BROOKHAVEN NATIONAL LABORATORY
PROPOSAL INFORMATION QUESTIONNAIRE
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT PROGRAM

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DEPARTMENT/DIVISION	Physics/CS - NPP/CSI	**DATE**	6/11/2021
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TITLE OF PROPOSAL	Lattice QCD using accelerators and machine learning		
TYPE A			
PROPOSAL TERM (month/year)	From **10/2021**	Through **09/2024**	

SUMMARY OF PROPOSAL

Description of Project:

Develop new algorithms and machine learning approaches to numerical sampling of the Feynman path integral for QCD, applying these to DOE Exascale computers to enable a decadal programme of research including dynamical charm quarks at fine lattice spacings. The proposal is twin track: Firstly to deploy a lower risk but mission critical baseline of new GPU aware algorithms that transform the level of locality by factoring the Fermion determinant to change the balance between interconnect speed and computing throughput. Secondly, to combine this with a higher risk, but high potential reward machine learned change of variables to accelerate the sampling and avoid critical slowing down.

Expected Results:

The Exascale-aware baseline algorithm is estimated to be a factor of ten faster than current algorithms on the DOE Aurora supercomputer at ANL, by evading communication. The machine learned algorithm field transformation can augment this gain further. These improvements will enable science that aligns with major lab priorities:

- Enable theoretical simulations using chiral fermion discretisations to be performed on substantially finer “grids” than ever before, allowing the inclusion of charm quarks and use of larger momenta.
- Enable theoretical predictions of the standard model hadronic contribution to muon g-2 to include charm quark loop effects and have reduced discretisation systematic errors, and help resolve whether muon g-2 is in tension with the standard model.
- Enable ab initio theoretical predictions of polarised hadron structure needed by the EIC.
- Enable simulations for B and D meson mixing and semileptonic decay form factors providing theoretical input to lepton flavour universality tests at Belle II

PROPOSAL

High Energy Theory (HET) and Nuclear Theory (NT) have significant common underpinning scientific methods. BNL is the worldwide leader in simulations of non-perturbative quantum chromodynamics (QCD) with discretized Fermions that respect physical symmetries between left-handed and right-handed spins. We develop software[1] for these chiral Fermion simulations[2] that is used world-wide, including the US, the UK, Germany and Japan[3].

Some of the key algorithms that underpin much of statistical computing, including Markov Chain Monte Carlo and Metropolis algorithms have emerged from theoretical high energy and statistical physics. More recently, the Hybrid Monte Carlo algorithm[4] was developed to sample the Lattice QCD path integral and has found cross-over and application to fields like statistics and machine learning. This proposal spans the interests of both CSI and Physics and builds on two grass-roots collaborations that have emerged in both new-but-conventional and also new machine learning capable algorithms for efficient sampling on accelerator hardware.

The project will exploit HET expertise in chiral fermion algorithms and B-physics, CSI expertise in numerical algorithms and machine learning and will exploit NT expertise in nucleon and EIC physics. New connections to Nuclear Theory at Argonne National Laboratory, and opportunities with Argonne computing give this approach a significant competitive advantage. These theoretical calculations support theoretical input to major DOE experimental projects including E989, Belle-II and the EIC.

Being able to generate large and fine lattices is also crucial to the reliable lattice determination of the hadronic vacuum polarization contribution to the muon g-2. Currently, there is a tension between the recent BMW 20 lattice result [5] with the dispersive data-driven approach. The major uncertainty of the BMW 20 lattice result is the systematic uncertainty from the continuum extrapolation. Finer lattices and calculations with different discretisation schemes are needed to further improve the accuracy of the lattice calculations and confirm or resolve the current tension. This is critical to claim new physics from the Fermilab muon g-2 experiment E989. Calculations of the hadronic vacuum polarisation contribution by the RBC UKQCD collaboration [6-10] have so far not been able to include charm quark loops in the gauge configuration sampling, and this proposal aims to develop algorithms that will enable these to be included in future calculations.

