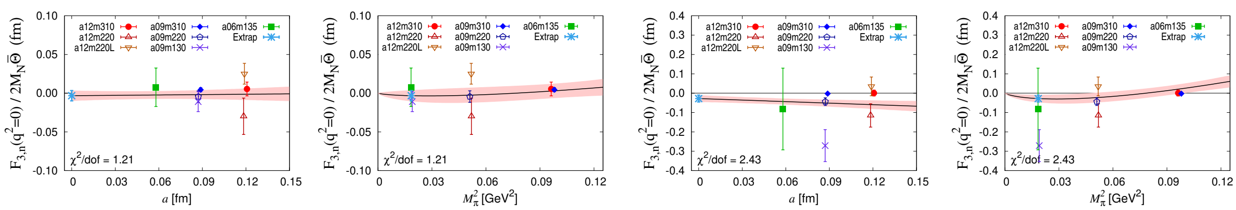

FIG. 7: Simultaneous chiral-continuum fit to $d_n = F_3^\Theta/2M_N$ plotted versus a and M_π^2 without (left 2 panels) and with (right 2) inclusion of $N\pi$ state in removing ESC. This clover-on-HISQ formulation data are reproduced from Ref. [7]. The continuum limit value is marked with a blue star.

Results for the Θ-term contribution to nEDM from the non-unitary clover-on-HISQ formulation have been presented in Ref. [7]. A χPT analysis showed that the contribution of $N\pi$ state can be significant. The resulting chiral-continuum extrapolation of $F_3^\Theta/2M_N\tilde{\Theta}$ without and with the $N\pi$ state is reproduced in Fig. 7. Overall, the statistical errors are large and the continuum value depends strongly on the strategy for removing ESC. The ongoing unitary Clover-on-Clover calculation with higher statistics (preliminary Figs. 8 and 9) will play a crucial role in clarifying the dependencies observed in the Clover-on-HISQ calculation, and possibly a robust result.

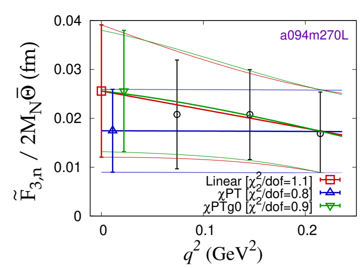

FIG. 8: The CP violating F_3 form factor induced by the QCD θ-term calculated on the $a094m270L$ ensemble and its extrapolation in Q^2.

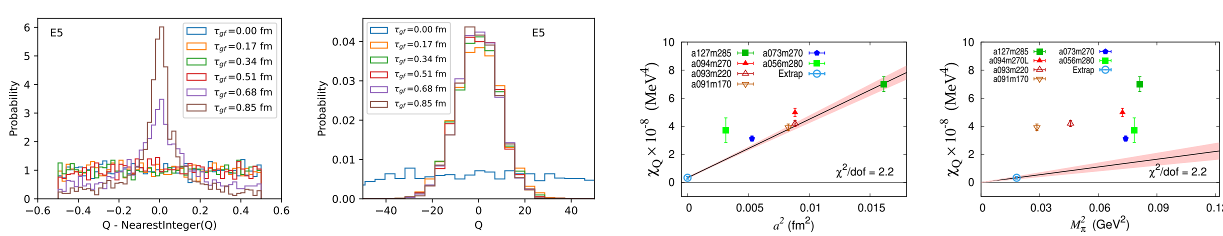

FIG. 9: (Left two) The distribution of the difference between the topological charge Q and its nearest integer, and the distribution of Q for different gradient flowtimes $\tau_{\rm gf}$ on the $a073m270$ ensemble. They show that Q takes a long flowtime ($\tau_{\rm gf} \gtrsim 0.7$ fm) to converge to an integer, but the distribution of Q converges at short flowtime. (Right two) Fits to the data for the topological susceptibility χ_Q. Our preliminary result of $\chi_Q = [76(5)\ {\rm MeV}]^4$ is consistent with our previous results $\chi_Q = [66(9)(4)\ {\rm MeV}]^4$ obtained using Clover-on-HISQ formulation [7]. In this project, we will increase the statistics by a factor of 2 and analyze smaller pion mass ensembles at $a \approx 0.07$ and 0.056 fm to significantly improve the precision.

VIII Software Development, Code Performance and Computational Readiness

The proposed work has two components: (i) to generate $O(1000)$ configurations separated by 4 molecular dynamics trajectories for the ensembles $a055m170$ and $a055m135$ described in Table I and (ii) to measure the correlations functions on these lattices needed to extract various physics results. The first part is sequential while the second part, once configurations exist, consists of independent simulations constituting statistics, and can be bundled together to run on large number of nodes. Leadership-class resources are required for both because of the large integrated flop count.

Our computations use the *Chroma* [53] code, which has been widely used for lattice gauge calculations in nuclear physics. *Chroma* GPU support is built over *QDP-JIT* originally described in Ref. [54], but which has since been further developed to generate GPU kernels using the LLVM compiler framework [55] at run-time in a just-in-time fashion, using the expression template mechanisms of the domain-specific data-parallel framework known as QDP++ (QCD Data Parallel in C++) developed under the DOE SciDAC program. NVIDIA GPUs are supported via the NVPTX back-end of LLVM, while for AMD GPUs the AMDGCN back-end is used to generate code objects which then need to be dynamically loaded. An Intel GPU implementation based on utilizing the Khronos SPIR-V standardized intermediate representation and the Intel oneAPI Level-Zero is underway. QDP-JIT also implements a data cache allocated on the GPUs and moved to the CPU via a-least-recently-used algorithm if the cache becomes full or when required for communications and I/O. Finally, the framework implements auto-tuning of the generated kernels, for optimized performance on the GPUs. The porting of QDP-JIT to AMD and Intel GPUs was carried out under the Exascale Computing Project (ECP).

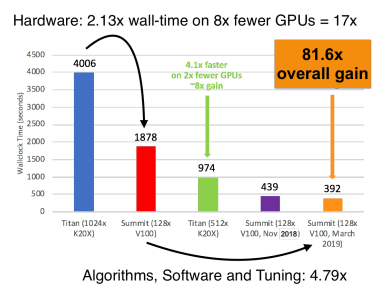

FIG. 10: Impact of algorithmic and architecture improvements on a benchmark gauge generation on moving from Titan to Summit.

Chroma and QDP-JIT interface with the QUDA library [56–58], maintained by NVIDIA, and which implements a variety of Krylov subspace solvers such as the Conjugate Gradients (CG) [59], the Stabilized Bi-Conjugate Gradients (BiCGStab) [60] algorithms and most importantly for our purposes, an implementation of the Generalized Conjugate Residuals (GCR) [61] with a mulltigrid preconditioner. The variant of multi-grid used is based on adaptive smoothed aggregation [62] and adaptations to the Wilson-Clover formulation of Lattice QCD are described in [63–66]. The ≈ 10X speedup of multigrid over traditional multi-precision BiCGStab is documented in the Figs 10 and 11. The QUDA Library has been considerably refactored over the last few years under ECP and now also supports AMD GPUs via a HIP Back-end, with a port to Intel GPUs being in an advanced state. The combination of QDP-JIT and QUDA allows for a complete port of Chroma to Frontier and has enabled the results shown in Fig.11.

The lattice generation code uses the hybrid Monte Carlo Algorithm (HMC). It is optimized for Summit (and Crusher=Frontier) with key contributions by Kate Clark (NVIDIA), Bálint Jóo, Frank Winter and Boram Yoon, and has been used to generate all the ensembles listed in Table I. The setup of the Chroma code, QDP-JIT, and the QUDA library with a multiple step-size force-gradient integrator has been employed on Summit for lattice generation for the last three years.

Strong-scaling studies used to determine the sweet spots on Crusher (Frontier) is shown in Fig. 11 (right) for $64^3\times128$, $72^3\times192$ and $96^3\times192$ lattice volumes. Analogous to Summit, in each case the most efficient (cost in node hours) is with the least number of nodes, which is used to get the cost estimates given in Table III. Bundling multiple streams of a given ensemble generation to utilize more nodes at a given time was found to be inefficient for two reasons. The time for a given trajectory has up to 10% variation, which results in some of the processors idling. Second, if one stream crashes, then either all do or the job does not release the nodes cleanly and resources are wasted.

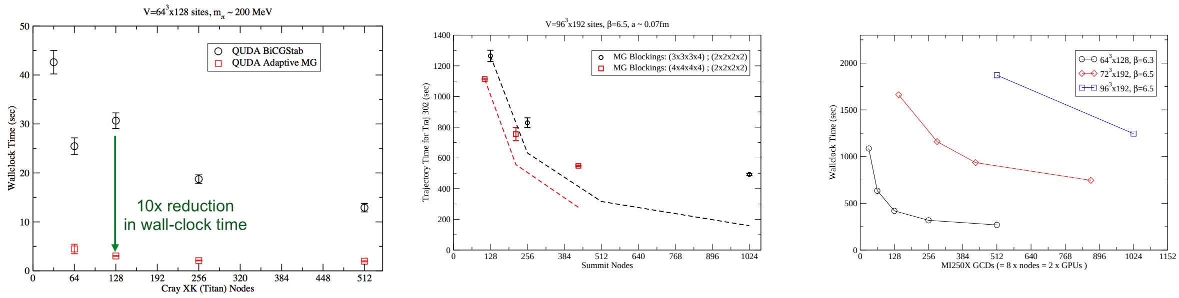

FIG. 11: (Left) Speed up from Algebraic MultiGrid over traditional multi-precision BiCGStab in the QUDA library, as a function of the quark mass for Clover Fermions on a lattice with $64^3 \times 128$ sites (data from [67] replotted). (Center) Strong-scaling performance of $96^3 \times 192$ lattice generation on Summit, using two multi-grid-blocking schemes. Blockings with power-of-2 block sizes are shown in red, and Blockings on power of 2 nodes (with factors of 3 in the blocking) are shown in black. (Right) Chroma strong-scaling performance for $96^3 \times 192$, $72^3 \times 192$ and $96^3 \times 192$ lattices on Crusher.

Based on the very good throughput on Summit, we have run each stream independently in auto-resubmit jobs of 2–12 hour duration, each generating 6–22 trajectories, with daily integrity checks.

In our HMC simulations, the Multi-Grid solver runs at a performance of of 428 GFLOPS/GPU–502 GFLOPS/GPU (2.57 TFLOPS–3.01 TFLOPS per node) on $96^3 \times 192$ sites on 648 GPUs/108 Summit nodes. In absolute terms, the solver on the large runs sustain over 267–313 TFLOPS on 108 nodes depending on the quark masses used. Our trajectory times range between roughly 800 sec on the smaller volumes to around 1250 sec on the largest volumes. These numbers include a $\approx 15\%$ improvement gained from a combination of optimizations of QDP-JIT software by our team member Frank Winter, and to the QUDA library implemented by our colleague Kate Clark. On Crusher we have seen absolute performances of 300 TFLOPS in our Multigrid solver on 64 nodes, or about 4.7 TFLOPS per node on a lattice with volume $96^3 \times 192$. In an initial attempt at a lattice with $128^3 \times 256$ sites we have sustained 500–700 TFLOPS on 128 nodes. Our comparison of timings and node counts indicates that on Crusher, we have already achieved ≈ 1.7 reduction in node-hours per trajectory compared to Summit. A very significant effort driven by Frank Winter is being devoted to optimizing the measurements code, especially on the GPUs, for the various components (source smearing, propagator inversion, contractions) described in the original proposal.

Measurement Optimizations Done: The latest version of QDP-JIT, having made the move to utilizing LLVM v12, features several new code optimizations. The GPU kernel launcher code has been restructured and modified to remove the CUDA/HIP context synchronization points after each kernel launch completely. We eliminated frequent small memory allocations and associated memory copies in expressions involving small scalars. Expressions requiring data access to neighboring compute nodes have been improved by removing not required conditional statements based on the virtual node geometry. We removed the auto-tuning facility for pure streaming kernels as these perform best at a certain block size set by the GPU architecture. Expressions which include multiplication with Dirac gamma matrices use an optimized code which implements sparse matrix multiplication. We changed the memory management of small scalars such that the global reductions across sets have a faster implementation. A cosmetic change we adopted was the introduction of helper objects for building JIT functions which mimic high level language constructs such as: 'if', 'for', and 'switch'. With these optimizations we see a 40% time reduction on hadron spectrum calculation, and about 10–15% reduction in three-point (building block) and sequential source parts. The overall performance improvement of the full measurement code is roughly 2X.

Optimizations under development: We continue to work on reducing the stack consumption of kernels for baryon contractions. Currently the kernels are built by unrolling the site-level operations all the way to the virtual register level of LLVM IR. In case of contracting propagators for baryon correlation functions this results in very long program code which the LLVM backend lowers to the target architecture by allocating big stack areas for register spilling. As a result the JIT compilation step also represents a significant time overhead. Our proposed way to alleviate these short comings is to install loops into kernels working with propagators—these have been identified to cause high stack usage and compile time. We already have a proof-of-concept and are ironing out the last bugs. The advantage of these changes are that the time overhead cause by JIT compilation of these large baryon functions will be significantly reduced and the stack usage of these kernels will be dramatically reduced—currently we leave around 4GB of GPU memory free for kernels' local memory. On the other hand, the runtime of the baryon kernels might be slightly increased.

The calculations are organized to minimize I/O cost in both generation and measurement. In both cases, only a gauge configuration is read in and the output is the next configuration in generation, and the correlation functions in the measurement part. Each job requires 25–50 minutes of wall clock time, so no checkpoint is done. This strategy has been validated by runs over the last 3 years. No propagators are written out as the I/O and storage overhead is large.

The long-term storage cost is only for the gauge configurations of size $576 \times L^3 \times T$ bytes that are archived in HPSS. Each $96^3 \times 192$ ($128^3 \times 256$) lattice is about one (3.2) TB. The correlation functions are about 50GB per configuration. Thus, the storage requirement of 4PB will grow over the two years as statistics are accumulated. We plan to develop a long-term archive of all the gauge configurations as a publicly available resource for the US lattice community. The correlation functions will be stored for 1–2 years after the duration of the award to finish a comprehensive analysis.

IX Proposed Work and Breakup of Resources Requested for 2023-24

As of June 15, 2022, the project has used 53% of the allocation of 440K Summit node hours for year 2022. Our goal for 2022 is to finish the analysis of isovector quantities, the Θ-term and the Weinberg operator on at least 2000 configurations on each of the 13 ensemble listed in Table I. The calculation of disconnected contributions will also continue opportunistically. The work proposed for 2023–24 is to generate and analyze 1000 configurations on the two $a055m170$ and $a055m135$ ensembles. All the code optimization for simulating $128^3 \times 256$ $a055m135$ lattices has been completed and tested as part of the thermalization process. We propose to generate and analyze the $96^3 \times 192$ $a055m170$ lattices on Summit and the $128^3 \times 256$ $a055m135$ lattices on Frontier.

Estimates of resources required are listed in Table III, and have been derived from current production runs on Summit and timing estimates on Crusher (Frontier). The cost of generation and analysis of each $a055m170$ configuration (separated by 4 trajectories) is 162 and 245 Summit node hours. The cost of generation and analysis of each $a055m135$ configuration (again separated by 4 trajectories) is 400 and 610 Frontier node hours. We propose to make 96 measurements on each lattice from randomly selected source points to increase statistics while keeping auto-correlations small. Our total request (rounded up) therefore is 205K Summit node hours and 505K Frontier node hours for each of the two years 2023 and 2024.

Ensemble	Volume	Lattices *Gen+* Analysis	Generation/lattice		Measurements/lattice		Node hours for 1000 lattices
			Sweet Spot # Nodes	Cost Node-hrs	Source-sink separations τ	Cost Node-hrs	
$a055m170$	$96^3 \times 192$	1000	108	162	5	245	407K Summit
$a055m135$	$128^3 \times 256$	1000	192	400	5	610	1010K Frontier

TABLE III: Cost estimates in Summit (Frontier) node hours for lattice generation and analysis of $a055m170$ ($a055m135$) ensembles. We propose to generate and analyze 1000 lattices on each ensemble. The number of nodes used and cost estimates are given in columns 4-7. The cost scales essentially linearly with the lattice volume with the multigrid inverter, ie, it is not sensitive to the pion mass or the lattice spacing. These lattices are separated by 4 molecular dynamics accept/reject trajectories with 92–94% acceptance rate.

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XI PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

The team has a well-established history of working together on lattice QCD projects and represents a balance between experts in lattice QCD (Tanmoy Bhattacharya, Rajan Gupta, Huey-Wen Lin), code development on latest HPC, in particular Summit (Balint Joo, Frank Winter, Boram Yoon), and phenomenology (Vincenzo Cirigliano, Emanuele Meregetti), with most member's interests spanning all three areas. They will work with and continue to mentor the four postdocs and graduate students at MSU.