In HET the electroweak couplings to W bosons are purely left-handed. CP violation is an asymmetry between the behaviour of matter and antimatter: in the standard model this is heavily suppressed and arises on through the unitary Cabibbo Kobayashi Maskawa (CKM) matrix encoding the W-couplings to quarks. Probing CP violation, both theoretically and experimentally, is a critical discovery opportunity since the standard model does explain the observed excess of matter in our universe. We believe that new sources of CP violation are needed and hope will be detectable against this small standard model contribution. Chiral fermion approaches are ideal for flavor physics amplitudes since we can treat the weak interactions as a purely left-handed four fermi interaction.

This proposal aims to develop technology and know-how that enables the generation of a series of simulations, sampling the most likely quantum fluctuations of the gluon fields using a Markov Chain Monte Carlo (MCMC) technique. These simulations should have inverse lattice spacings in the range 3GeV – 5GeV and Nyquist frequencies covering practical momenta from 9-15 GeV.

Physics enabled: This will enable calculations in both HET and in NT covering new physics and in support of important DOE experimental programs. Both groups have common base requirements, which are simulations on fine lattices (i.e. mesh grids) with chiral fermions.

In recent years, with the development of factorization or effective theory expansion approaches, especially the large-momentum effective theory (LaMET), it is now realistic to calculate the x-dependence or higher Mellin moments of the PDFs and GPDs with controlled systematic uncertainties. Moreover, one can also calculate the TMDs and their nonperturbative evolution information from the lattice. In these calculations, in order to access a wider range of x and higher moments, one must simulate the proton moving at very large momentum, which is limited by the momentum cut-off imposed by the finite lattice spacing. With 5 GeV inverse lattice spacing, it is promising to calculate the PDFs and GPDs within the range of $0.1<x<0.9$ to complement the measurements at EIC.

The lattice calculation of polarized proton observables, including the PDFs, GPDs and TMDs, can have huge impact on EIC in the following aspects:
1) Flavor asymmetry and in the sea quark helicity and transversity distributions.
2) Flavor separation of valence and sea quarks, including the strange and charm contributions.
3) the gluon distribution in the large-x region and the total gluon helicity contribution to the proton spin.
4) Nonperturbative input for TMD evolution in global analysis.
5) Sivers function in single transverse-spin asymmetry, as well as the worm-gear TMDs.

These fine lattices should enable to simulate with domain wall fermions as a heavy quark [11,12] on DOE Exascale computers and will enable for significant simultaneous coverage of mass difference and recoil kinematic space in B to D semileptonic transition form factors. In addition to precise determination of CKM matrix element Vcb, this will enable a program of form factor determination where lattice results may be combined with experimental data to improve predictions of lepton flavor ratios between tau and electrons or muons: R(D) and R(D*) [13]. The parametrization of the form factor is a key systematic effect, and has been associated with tensions between theory and experiment. Model independent parametrization is enabled by fit to lattice QCD data, and tensions have been resolved by incorporating lattice results in the analysis [14]. Continued theoretical error reduction is important to match the ongoing experimental program.

Program of work: The project will develop new multi-level algorithms, know-how, and software required to use the Exaflop computer that the DOE is constructing at Argonne National Laboratory under a $500M dollar contract. The development effort has recently started as a new direct collaboration project between Kelly (CSI), Boyle (HET) with partial Exascale Computing Project funding. Deploying and tuning these algorithms and developing the four flavour (u,d,s,c) physical point simulations is a considerable effort that requires post-doctoral support. The corresponding three flavour effort took place in 2005/6 and was foundational to 15 years of international theoretical research.

The proposed research directions are two fold: firstly to adapt algorithms to the constraints and limits of computers, and secondly to address the intrinsic tendency for algorithms to slow down and as the simulated grids become finer. The former is required to realise the potential of exascale hardware - and can address the need for greater statistical precision - while the latter is required to address systematic errors like include charm quarks (so far neglected) or larger momenta in our calculations.

Divide and conquer: The algorithms and software are being designed to work well with modern multi-GPU (graphics processor) computing nodes. While these feature new programming environments and complex programming models, the fundamental difficulty lies in the large disparity between the GPU memory performance and the performance of connections between nodes. Independent of how the software is programmed, the algorithms must be conceptually redesigned to be cellular: this implies a hierarchy of length scales, exploiting multiple islands of good performance.