Rajan Gupta (PI) has lead the Lattice QCD effort at Los Alamos since 1985, has performed pioneering calculations, and contributed to the development of high performance computing. He will be responsible for the overall management of the project and mentoring of the postdocs.

Tanmoy Bhattacharya (Co-PI) and **Huey-Wen Lin** are experts in lattice QCD and have made a number of contributions to lattice QCD, in particular to nucleon matrix elements, and to high performance computing. They will mentor the postdocs on the physics and data analysis.

Vincenzo Cirigliano (Co-PI) and **Emanuele Meregetti** are experts in effective field theory methods including chiral perturbation theory, low-energy probes of physics beyond the Standard Model, and their connection with the physics of the Early Universe, including baryogenesis mechanisms. They will lead the phenomenology effort.

Balint Joo, **Frank Winter** and **Boram Yoon** are computational scientists with many contributions to lattice QCD. Joo is the co-developer of the CHROMA software suite, and instrumental in developing and optimizing the lattice generation code and multi-grid inverter on Summit, Frontier and Perlmutter. Yoon is an expert in parallel computing and analysis of CP violation in neutron electric dipole moment. He will be responsible for cross-checking all calculations and analysis codes. Winter is an expert in the optimization of codes on GPUs. He is the author and maintainer of QDP-JIT/LLVM.

Postdocs: (i) Yong-Chull Jang is currently a postdoc at Columbia University and working on this project at 20%. **(ii) Santanu Mondal** is currently in India on paternity leave but continuing to work on this project. **(iii) Sungwoo Park** is a postdoc at JLAB and working at 25–50%. **(iv) Jun-sik Yoo** joined LANL as a postdoc in May 2022. They are responsible for the simulations, analysis, code optimizations and data management.

A MANAGEMENT PLAN

The PI, Rajan Gupta, will be the PoC. The two Co-PIs, T. Bhattacharya and Vincezo Cirigliano, will serve as backups. Together, they will be responsible for project execution and for providing updates on the status of the work including publications, awards, highlights and accomplishments.

We work closely together as a small tight knit team. Most members of the team participate in all aspects of the project and are expected to be able to do the full calculation on their own. Members at LANL discuss daily. The team gets together via teleconferencing four time a week during a dedicated hour to discuss the SIMULATIONS analysis and analytical calculations. Once COVID-19 travel restrictions are lifted, we will encourage and organize visits. The allocation of time, run priorities, simulation and analysis strategies are decided as a team. The junior members and postdocs are expected and encouraged to spend time pursuing independent ideas and directions. Senior members share in running, developing, debugging and optimization of the code.

The generation of the ensembles is costly and many different physics analyses beyond those proposed here can be performed. To facilitate these calculations, we have already made available 1000 configurations on each of the 13 ensembles through the USQCD Collaboration, and will open up the full set at the end of 2022. These lattices are stored in HPSS at OLCF and a long-term community archive is under discussion.

XII MILESTONES TABLE

Project Title: Precision calculations of matrix elements for Novel CP Violation Experiments

Year 1 (CY2023)		
Milestone	Details	Dates
(i) Start generation of $a055m135$ and $a055m135$ configurations (ii) Start measurements in Q2 (iii) Finish analysis of 13 ensembles and submit papers for publication (iv) Present preliminary results including the 2 new ensembles at Lattice 2023	Resource: Summit and Frontier Node-hrs: 205K (Summit) 505K (Frontier) Filesystem storage(TB & dates): 200 Archival storage: 250TB/Quarter Software Application: Chroma Tasks: Generation and Measurement Dependencies: None	Lattice generation will start in Q1 Generation and measurements continue throughout Q2, Q3, Q4 in 2023

Year 2 (CY2024)		
Milestone	Details	Dates
(i) Complete generation of 1000 configs for the two ensembles (rows 14-15 in Table I) (ii) Perform analysis of 1000 configurations on the 2 ensembles. (iii) Present preliminary results at Lattice 2024 (iv) Write papers based on all 15 ensembles	Resource: Summit and Frontier Node-hrs: 205K (Summit) 505K (Frontier) Filesystem storage(TB & dates): 200 Archival storage: 250TB/Quarter Software Application: Chroma Tasks: Generation and Measurement Dependencies: None	Lattice generation, measurements, and physics analysis will proceed throughout the year

TABLE IV: CY2023: Start generation of $a055m170$ and $a055m135$ ensembles immediately as optimized codes are ready and tested. Start measurements in Q2 while continuing generation. Complete writing papers based on 13 ensembles and present results at Lattice 2023 and other conferences. (Include $a055m170$ and $a055m135$ ensembles as a reliable statistics signal is obtained.) Archival storage will increase by about 250 TB per quarter to store generated lattices.
CY2024: Continue generation and measurements on the $a055m170$ and $a055m135$ ensembles. Present preliminary from 15 ensembles at Lattice 2024 and at other conferences. Present final results at the end of 2024.

XIII PUBLICATIONS RESULTING FROM INCITE AWARDS

The PI and the Co-PIs were part of the 2020 umbrella USQCD INCITE award to generate clover ensembles to generate the $a071m170$ and the $a056m270$ ensembles and to carry out measurements of correlations functions needed for the analyses of nucleon structure. The major progress has been made with the current two year INCITE award, 2021 and 2022. Over this time, we have five publications [3, 7, 8, 30, 68] on the various nucleon matrix elements discussed in this proposal:

1. "*Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD*," S. Park, et al, Phys. Rev. D 105, 054505 (2022)
2. "*Contribution of the QCD Θ-term to neutron electric dipole moment*," T. Bhattacharya, V. Cirigliano, R. Gupta, E. Mereghetti, and B. Yoon, Phys. Rev. D 103, 114507 (2021)
3. "*The pion-nucleon sigma term from lattice QCD*," NME Collaboration, R Gupta, S. Park, M. Hofericter, E. Mereghetti, B. Yoon, T. Bhattacharya, Phys. Rev. Lett. 127, 242002 (2021)
4. "*Nucleon Momentum Fraction, Helicity and Transversity from 2+1-flavor Lattice QCD*", S. Mondal, R. Gupta, S. Park, B. Yoon, T. Bhattacharya, B. Joó, F. Winter, JHEP 04, 44 (2021)
5. "*Moments of nucleon isovector structure functions in 2+1+1-flavor QCD*", S. Mondal, R. Gupta, S. Park, B. Yoon, T. Bhattacharya, H. Lin, Phys. Rev. D 102, 054512 (2020)

An equally important product of these INCITE awards is the library of ensembles specified in Table I. These are archived at OLCF and we have already made available 1000 configurations from each ensemble through USQCD in May 2022 and the rest will be made available at the end of 2022. We consider these ensembles as a long-term resource for the US lattice QCD community to facilitate calculations of many other quantities. This set of ensembles is large enough to facilitate simultaneous CCFV fits to get results at the physical point with quantified uncertainty in extrapolations in all three parameters, $\{M_\pi, a, M_\pi L\}$.

XIV Curriculum Vitae

Rajan Gupta

Laboratory Fellow, Nuclear and Particle Physics Cosmology and Astrophysics Group T-2
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545
e-mail: rajan@lanl.gov

Professional Preparation

Ph. D. in Theoretical Physics	1982	California Institute of Technology, Pasadena, USA
M. Sc. in Physics	1975	University of Delhi, Delhi, India

Appointments and Awards

2000–	Program Manager, High Energy Physics, Los Alamos National Laboratory
1988–	Staff Scientist, Theoretical Division, Los Alamos National Laboratory
2001–2008	Group Leader, T-8, Theoretical Division, Los Alamos National Laboratory
1991	Visiting Lecturer, California Institute of Technology, Pasadena, CA, USA
1985–1988	J. Robert Oppenheimer Fellow at Los Alamos National Laboratory, Los Alamos, New Mexico
1987	Guest Professor, University of Wuppertal, Germany
1983–1986	Honorary Post-doctoral fellow at Harvard University, Boston
1982–1985	Post-doctoral fellow at Northeastern University, Boston
2006	Elected Fellow, Los Alamos National Laboratory
1994	Elected Fellow, American Physical Society

Publications Most Relevant to This Proposal

($>$ 14500 *citations,* **H index=55** *(Google Scholar)*
4 Topcite 500+; 36 Topcite 100–499; 19 Topcite 50–99)

1. "Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD," S. Park, et al,
arXiv:2103.05599 [hep-lat]. To appear in PRD.
2. "Contribution of the QCD Θ-term to neutron electric dipole moment," T. Bhattacharya, V. Cirigliano, R. Gupta, E. Mereghetti, and B. Yoon, Physical Review D103:11 (2021) 114507.
3. "The pion-nucleon sigma term from lattice QCD" NME Collaboration, R Gupta, S Park, M. Hofericter, E. Mereghetti, B Yoon, T Bhattacharya *Phys. Rev. Lett.* **127** (2021), 242002.
4. "Nucleon electromagnetic form factors in the continuum limit from (2+ 1+ 1)-flavor lattice QCD," PNDME Collaboration,Yong-Chull Jang, Rajan Gupta, Huey-Wen Lin, Boram Yoon, Tanmoy Bhattacharya, *Phys. Rev.* **D101** (2020), 094512.
5. "Axial Vector Form Factors from Lattice QCD that Satisfy the PCAC Relation," PNDME Collaboration, Yong-Chull Jang, Rajan Gupta, Boram Yoon, Tanmoy Bhattacharya, *Phys. Rev. Lett.* **120** (2020) 072002
6. "Flavor diagonal tensor charges of the nucleon from from 2+1+1-flavor lattice QCD" PNDME Collaboration, R Gupta, B Yoon, T. Bhattacharya, V Cirigliano, Y-C Jang, H-W Lin, *Phys. Rev.* **D98** (2018), 034503

Research Interests and Expertise

My interests are to obtain phenomenologically relevant results for probing physics beyond the standard model using large scale simulations of lattice QCD, understanding QCD, elucidating the properties and interactions of hadrons and mesons, and to develop high-performance computing.

Synergistic Activities

NSF; HEP Comparitive Review Panel; Reviewer for the NSF and DOE Proposals
Referee for *PRL*, *PRD*, *PLB*, *NPB*, *JHEP*
Divisional Associate Editor, Physical Review Letters, *Particles and Fields*, 2000-2002
Member, Local Organizing Committee, LATTICE 1998, 2000
Member, International Advisory Committee, LATTICE 1997, 1999, 2017, 2018
Organizer, *Santa Fe Workshops on topics in HEP*, 1993-1998, 2017, 2019
Scientific Director, Les Houches School, *Probing the standard model of particle interactions*, 1997.

Collaborators over the last 5 years

S. Aoki (Kyoto University, Japan), Y. Aoki (KEK, Japan), D. Becirevic (University Paris-Sud, France), Tanmoy Bhattacharya (Los Alamos National Lab), T. Blum (University of Conneticut), Norman H. Christ (Columbia University), Vincenzo Cirigliano (Los Alamos National Lab), Saul Cohen(NVIDIA), G. Colangelo (University of Bern, Switzerland), Sara Collins (University of Regensburg), M. Della Morte (University of Southern Denmark), Carleton DeTar(University of Utah), William Detmold (M.I.T), P. Dimopoulos (Universita di Roma Tor Vergata), S. Durr (University of Wuppertal, Germany), Michael Engelhardt (New Mexico State University), H. Fukaya (Osaka University, Japan), Steven Gottlieb (Indiana University), M. Golterman (San Francisco State University), Jeremy Green(CERN, Switzerland), S. Hashimoto (KEK, Japan), U. M. Heller (American Physical Society (APS)), G. Herdoiza (Universidad Autonoma de Madrid, Spain), R. Horsley (University of Edinburg), Balint Joo (JLab), A. Juettner (University of Southhampton, UK), T. Kaneko (KEK, Japan), Andreas Kronfeld Fermilab), C.-J. D. Lin (National Chiao-Tung University, Taiwan), Keh-Fei Liu University of Kentucky), Weonjong Lee(Seoul National University, Korea), Huey-Wen Lin (Michigan State University), E. Lunghi (Indiana University), R. Mawhinney (Columbia University), Aaron Meyer (Brookhaven National Lab), John Negele (M.I.T), A. Nicholson (University of North Carolina), T. Onogi (Osaka University, Japan), C. Pena (Universidad Autonoma de Madrid, Spain), Andrew Pochinsky (M.I.T), A. Portelli (University of Edinburg), Kostas Orginos (College of William and Mary), Gabriel Perdue (Fermilab), A. Ramos (Trinity College Dublin, Ireland) David Richards (JLab), Alessandro Roggero (University of Washington), Andreas Schaefer (University of Regensburg), Stephen Sharpe (University of Washington), J. N. Simone (Fermilab), S. Simula (INFN, Sezione di Roma Tre, Italy), R. Sommer (DESY, Zeuthen, Germany), Raza Sufian (JLab), Sergey Syritsen (University of Stonybrook), R. Van De Water (Fermilab), A. Vladikas (Universita di Roma Tor Vergata, Rome), M. Wagner (Indiana University), U. Wenger (University of Bern, Switzerland), Frank Winter (JLab), H. Wittig (University of Mainz, Germany), Hantao Yin (Columbia University), Boram Yoon (Los Alamos National Lab)

Thesis Advisor:

Geoffrey Fox: Currently at the University of Virginia

Post-docs Mentored

David Daniel (1990-1993, LANL), Tanmoy Bhattacharya (1992-1995, LANL), Jeffrey Grandy (1992-1994, LLNL), Shailesh Chandrasekharan (1997-1998, Duke University), Weonjong Lee (1997-2002, Seoul National University, South Korea), Anosh Joseph (2011-2013, IISER, Mohali, India), Huey-Wen Lin (2010-2016, Michigan State University), Saul Cohen (2010-2014, NVIDIA), Boram Yoon (2013-2016, LANL), Yong-Chull Jang (2016-2017, Columbia University), Sungwoo Park (2018–2021, JLab), Shantanu Mondal (2019–2021, MSU), Jun-sik Yoo (2022–)

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Professional Preparation

1989 Ph.D. in Physics, Tata Institute of Fundamental Research, Bombay, India
1984 M.Sc. in Physics, IIT, Kharagpur, India
1982 B.Sc. in Physics, IIT, Kharagpur, India

Appointments

2006–present Professor at Santa Fe Institute
1995–present Scientist at Los Alamos National Laboratory
1992–1995 Post-doctoral Researcher at Los Alamos National Laboratory
1991–1992 Post-doctoral fellow at Centre de Energie Atomique, Saclay
1989–1991 Post-doctoral fellow at Brookhaven National Laboratory

Publications Most Relevant to This Proposal

1. "Precision Nucleon Charges and Form Factors Using (2+1)-flavor Lattice QCD," S. Park, R. Gupta, B. Yoon, S. Mondal, T. Bhattacharya, Y.-C. Jang, B. Joó, and F. Winter (NME Collaboration), arXiv:2103.05599 [hep-lat], Physical Review D105:05 (2022) 054505.
2. "Pion-nucleon sigma term from lattice QCD," R. Gupta, S. Park, M. Hoferichter, E. Mereghetti, B. Yoon, and T. Bhattacharya, arXiv:2105.12095 [hep-lat], Physical Review Letters 127:24 (2021) 242002.
3. "Contribution of the QCD Θ-term to neutron electric dipole moment," T. Bhattacharya, V. Cirigliano, R. Gupta, E. Mereghetti, and B. Yoon, arXiv:2101.07230 [hep-lat], Physical Review D103:11 (2021) 114507.
4. "Axial Vector Form Factors from Lattice QCD that satisfy PCAC Relation," Y.-C. Jang, R. Gupta, B. Yoon, and T. Bhattacharya, PRL124:07 (2019) 072002.
5. "Nucleon Electromagnetic Form Factors in the Continuum Limit from (2+1+1)-flavor Lattice QCD," Y.-C. Jang, R. Gupta, H.-W. Lin, B. Yoon, and T. Bhattacharya (PNDME Collaboration), PRD101:01 (2020) 014507.
6. "Axial-vector Form Factors of the Nucleon from Lattice QCD," R. Gupta, Y.-C. Jang, H.-W. Lin, B. Yoon, and T. Bhattacharya (PNDME Collaboration), PRD96:11 (2017) 114503.
7. "Neutron Electric Dipole Moment and Tensor Charges from Lattice QCD," T. Bhattacharya, V. Cirigliano, R. Gupta, H.-W. Lin, and B. Yoon (PNDME Collaboration), PRL115:21 (2015) 212002.
8. "Controlling Excited State Contamination in Nucleon Matrix Elements," B. Yoon, R. Gupta, T. Bhattacharya, M. Engelhardt, J. Green, B. Joó, H.-W. Lin, J. Negele, K. Orginos, A. Pochinsky, D. Richards, S. Syritsyn, and F. Winter (NME Collaboration), PRD93:11 (2016) 114506

Research Interests and Expertise

My relevant research interests and expertise are in Lattice Field Theories and high-performance computing. I have been working on these topics for about 30 years. For the last 9 years, I am investigating baryonic matrix elements, especially those allowing low-energy experiments to bound or constrain theories beyond the standard model.