The determinant of the lattice Dirac operator enters the MCMC probability weight and is a fundamentally non-local object since it is totally antisymmetric to encode the Pauli exclusion principle. However, Schur decomposition of the matrices leads to a clever factorization [15] into determinants of a *local truncation* of the Fermion matrix and a more complicated “boundary” term that connects domains. The key idea is to use the huge single node performance available on these local determinants, integrating these on a fine timestep, while suppressing the size of the forces from the boundary terms by a physical distance from the boundary. This is the natural marriage of locality in the theory to the “performance island” characteristic of large, modern GPU nodes. We have good reason to predict the ideas will work significantly better giving an estimated 10x speed up.

Critical slowing down: The algorithms must also address critical slowing down that arises as the discretization is made finer. The approaches proposed address this can be thought in some way as either a form of “Fourier acceleration” or the intelligent identification of important collective degrees of freedom in our algorithms [22,23,24].

The simplest explanation of critical slowing down might be seen if we applied our sophisticated algorithms for Quantum Chromodynamics to a simple case like the violin string. We seek to evolve the different modes of the system in randomly selected directions to sample all states under some probability weight. But, the different wavelength harmonics oscillate periodically at very different frequencies (and with very different forces), meaning that there is no single optimal distance for a new state proposal. Whatever time evolution distance you choose, some modes will decorrelate faster than others. The idea of Fourier acceleration is to choose the evolution rate in a wavelength dependent way, such that all modes decorrelate at the same rate.

In a complex, non-linear gauge theory, the important modes are not as simple as Fourier modes. In fact, phase is ill-defined in a gauge theory - as the phase of the wavefunction is unobservable- and Fourier transformation becomes meaningless! One cannot pre-suppose that nature of the accelerated degrees of freedom - they must be discovered in a data dependent way. Our first critical slowing down proposal, Riemannian Manifold HMC (RMHMC), uses the data dependent gauge *covariant* Laplacian to define its acceleration.

RMHMC is a complementary method under research by Jung that can in principle be combined with Domain Decomposition and allows to accelerate different degrees of freedom if they can be identified. So far forms of gauge covariant "Fourier" acceleration have been tried, but the method has considerable freedom that could be exploited and optimized in a machine learning context. These steps can also be combined with open boundary conditions to ensure sampling of topological sectors that are difficult to explore and ensure the full space is sampled. RMHMC is based on the simplest analogue to the Fourier transformation in a gauge theory - the modes of the gauge *covariant* Laplacian operator.

Machine learning:

However, non-abelian gauge theories have a strong non-perturbative sector that defies easy human interpretation. There are known semi-classical topological objects, called instantons, that are physically important but defy simple plane wave analyses in the same way that "Hurricanes" defy a simple sound wave analysis. These are the "known-unknowns". A Quantum Field theory also has intrinsic not-even-semi-classical effects: the typical field configuration isn't even differentiable let alone interpretable in terms of plane wave analysis. These are our "unknown-unknowns".

The second, more ambitious strand of our proposal to address critical slowing down is to use machine learning to figure out our "unknown-unknowns" with a machine-learned free-form "data dependent acceleration". This is expressed as a change of variables in our HMC integration. The "Field transformation HMC" is described in more detail below. Since the "unknown-unknowns" are known to exist (please excuse the linguistic abuse, as we are reducing a complex topic to words), there is good reason the "data driven machine discovery" might do significantly better than a human created and approximation inspired guess at the right transformation. Since the human and approximation inspired guess will be demonstrated below to give a 2x gain the ML version could give significantly more than 2x. We cannot place an upper bound on the potential gain, and for this reason it is very exciting indeed.

Postdoc-1:
We request funding for a post-doctoral researcher and have at least one qualified and interested candidate who would be appropriate to fill the position. The post will undertake the research and development tasks related to developing simulations with a new 2+1+1 flavor program with u, d, s, c quarks. This will include integrating and using new multiscale aware algorithms for sampling domain wall Fermions, and they will match recent BNL algorithms work to the properties of the DOE Aurora computer. For example, we seek to use the "domain decomposed HMC algorithm" [15], and tune this in a new, large subdomain context where the domain is large and the executed on a sub-lattice appropriate to an entire multi-GPU (graphics processor unit) high performance computer node – a processing island.