Synergistic Activities

1. Chair of the Scientific Program Committee for USQCD.

2. Serve as moderator for the hep-lat category on the arXiv.
3. Served on review teams for US DOE and NSF, HEP and CompPhys.
4. Peer reviewed for over 30 journals.
5. Co-organizer of various meetings.

Collaborators (*past 5 years*) W.P. Abfalterer[0], J.C. Abundo[1], S.M. Alam[2], H.J. Alter[3], J.P. Arche[4], G. Arya[5], G. Athreya[6], R.T. Bailer[3], J.A. Bailey[7], K.J. Bar[8], D.H. Barouch[9], J.D. Barry[10], M. Bayne[9], A. Bazavov[11], E. Begoli[12], A. Berea[13], R.J.O. Barnard[14], D. H. Barouch[9], M. Bayne[9], M. Berrong[2], J. Bilmes[15], L.M. Blair[16], D.E. Blasi[17], R.A. Blythe[18], J. Bono[19], M. Bonsignori[2], S. Branford[20], T. Brettin[21], M.I. Buchoff[22], D.R. Burton[23], M.P. Busch[24], F. Cai[2], B.J. Callahan[25], O. Carja[26], Y. Chen[27], M. Cheng[22], G. Chennupati[0], L.Y. Chew[1], N.H. Christ[28], B. Christian[12], N.N. Chung[1], Y.-S. Chung[29], V. Cirigliano[0], M.S. Cohen[30], S.D. Cohen[15], M.P. Cox[31], W. Croft[33], L. Cuellar-Hengartner[0], M. Cysouw[34], Z. Davousi[13], C. DeTar[35], H.-T. Ding[36], W. Ding[8], J.H. Doroshow[37], S.S. Downey[38], M. Engelhardt[39], C.M. Evans[80], Y. Evrard[40], G. Ferrari[2], D.S. Fierer[41], W.M. Fischer[0], B.T. Foley[0], L. Fortunato[42], T.M. Freeman[79], H. Gaffer[43], V.V. Ganusov[44], F. Gao[2], H. Gao[2], J. Garrity[9], A.R. Geonnotti[2], E.E. Giorgi[0], S. Gnanakaran[0], M.G. Gonzalez[27], N. Goonetilleke[30], S. Gottlieb[45], J. Grana[46], J. Green[47], K.M. Greene[2], E.J. Greenspan[37], S. Grigoryev[48], A.L. Gryshuk[22], E.G. Guillot[49], R. Gupta[0], P. Hägler[50], B.H. Hahn[8], L. Harris[51], K.M. Hastie[78], B.F. Haynes[2], P. Hegde[36], U.M. Heller[52], N. Hegartner[0], T.T. Hoang[53], B. Hora[2], P.T. Hraber[0], D.J. Hruschka[54], S. Imari-Walker[54], T. Izubuchi[55], S.S. Iyer[8], G.S. Jacobs[1], Y.-C. Jang[55], H. Jeong[7], C. Jiang[56], B. Joó[57], M. John[58], A. Joseph[59], C. Jung[55], A. Kandler[60], J. Kappes[27], S.A. Karim[61], F. Karsch[55], R. Ke[0], B.F. Keele[8], E.-Y. Kim[29], J.H. Kim[62], A. Kolchinsky[46], W. Kong[56], R. Kong[3], B.T.M. Korber[0], D. Kusnezov[53], C.C. LaBranche[2], J.S. Lansing[1], W. Lee[7], J.-H. Leem[7], H. Li[8], X. Li[2], H.-Y. Lin[63], D. Liu[2], M.K.P. Liu[64], M.K. Louder[3], J. Mackory[65], C. Mathis[54], I. Maddieson[33], I. Maliijkovic Berry[29], J.R. Mascoal[3], C. McDanal[2], A.J. McMichael[64], S.E. Michalak[0], J. Mohd-Yusof[0], S. Mondal[0], D.C. Montefiori[2], A Moon-Walker[78], C. Moore[46], L. Morris[61], L. Müller[66]; B.U. Munsch[50], J.W. Negele[67], D. Nisley[3], M.C. Nussenzweig[68], C. Ochsenbauer[27], K. Orginos[57], S. Park[0], M.D. Parker[79], D.G. Partridge[80], L. Pennberthy[37], A.S. Perelson[0], L.G. Perez[2], A.V. Pochinsky[67], J. Qiu[12], C. Rademeyer[69], N. Retzlaff[70], R.M. Ribeiro[0], D. Richards[57], M. Rist[9], A. Robles[9], E. Romero-Severson[0], J.F. Salazar-Gonzalez[27], E.O. Saphire[78], A. Schäfer[50], M. S. Seaman[9], P. Shanahan[67], G.M. Shaw[8], E. Smith[71], H. Song[81], P.F. Stadler[66], E. Stahlberg[37], G. Starostin[72], D. A. Steck[65], R. Stevens[21], T.I. de Silva[80], F. Streitz[22], H. Sudoyo[73], L. Sutton[33], S.N. Syritsyn[74], H. Tang[2], J.P. Theiler[0], S. Thulasisasan[0], S. Thurner[1], G. Tourassi[12], C.B. Vea Lauzon[53], M. Wagman[67], S.I. Walker[54], T.C. Wallstrom[0], C. Wang[2], S. Wang[8], S.P. Whelan[15], D. Wolpert[46], J.G. Wilkins[75], C. Williamson[69], F. Winter[57], X.-C. Wu[76], F. Xia[21], B. Yoon[0], H. Yoon[0], H. Youn[29], X. Yu[56], G. Zaki[40], T. Zuo[2]

Graduate and Postdoctoral Advisors and Advisees: Graduate Advisor: P. Roy[77]; Postdoctoral Advisors: W. Marciano[55], A. Morel*, R. Gupta[0]; Postdoctoral Advisee: A. Chamblin*, U. Smith†, B. Yoon[0], E. Mereghetti[0], Y.C. Jang[55], S. Park[0], S. Mondal[0], L. Fortunato[42], A. Kandler[70]; Interns, Summer Students and REUs: L. Blair[16], M. Odigi[3], O. Carja[26], R. Elliott Smith[5], C. Williams[0]

[0]LANL, [1]Nanyang Technological University, [2]Duke University, [3]NIH, [4]University of Manchester, [5]UCSD, [6]Kuali Foundation, [7]Seoul National University, [8]U. Penn, [9]Beth Israel, [10]University of Glasgow, [11]University of Iowa, [12]ORNL, [13]University of Maryland, [14]Merck & Co, [15]University of Washington, [16]Karius Inc, [17]Universität Zürich, [18]University of Edinburgh, [19]American University, [20]University of Reading, [21]ANL, [22]LLNL, [23]Scripps, [24]UCSF, [25]Stanford University, [26]Carnegie Mellon, [27]University of Alabama, [28]Colombia University, [29]Northwestern, [30]UNC, [31]Massey University, [33]University of New Mexico, [34]University of Marburg, [35]University of Utah, [36]Central China Normal University, [37]NCI, [38]OSU, [39]NMSU, [40]Frederick National Lab for Cancer Research, [41]Mt. Sinai, [42]Cambridge University, [43]Coldspring Harbor, [44]University of Tennessee, [45]Indiana University, [46]Santa Fe Institute, [47]University of Mainz, [48]Penn State University, [49]University of Lausanne, [50]University Regensburg, [51]Fred-Hutchinson, [52]APS, [53]DOE, [54]ASU, [55]BNL, [56]Jilin University, [57]JLab, [58]Murdoch University, [59]DESY, [60]University College, London, [61]University Kwazulu Natal, [62]Walter Reed, [63]MSU, [64]Oxford University, [65]University of Oregon, [66]University Leipzig, [67]MIT, [68]Rockefeller University, [69]University of Cape Town, [70]MPI, Leipzig, [71]Georgia Tech, [72]Russian State University for the Humanities Moscow, [73]University of Indonesia, [74]Stony Brook, [75]Ronin Institute, [76]LSU, [77]Bose Institute, [78]La Jolla Institute for Immunology, [79]University of Sheffield, [80]Sheffield Teaching Hospitals, [81]Institute of Human Virology, †self-employed, *expired.

Vincenzo Cirigliano

Institute for Nuclear Theory
University of Washington
Seattle, WA 98195 USA

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E-mail: cirigv@uw.edu

Professional Preparation

- Undergraduate: University of Pisa (Italy), Physics "Laurea" (M.S. equiv.), 1996
- Graduate: University of Pisa (Italy), Ph.D., 2000
- Postdoctoral: Institute for Theoretical Physics, University of Vienna, Austria (2000-2001); IFIC, University of Valencia, Spain (2001 - 2003); Sherman Fairchild Fellowship, California Institute of Technology (2003-2006).