The postdoctoral researcher will study and tune the performance of combinations of these algorithms, boundary conditions and choice of gauge and fermion action that maximises sampling for lattice spacings in the 4 GeV range (M1). The lattice spacing and interacting quark masses are a measured output of a simulation in a lattice field theory, so must be measured and the bare coupling and input masses tuned to find the right simulation point as the second milestone (M2).

Milestones 3 will develop methods for calculating correlation functions required to extract observables. These will likely use Grid Python Tools, a newly started python library by BNL/Regensburg providing a friendly high-level interface to Grid. Milestone 5 will be the implementation and demonstration of well performing software for the above on the DOE Aurora computer.

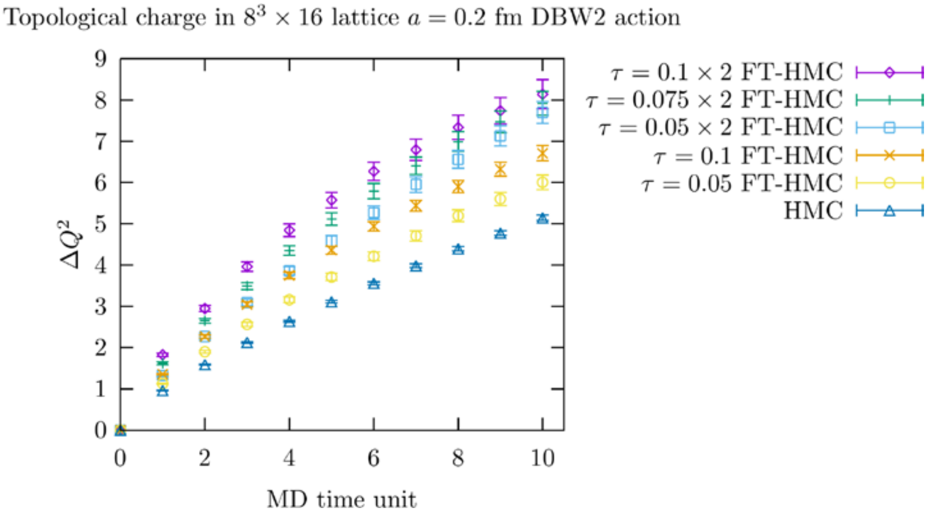
Post-doc 2

To address the critical slowing down issue, we would like to pursue another improvement to the HMC algorithm, which we shall refer to as the Field Transformation HMC (FT-HMC), in parallel to the aforementioned Riemannian Manifold HMC (RM-HMC). HMC is the standard algorithm to generate lattice gauge field configurations U following the needed distribution density $e^{-S[U]}$. We can apply an invertible transformation to U and obtain new gauge field configurations $U_0 = \mathcal{F}^{-1}U$, which satisfy a new distribution density, $e^{-S_{\mathcal{F}}[U_0]}$. The standard HMC algorithm can then be used to generate configurations U_0 with the new distribution, to avoid the critical slowing down issue with the old distribution. This idea was proposed by Martin Lüscher in 2009 [16]. In that work, he has proved, constructively, the existence of trivializing maps, which refer to field transformations that lead to trivial uniform distribution, i.e. $S_{\mathcal{F}}[U_0] = \mathrm{constant}$. At leading order, the Wilson flow operation is the trivializing map for the Wilson pure gauge action. It is then proposed to use Wilson flow as the transformation in the FT-HMC to reduce the auto-correlation length in the generated configurations.

We have implemented the FT-HMC algorithm with a “human guessed” field transformation taken as the Wilson flow (the flow is decomposed into a few stout smearing steps). We studied the tunnelling of topological charge in the HMC evolution process with different Wilson flow time τ and compared it with the standard HMC (equivalent to $\tau = 0$). The result of a small scale pure gauge test with close to realistic parameters is shown in the plot below.

The x-axis is the HMC evolution time, the y-axis is the average of topological charge change’s square. It can be seen that with Wilson flow as the transformation, the tunnelling rate of the topological change can increase by more than a factor of two. Also, we find that after the transformation, the total force is reduced for flow time $\tau \lesssim 0.2$.

In this proposal, we would like to explore more effective field transformations by incorporating multiple layers of more general convolutional neural network kernels [M6], and use machine



learning techniques to train the parameters of the transformation [M7]. The resulting field transformation is similar to a 4D (our lattice spans space and time) convolutional neural network.

This is very challenging, but if successful, we will have a dramatic speed up compared with the current standard HMC, which is needed for the next stage physics goals. Compared to the recent work by the MIT group [17-20], which tries to train a neural-trivializing map directly, our proposed approach allows transformation of much less accuracy to have a positive impact to the performance of the gauge field configuration generation. This property makes it possible to use the algorithms to generate the needed large and fine lattices. The trained transformation using a modest size lattice, is expected to work for large lattice sizes and a range of different parameters.

Finally, we would like to combine the RHMC or FT-HMC and DD-HMC to benefit from the acceleration from both ML/Fourier and hardware aware improvements.

Visiting PhD Student: The visiting PhD student will work with Post-doc 1,Mukherjee and Boyle to implement Milestone 3 in the GPT framework and prepare BNL to translate the opportunity created into scientific input to the EIC.

Milestones

- M1. Algorithm for multiscale capable HMC for 2+1+1f simulation
- M2. Determine simulation action parameters for 2+1+1f simulation
- M3. Methods for polarized PDFs, gluon helicity and GPD's and TMD's.
- M4. Performant software implementations of M1-3 on Aurora computer
- M5. Flow transformation HMC with convolutional kernels
- M6. ML trained flow transformation HMC.

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Education and Training:

PhD in Theoretical Particle Physics, The University of Edinburgh, 1997 (Carnegie Scholarship)
First Class BSc Combined Honours Mathematics and Physics, The University of Glasgow, 1994

Research and Professional Experience

Sept 1997 - Sept 2000 : PPARC Personal fellowship, University of Glasgow
Sept 2000 - April 2005: Postdoctoral researcher, University of Edinburgh
Jan 2001- Nov 2004: Columbia University visiting scholar
April 2005 - Sept 2010: University of Edinburgh Lecturer
April 2005 - Sept 2010: RCUK Fellow
Sept 2010 - Sept 2014: UoE Reader
Sept 2014 - Oct 2019: UoE Professor
Oct 2019 – Present: BNL Scientist

Select Recent Publications

"Direct CP violation and the ΔI=1/2 rule in K→ππ decay from the standard model", Phys.Rev.D 102 (2020) 5, 054509.
"Calculation of the hadronic vacuum polarization contribution to the muon anomalous magnetic moment" Phys.Rev.Lett. 121 (2018) no.2, 022003
"Neutral kaon mixing beyond the Standard Model with Nf = 2 + 1 chiral fermions. Part 2: non perturbative renormalisation of the ΔF = 2 four quark operators". JHEP 1710 (2017) 054
"Domain wall QCD with physical quark masses" Phys.Rev. D93 (2016) no.7, 074505.
"Calculation of the hadronic vacuum polarization disconnected contribution to the muon anomalous magnetic moment" Phys.Rev.Lett. 116 (2016) no.23, 232002
"The decay constants fD and fDs in the continuum limit of Nf = 2 + 1 domain wall lattice QCD" JHEP 1712 (2017) 008

Fellowships and honours

2013 Gordon Bell prize finalist (Supercomputing 2013)
2012 Ken Wilson Lattice Award (Lattice 2012)
2012 Gauss Award (International Supercomputing Conference 2012)
2004 Gordon Bell prize finalist (Supercomputing 2004)
2016 Visiting Scientist Brookhaven National Laboratory
2016 Royal Society Wolfson Research Merit Award
2016 - 2019 Alan Turing Institute Faculty Fellow

Synergistic Activities

Led the development of the Grid LQCD software library, under DOE Exascale Computing Project Chair of the STFC DiRAC Technical Working Group (2011-2019)
Led Alan Turing Institute Intel codesign project (2016-2019).
Led Edinburgh-Columbia Intel Sponsored Research Project (2016-2020).
Lattice Conference IAC - 2016, 2021

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Education and Training:

University of Tokyo, Ph.D. (1997), M.S. (1994), Theoretical Physics, B.S., Physics (1992)

Research and Professional Experience

Dec 2008 - present Assistant (2008-), Associate (2010-), Tenured (tenure 2013-), Senior Scientist
Oct 2011 - present Founding Group Leader, Computing Group, RIKEN BNL Research Center
Oct 2008 - present RIKEN fellow, RIKEN BNL Research Center
Dec 1999 - Sep 2008 Assistant Professor (tenured), Department of Physics Kanazawa University