Appointments

- 2022– present: Senior Fellow, Institute for Nuclear Theory, University of Washington.
- 2020–2022: Deputy Group Leader, T-2 (Nuclear and Particle Physics, Astrophysics, and Cosmology), Los Alamos National Laboratory.
- 2008–2020: Staff Scientist, Los Alamos National Laboratory.
- 2006–2008: Limited Term Staff Member, Los Alamos National Laboratory.

Five Publications Most Relevant to This Proposal

1. *New Leading Contribution to Neutrinoless Double-beta Decay*, V. Cirigliano, W. Dekens, J. De Vries, M. L. Graesser, E. Mereghetti, S. Pastore and U. Van Kolck, Phys. Rev. Lett. **120**, no. 20, 202001 (2018) [arXiv:1802.10097 [hep-ph]]
2. *Neutron Electric Dipole Moment and Tensor Charges from Lattice QCD*, T. Bhattacharya, V. Cirigliano, R. Gupta, H. W. Lin and B. Yoon, Phys. Rev. Lett. **115**, no. 21, 212002 (2015) [arXiv:1506.04196 [hep-lat]]
3. *Probing Novel Scalar and Tensor Interactions: from UCNs to the LHC*, T. Bhattacharya, V. Cirigliano, S. D. Cohen, A. Filipuzzi, M. Gonzalez-Alonso, M. L. Graesser, R. Gupta and H. -W. Lin, Phys. Rev. D **85** (2012) 054512, arXiv:1110.6448 [hep-ph]
4. *An Evaluation of $|V_{us}|$ and precise tests of the Standard Model from world data on leptonic and semileptonic kaon decays*, M. Antonelli, V. Cirigliano *et al.* [FlaviaNet Working Group on Kaon Decays], Eur. Phys. J. C **69**, 399-424 (2010), [arXiv:1005.2323 [hep-ph]]
5. *Two-loop effective theory analysis of $\pi(K) \to e\bar{\nu}[\gamma]$ branching ratios*, V Cirigliano and I. Rosell, Phys. Rev. Lett. **99** (2007) 231801, arXiv 0707.3439 [hep-ph]

Research Interests and Expertise

- Low energy probes of electroweak interactions and fundamental symmetries
- Effective field theories: from QCD to physics beyond the Standard Model
- Flavor physics in the quark and lepton sector
- Baryogenesis mechanisms and their experimental probes
- Neutrino physics and astrophysics

Selected Synergistic Activities

- Member, Nuclear Science Advisory Committee (2013-2016)
- Member, INT National Advisory Committee (2011-2014)
- Referee for European Physics Journal C, Journal of High Energy Physics, Physical Review D, Physical Review Letters, Physics Letters B, Reviews of Modern Physics
- Frontiers in Science Public Lecture (November 2013): Los Alamos, Albuquerque, Santa Fe, Taos. Title: *Matter versus antimatter: how did we survive the Big Bang?*
- Organizer, Institute for Nuclear Theory programs INT-08-3 *Low-energy electroweak precision physics in the LHC era* and INT-17-2a *Neutrinoless double beta decay* 2008

Collaborators

Collaborations in the past 60 months (22): T. Bhattacharya (LANL), J. Carlson (LANL), A. Celis (Munich), A. Crivellin (PSI), W. Dekens (UCSD), A. Falkowski (Paris), G. Fuller (UCSD), K. Fuyuto)LANL), S. Gandolfi (LANL), M. Gonzalez-Alonso (Lyon), M. Graesser (LANL), R. Gupta (LANL), M. Hoferichter (INT), U. van Kolck (Arizona), H. W. Lin (MSU), E. Mereghetti (LANL), E. Passemar (Indiana), S. Pastore (Washington U., St. Louis), F. Pederiva (Trento), M. J. Ramsey-Musolf (UMass Amherst), A. Rodriguez (Lund), S. Shalgar (Niels Bohr Institute), J. de Vries (UMass), R. Wiringa (ANL), B. Yoon (LANL),

Graduate Advisors and Postdoctoral Sponsors (6): G. Paffuti (University of Pisa) and John F. Donoghue (UMass Amherst), graduate advisors.
G. Ecker (University of Vienna), A. Pich (University of Valencia), M. J. Ramsey-Musolf (UMass Amherst), M. B. Wise (Caltech), postdoctoral sponsors.

Thesis Advisor and Postgraduate-Scholar Sponsor (12): Alejandro Celis, Alberto Filipuzzi, Martin Gonzalez-Alonso, Ignasi Rosell, Paula Tuzon, student advisees.
W. Dekens (LANL / NMC), M. Giannotti (Barry University), J. Jenkins (LANL), E. Mereghetti (LANL), G. Ovanesyan (UMass), E. Passemar (Indiana), R. Sharma (TIFR), postdoctoral advisees.

Emanuele Mereghetti

Theoretical Division, T-2, MS B283
Los Alamos National Laboratory
Los Alamos, NM 87545, USA

Phone: (505) 665-9850
E-mail: emereghetti@lanl.gov

Education and Training:

- Undergraduate: Università degli Studi di Milano, Physics, Bachelor of Science, 2005
- Graduate: University of Arizona, Physics, Ph.D., 2011
- Postdoctoral training: Lawrence Berkeley National Laboratory (LBNL), Physics, 2011
- Postdoctoral training: Los Alamos National Laboratory (LANL), Physics, 2014

Professional Experience:

- 9/2017–present: *Staff scientist* in the T2 group at Los Alamos National Laboratory.

Five Publications Most Relevant to This Proposal:

1. E. Mereghetti, C. Monahan, M. Rizik, A. Shindler, P. Stoffer, *"One-loop matching for quark dipole operators in a gradient flow scheme"* JHEP 04 (2022) 050.
2. R. Gupta, S. Park, M. Hoferichter, E. Mereghetti, B. Yoon, T. Bhattacharya, *"Pion-nucleon Sigma Term from Lattice QCD"*, Phys. Rev. Lett. 127 (2021) 24.
3. V. Cirigliano, E. Mereghetti, P. Stoffer, *"Non-perturbative renormalization scheme for the CP-odd three-gluon operator"*, JHEP 09 (2020) 094.
4. S. Alioli, V. Cirigliano, W. Dekens, J. de Vries, E. Mereghetti, "*Right-handed charged currents in the era of the Large Hadron Collider"*, JHEP 05 (2017) 086.
5. J. de Vries, E. Mereghetti, R. G. E. Timmermans, U. van Kolck *"The Effective Chiral Lagrangian from dimension-six parity and time-reversal violation"*, Annals Phys. 338 (2013) 50-96.

Research Interests and Expertise

- Low-energy probes of physics beyond the Standard Model,
- Standard Model Effective Field Theory and its application to collider processes,
- Hadronic and nuclear effective field theories
- Interface between lattice QCD and perturbative QCD

Synergistic Activities:

- member of the DOE topical collaboration "Nuclear Theory for Double Beta Decay and Fundamental Symmetries"
- Organizer of: INT Program "Beyond the Standard Model Physics with Nucleons and Nuclei", July 13 - August 7 2020, University of Washington, Seattle; ECT* Workshop "Progress and challenges in the theory of neutrinoless double beta decay", July 2019, "XII$^{\text{th}}$ Annual Workshop on Soft-Collinear Effective Theory", March 2015 Santa Fe.
- Convener of Section E "QCD and New Physics" of the XII$^{\text{th}}$, XIII$^{\text{th}}$ and XIV$^{\text{th}}$ Quark Confinement and the Hadron Spectrum conferences.
- Member of the DNP Program Committee, 2021-22
- Referee for Physical Review Letters, Physical Review C, Physical Review D, Physics Letters B, Nuclear Physics A, Journal of High Energy Physics

- Grant Reviewer for the DOE Office of Science, Nuclear Physics, the Natural Sciences and Engineering Research Council of Canada and the Dutch Research Council.