Select Recent Publications

"The hadronic light-by-light scattering contribution to the muon anomalous magnetic moment from lattice QCD,"

"Novel |Vus| determination using inclusive strange tau decay and Lattice Hadronic Vacuum Polarization Function," Phys. Rev. Lett. 121, 202003 (2018)

Calculation of the hadronic vacuum polarization contribution to the muon anomalous mag- netic moment," Phys. Rev. Lett. 121, 022003 (2018

"Lattice Calculation of Electric Dipole Moments and Form Factors of the Nucleon," Phys. Rev. D96, 014501 (2017)

"Direct CP violation and the ΔI=1/2 rule in K→ππ decay from the standard model", Phys.Rev.D 102 (2020) 5, 054509.

"Connected and Leading Dis- connected Hadronic Light-by-Light Contribution to the Muon Anomalous Magnetic Moment with a Physical Pion Mass," Phys. Rev. Lett. 118, 022005 (2017)

"Calculation of the hadronic vacuum polarization disconnected contribution to the muon anomalous magnetic moment," Phys. Rev. Lett. 116, 232002 (2016)

Fellowships and honours

2019 BNL Science and Technology Award
2018 APS fellowship
2018-20 International Advisory Committee member, Lattice 2019, 2020, Selection Committee member, The Ken Wilson Lattice Award 2020
2012-present As PI and co-PI, two BNL LDRD grants, one PD grant
2011-present Successfully proposed and hosted joint tenure track professors between U.S. universities and RIKEN/RBRC, one joint fellow with KEK, Japan, and 8 RBRC PostDocs.
2005-present As a PI, 6 grants from Japan Society for the Promotion of Science
2016-2017 PI of BNL, DOE SciDAC program
2013-2015 Member of Scientific Program Committee of USQCD
2012 The Ken Wilson Lattice Award

Assistant Professor Luchang Jin
Physics Department
University of Connecticut
Storrs, CT

Tel: +1 (917) 705 8827
Email: ljin.luchang@gmail.com

Education and Training:

PhD in Theoretical Particle Physics,	Columbia University, 2016
BS in Physics,	Peking University, 2011

Research and Professional Experience
2016 – 2017: Brookhaven National Laboratory, Research Associate
2017 – Present: University of Connecticut, Assistant Professor

Select Recent Publications

- “Field sparsening for the construction of the correlation functions in lattice QCD,” Phys. Rev. D 103, no.1, 014514 (2021) arXiv:2009.01029.
- “First-principles calculation of electroweak box diagrams from lattice QCD,” Phys.Rev.Lett. 124, no.19, 192002 (2020) arXiv:2003.09798.
- “Hadronic Light-by-Light Scattering Contribution to the Muon Anomalous Magnetic Moment from Lattice QCD,” Phys.Rev.Lett. 124, no.13, 132002 (2020) arXiv:1911.08123.
- “Long-distance contributions to neutrinoless double beta decay π – → π + ee,” Phys. Rev. D 100, no.9, 094511 (2019) arXiv:1909.13525.
- “QED self energies from lattice QCD without power-law finite-volume errors,” Phys. Rev. D 100, no.9, 094509 (2019) arXiv:1812.09817.
- “Factorization Theorem Relating Euclidean and Light-Cone Parton Distributions,” Phys. Rev. D 98, no.5, 056004 (2018) arXiv:1801.03917.

Grants and Awards

- DOE Early Career Award, 2020
- Kenneth G. Wilson Award for Excellence in Lattice Field Theory, 2019
- Three year DOE Grant in High Energy Physics as Co-PI, 2019
- Intel Fellowship for exceptional research achievements by a PhD student, 2016.
- Champion of Battlecode – MIT AI programming competition (teamed with Greg McGlynn), 2016
- Joseph C. Pfister Fellowship Fund, 2013-2014.
- Faculty Fellowship in Physics Department, 2011-2013.