Collaborators and Co-Editors in the last 5 years:

Simone Alioli	Universitá degli Studi di Milano-Bicocca
Radja Boughezal	Argonne National Laboratory
David Brantley	Lawrence Livermore National Laboratory
Andreas Crivellin	Paul Scherrer Institut, Villigen
Wouter Dekens	University of California San Diego
Jordy de Vries	University of Massachussetts Amherst
Guo-Xiang Dong	Huzhou University, Huzhou
Christian Drischler	University of California Berkeley and Lawrence Berkeley National Laboratory
Evgeny Epelbaum	Ruhr Universität, Bochum
Michael Fickinger	private industry
Sean Fleming	University of Arizona, Tucson
Michael Girard	private industry
Luca Girlanda	Universita' del Salento, Lecce
Alex Gnech	Gran Sasso Science Institute, L'Aquila
Wick Haxton	University of California Berkeley and Lawrence Berkeley National Laboratory
Martin Hoferichter	Institute of Nuclear Physics, Seattle
Balint Joo	Thomas Jefferson National Accelerator Facility
Ekaterina Mastropas	College of William and Mary
Ken McElvain	University of California Berkeley and Lawrence Berkeley National Laboratory
Henry Monge-Camacho	University of North Carolina, Chapel Hill
Christopher Monahan	College of William and Mary
Amy Nicholson	University of North Carolina, Chapel Hill
Saori Pastore	Washington University, St. Louis
Frank Petriello	Northwestern University, Evanston
Maria Piarulli	Washington University, St. Louis
Lucas Platter	University of Tennessee, Knoxville
Matthew Rizik	Michigan State University
Matthias Schindler	University of South Carolina
Andrea Shindler	Michigan State University
Peter Stoffer	University of California San Diego
Brian Tiburzi	City College of New York
Ubirajara van Kolck	University of Arizona, Tucson and Institut de Physique Nucléaire, Orsay
Jared Vanasse	Fitchburg State University
Michele Viviani	Istituto Nazionale di Fisica Nucleare, Pisa
Pavlos Vranas	Lawrence Livermore National Laboratory
Andre Walker-Loud	Lawrence Berkeley National Laboratory
Xiao Bao Wang	Huzhou University, Huzhou
Robert Wiringa	Argonne National Laboratory
Zichao Yang	University of Tennessee, Knoxville
Guanghui Zhou	University of Massachussetts Amherst

Curriculum Vitae
BÁLINT JOÓ

Contact Information
Scientific Computing Group, IT Division phone: (757) 269-5339
Thomas Jefferson National Accelerator Facility
Newport News, VA 23606 email: bjoo@jlab.org, joobalint@gmail.com

Professional Preparation

Ph.D. Physics, Edinburgh University, 2000 (Advisors: Richard D. Kenway, Anthony D. Kennedy).

B. Sc. (Hons.) 1st class, Computer Science and Physics, Edinburgh University, 1996

Appointments

Staff Computer Scientist, Jefferson Lab, 2005-2020

Post Doctoral Research Associate, University of Edinburgh, 2002-2005

Post Doctoral Research Associate, University of Edinburgh (at Columbia University), 2000-2002

Post Doctoral Research Asssociate, University of Kentucky, 2000

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)

Professional Activities

SC'20 Program committee

Co-PI of SciDAC-4 Project: Computing the Properties of Matter with Leadership Computing Resources (2017-present)

Co-PI of NERSC NESAP-2 Lattice QCD Project for Perlmutter (2019-present)

PI of NERSC NESAP Chroma Project for Cori KNL (2014-2018)

Vice Chair of NERSC User Group Executive, 2019

Panel Member: OLCF-4 Acceptance Test Review, Dec 2018

Panel Member: NERSC-9 Technical Design Review, May, 2018

NERSC Summer Associate, July 2017

Panel Chair: ALCF Theta Acceptance Review, Sept. 2016

Panel Member: NERSC Operational Assessment Review, 2016

Panel Member: OLCF Operational Assessment Review, 2015

Reviewer for DOE/ASCR SciDAC 2017, 2016, 2014

Lecturer: INT Summer School on Lattice QCD for Nuclear Physics (INT-12-2b), 2012, Seattle, WA

Lecturer: INT Summer School on Lattice QCD and its Applications (INT-12-2b), 2007, Seattle, WA

Summer School Lecturer, HackLatt Sumer School (2008,2009,2012), Edinburgh

Co-designer of QCDOC supercomputer (2000-2002)

Invited Talks

APS April Meeting 2017, *Lattice Calculations of the Hadron Spectrum*, Washington D.C., 2017

APS April Meeting 2012, *Lattice QCD and Graphical Processing Units*, Atlanta, GA, Mar. 2012

The 29th International Symposium on Lattice Field Theory, Lattice 2011 Plenary Talk, *GPUs for the Lattice*, Squaw Valley, Lake Tahoe, CA, 2011

Selected Publications

1. Sungwoo Park, Rajan Gupta, Boram Yoon, Santanu Mondal, Tanmoy Bhattacharya, Yong-Chull Jang, Bálint Joó, Frank Winter, *Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD*, Phys. Rev. D105 (2022) 054505, arXiv:2103.05599
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 the International Conference for High Performance Computing, Networking, Storage and Analysis (SC '16), Article 68 (November, 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 (IPDPS'14), Phoenix, USA, May 19-23, 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, Seattle WA, Nov 12-18, 2011
6. R.G. Edwards, B. Joo, *The Chroma Software System for Lattice QCD*, Nucl. Phys. Proc. Suppl. 140:832 (2005)

Huey-Wen Lin

Department of Physics and Astronomy &
Computational Mathematics, Science and Engineering
Michigan State University
East Lansing, MI 48824

Phone: (517) 884-5594
E-mail: hwlin@pa.msu.edu

Education and Training:

- Undergraduate: National Taiwan University (Taipei, Taiwan), Bachelor in Physics
- Graduate: Columbia University (New York, NY), Ph.D. in Physics
- Postdoctoral training: Postdoctoral Fellow, Theory group, Thomas Jefferson National Accelerator Facility

Professional Experience:

- 2009–2014: *Research Assistant Professor*, Department of Physics, University of Washington.
- 2015–2016: *Visiting Assistant Professor*, Department of Physics, University of California, Berkeley
- 2016–2021: *Assistant Professor*, Department of Physics & Astrophysics and Computational Mathematics, Science and Engineering, Michigan State University
- 2021–present: *Associate Professor*, Department of Physics & Astrophysics and Computational Mathematics, Science and Engineering, Michigan State University

Five Publications Most Relevant to This Proposal:

1. T. Bhattacharya, V. Cirigliano, R. Gupta, H.-W. Lin, B. Yoon, *"Neutron Electric Dipole Moment and Tensor Charges from Lattice QCD"*, Phys. Rev. Lett. 115 (2015) 212002
2. H.-W. Lin, W. Melnitchouk, A. Prokudin, N. Sato, H. Shows, *"First Monte Carlo Global analysis of Nucleon Transversity with Lattice QCD Constraints"*, Phys. Rev. Lett. 120 (2018) 152502
3. Z. Fan, Y. Yang, A. Anthony, H.-W. Lin, K. Liu, *"Gluon Quasi-PDF from Lattice QCD"* , Phys. Rev. Lett. 121 (2018) 242001
4. H.-W. Lin, J. Chen, L. Jin, Y. Liu, Y. Yang, J. Zhang, Y. Zhao, *"Proton Isovector Helicity Distribution on the Lattice at Physical Pion Mass"*, Phys. Rev. Lett. 121 (2018) 242003
5. H.-W. Lin *"Nucleon Tomography and Generalized Parton Distribution at Physical Pion Mass from Lattice QCD"*, Phys. Rev. Lett. 127 (2021) 18, 182001

Research Interests and Expertise

- Direct lattice-QCD calculation of the Bjorken-x dependence of parton distribution functions
- Precision QCD low-energy constants for probing BSM (e.g. dark matter, neutron electric dipole moment, novel interactions in neutron beta decay,neutron decay, neutrino cross section)
- Three-dimensional structure of nucleons, such as Generalized Parton Distributions

Synergistic Activities:

- Elected member, APS DNP Executive Committee, 2022–2024
- Elected member, USQCD Executive Committee, 2020–2022
- Convener of the topical group on "QCD and strong interactions: hadronic structure and forward QCD" of the Energy Frontier group of the next HEP Community Planning Exercise (a.k.a. Snowmass)
- Elected Chair, Gordon Research Conference on Photonuclear Reactions, Aug. 7–12, 2022, Holderness, NH, USA
- Lead Organizer for INT Summer School on Problem Solving in Lattice QCD, Jun. 28–Jul. 16, 2021, Institute for Nuclear Theory, Seattle, WA, US

Collaborators and Co-Editors in the last 5 years:

Christopher Aubin	Fordham U.
Gunnar Bali	U. Regensburg
Tanmoy Bhattacharya	Los Alamos Natl. Lab.
Jiunn-Wei Chen	Natl. Taiwan U., Taiwan
Vincenzo Cirigliano	Los Alamos Natl. Lab.
Martha Constantinou	Temple University
Luigi Del Debbio	U. Edinburgh
William Detmold	MIT, Cambridge, CTP
Jozef J. Dudek	Jefferson Lab and William-Mary Coll.
Robert G. Edwards	Jefferson Lab
Michael Engelhardt	New Mexico State University
Jeremy Green	Mainz U.
Rajan Gupta	Los Alamos Natl. Lab.
Luchang Jin	Connecticut U.
Bálint Joó	Jefferson Lab
Andreas S. Kronfeld	Fermilab
Keh-Fei Liu	Kentucky U.
Liuming Liu	Lanzhou, Inst. Modern Phys.
Stefan Meinel	Arizona U.
W. Melnitchouk	Jefferson Lab
Harvey B. Meyer	Mainz U.
Swagato Mukherjee	Brookhaven Natl. Lab.
John Negele	MIT
Emanuele R. Nocera	Nikhef Theory Group, The Netherlands
Fred Olness	Southern Methodist University
Kostas Orginos	Jefferson Lab and William-Mary Coll.
Peter Petreczky	Brookhaven Natl. Lab.
Andrew Pochinsky	MIT
Alexei Prokudin	Penn State U.
David Richards	Jefferson Lab
David G. Richards	Jefferson Lab
Sinéad M. Ryan	Trinity Coll., Dublin
N. Sato	Connecticut U.
Phiala Shanahan	MIT
Sergey Syritsyn	Stony Brook University
Frank Winter	Jefferson Lab
Yi-Bo Yang	Chinese Academy of Sciences
Boram Yoon	Los Alamos Natl. Lab.
Jian-Hui Zhang	Beijing Normal U.

FRANK WINTER
email: fwinter@jlab.org

Professional Preparation

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

Appointments

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

Publications Most Relevant to This Proposal

1. Sungwoo Park, Rajan Gupta, Boram Yoon, Santanu Mondal, Tanmoy Bhattacharya, Yong-Chull Jang, Bálint Joó, Frank Winter, *Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD*, Phys. Rev. D105 (2022) 054505, arXiv:2103.05599
2. Assumpta Parreño, Phiala E. Shanahan, Michael L. Wagman, Frank Winter, Emmanuel Chang, William Detmold, Marc Illa *The axial charge of the triton from lattice QCD*, Phys. Rev. D 103, 074511 (2021)
3. S. R. Beane, et. al. "Charged multi-hadron systems in lattice QCD+QED", submitted to PRL
4. Colin Egerer, et al. "Controlling Excited-State Contributions with Distillation in Lattice QCD Calculations of Nucleon Isovector Charges g_S^{u-d}", Phys. Rev. D 99, 034506 (2019)
5. Emmanuel Chang, et. al. "Nuclear modification of scalar, axial and tensor charges from lattice QCD", Phys. Rev. Lett. 120, 152002 (2018)
6. Michael L. Wagman, et. al. "Baryon-Baryon Interactions and Spin-Flavor Symmetry from Lattice Quantum Chromodynamics", Phys. Rev. D 96, 114510 (2017)
7. Brian C. Tiburzi, et. al. "Double-β Decay Matrix Elements from Lattice Quantum Chromodynamics", Phys. Rev. D 96, 054505 (2017)

Research Interests and Expertise

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

Synergistic Activities

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

Collaborators

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

P. E. L. Rakow, University of Liverpool
P. E. Shanahan, Massachusetts Institute of Technology
R. D. Young, University of Adelaide
R. Horsley, University of Edinburgh
R. Edwards, Thomas Jefferson National Accelerator Facility
S. R. Beane, University of Washington
W. Detmold, Massachusetts Institute of Technology
Y. Nakamura, RIKEN Center for Computational Science
Z. Davoudi, University of Maryland

Boram Yoon
boram@lanl.gov, 505-695-8180

Professional Preparation

PhD in Physics, 2013, Seoul National University, Seoul, South Korea
BS in Physics, 2007, Seoul National University, Seoul, South Korea

Appointments

2016–present, Postdoctoral Researcher, Los Alamos National Laboratory
2013–2016, Postdoctoral Researcher, Los Alamos National Laboratory

Publications Most Relevant to This Proposal

1. Sungwoo Park, Rajan Gupta, Boram Yoon, Santanu Mondal, Tanmoy Bhattacharya, Yong-Chull Jang, Bálint Jóo, Frank Winter, *Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD*, Phys. Rev. D 105, 054505 (2022)
2. Tanmoy Bhattacharya, Vincenzo Cirigliano, Rajan Gupta, Emanuele Mereghetti, Boram Yoon, *Contribution of the QCD θ-term to nucleon electric dipole moment*, Phys. Rev. D 103, 114507 (2021)
3. Yong-Chull Jang, Rajan Gupta, Boram Yoon, and Tanmoy Bhattacharya, *Axial Vector Form Factors from Lattice QCD that Satisfy the PCAC Relation*, Phys. Rev. Lett. 124, 072002 (2020)
4. Rajan Gupta, Boram Yoon, Tanmoy Bhattacharya, Vincenzo Cirigliano, Yong-Chull Jang, and Huey-Wen Lin, *Flavor diagonal tensor charges of the nucleon from 2+1+1 flavor lattice QCD*, Phys. Rev. D 98, 091501 (2018)
5. Huey-Wen Lin, Rajan Gupta, Boram Yoon, Yong-Chull Jang, and Tanmoy Bhattacharya, *Quark contribution to the proton spin from 2+1+1-flavor lattice QCD*, Phys. Rev. D 98, 094512 (2018)
6. Boram Yoon, Yong-Chull Jang, Rajan Gupta, Tanmoy Bhattacharya, Jeremy Green, Balint Joo, Huey-Wen Lin, Kostas Orginos, David Richards, Sergey Syritsyn, and Frank Winter, *Isovector charges of the nucleon from 2+1-flavor QCD with clover fermions*, Phys. Rev. D 95, 074508 (2017)
7. T. Bhattacharya, V. Cirigliano, R. Gupta, H.-W. Lin, and B. Yoon, *Neutron Electric Dipole Moment and Tensor Charges from Lattice QCD*, Phys. Rev. Lett., 115, 212002 (2015)

Research Interests and Expertise

I have 8+ years of experience in lattice QCD, high-performance computing and machine learning. My research is focused on QCD simulations unearthing novel interactions and related computational and machine-learning tools.

Synergistic Activities

1. Co-organizer of Santa Fe Workshop on Lattice QCD (2017, 2019)
2. Reviewer for Journal of High Energy Physics, Physical Review D, International Journal of Modern Physics E, and Journal of Computer Networks and Communications

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

Chia Cheng Chang (LinkedIn), Vincenzo Cirigliano (University Washington), Lukasz Cincio (Los Alamos National Laboratory), Zhouyou Fan (Michigan State University), Michael Graesser (Los Alamos National Laboratory), Martin Hoferichter (University of Bern), Yong-Chull Jang (Columbia University), Balint Joo (Jeferson Lab), Garrett Kenyon (Los Alamos National

Laboratory), Weonjong Lee (Seoul National University), Jaehoon Leem (Seoul National University), Ruizi Li (Michigan State University), Xuan Li (Los Alamos National Laboratory), Huey-Wen Lin (Michigan State University), Ming Liu (Los Alamos National Laboratory), Emanuele Mereghetti (Los Alamos National Laboratory), Santanu Mondal (Los Alamos National Laboratory), Duff Neill (Los Alamos National Laboratory), Sungwoo Park (Thomas Jefferson National Accelerator Facility), Ermal Rrapaj (University of California Berkeley), Matthew Sievert (New Mexico State University), Cesar da Silva (Los Alamos National Laboratory), Ivan Vitev (Los Alamos National Laboratory), Frank Winter (Thomas Jefferson National Accelerator Facility), Rui Zhang (Michigan State University)

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

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.

Notification by the DOE INCITE program and OLCF

Question #2

Suggested Reviewers

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

Stephen Sharpe, University of Washington

Maarten Goltermann, San Francisco State University

Aneesh Manohar, UCSD

Alex Friedland, SLAC

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_INCITE_2023_Gupta.pdf
The attachment is on the following page.

Proposal Title: Precision calculations of matrix elements for Novel CP Violation Experiments

PI: Rajan Gupta,
Co-PIs: Tanmoy Bhattacharya and Vincenzo Cirigliano

This is to certify that we are not requesting any testbed resources as part of this proposal. This proposal uses well-developed and tested methodology to solve a problem of high interest to both the high energy and nuclear physics communities.

We do have a very active research program on novel (both quantum and AI) technologies which use separate resources.