Synergistic Activities

- Chair of the Local Organizing Committee for the “Muon g – 2 Theory Initiative Hadronic Light-by-Light Working Group Workshop”, University of Connecticut, March 12th – March 14th, 2018

CHULWOO JUNG

High Energy Theory Group,
Department of Physics, Bldg. 510A,
Brookhaven National Laboratory,
Upton, NY 11973, U. S. A.
Tel: (631) 344-5254
e-mail: chulwoo@bnl.gov

Education and Training:

Ph.D. Physics, Columbia University, Feb. 1998 (Thesis Advisor: Robert D. Mawhinney)
M.Phil. Physics, Columbia University, 1995
B.S. Physics, Korea Advanced Institute of Science and Technology, Daejon, Republic of Korea, 1992

Research and Professional Experience:

October 2007 -, Physicist, Physics Department, Brookhaven National Laboratory,
October 2004 - September 2007 Associate Physicist, Physics Department, Brookhaven National Laboratory,
September 2002 - September 2004 Assistant Physicist, Physics Department, Brookhaven National Laboratory,
September 2001 - August 2002, Associate Research Scientist, Physics Department, Columbia University.
September 1999 - August 2001, Research Associate, Theoretical Quark, Hadron and Nuclei (TQHN) group, University of Maryland.

Honors and Awards

2012: Ken Wilson Lattice Award
1998: First prize, Gordon Bell prize (performance per dollar category),
IEEE Computer society (as a member of QCDSP group)

Selected Recent Publications

1. Hadronic Light-by-Light Scattering Contribution to the Muon Anomalous Magnetic Moment from Lattice QCD, T. Blum et al., Phys. Rev. Lett. 124, no.13, 132002 (2020) doi:10.1103/PhysRevLett.124.132002 [arXiv:1911.08123 [hep-lat]].
2. Calculation of the hadronic vacuum polarization contribution to the muon anomalous magnetic moment, T. Blum et al. [RBC and UKQCD Collaborations], Phys. Rev. Lett. 121, no. 2, 022003 (2018) [arXiv:1801.07224 [hep-lat]].
3. Using infinite volume, continuum QED and lattice QCD for the hadronic light-by-light contribution to the muon anomalous magnetic moment, T. Blum, N. Christ, M. Hayakawa, T. Izubuchi, L. Jin, C. Jung and C. Lehner, Phys. Rev. D 96, no. 3, 034515 (2017) [arXiv:1705.01067 [hep-lat]].
4. Connected and leading disconnected hadronic light-by-light contribution to the muon anomalous magnetic moment with physical pion mass, T. Blum, et al., Phys. Rev. Lett. 118, no. 2, 022005 (2017) [arXiv:1610.04603 [hep-lat]].
5. Domain wall QCD with physical quark masses, T. Blum et al. [RBC and UKQCD Collaborations], Phys. Rev. D 93, no. 7, 074505 (2016) [arXiv:1411.7017 [hep-lat]].

Christopher Brendan Kelly
Assistant Computational Scientist

Computational Science Initiative,
Brookhaven National Laboratory
Upton, NY 11973-5000

phone: (347) 263 6775
email: ckelly@bnl.gov

Education and training:

Ph.D. Theoretical Physics, University of Edinburgh, 2010, (advisor: Peter Boyle)
MPhys. 1st with Honours, The Queen's College, University of Oxford, 2007

Appointments:

March 2020 - present - Assistant Computational Scientist, Computational Science Institute, BNL
2016 - March 2020, Associate Staff Scientist, Columbia University (sponsored by Intel)
2013 - 2016, RIKEN Foreign Postdoctoral Research Fellow, RBRC, BNL
2010 - 2013, Postdoctoral Fellow, Columbia University

Honors and Awards:

RIKEN Foreign Postdoctoral Research Fellowship (2013)
Ken Wilson Lattice Award (2012)

Select Recent Publications:

Lattice determination of I=0 and 2 $\pi\pi$ scattering phase shifts with a physical pion mass, arXiv:2103.15131 , for submission to Physical Review D.

Chimbuko: A Workflow-Level Scalable Performance Trace Analysis Tool, ISAV 2020 (SC20) workshop [Corresponding author]

Direct CP violation and the $\Delta I=1/2$ rule in $K\rightarrow\pi\pi$ decay from the Standard Model, R. Abbott *et al* Phys. Rev. D 102 (2020) 5, 054509 [Corresponding author]

Lattice simulations with G-parity Boundary Conditions, N.H.Christ *et al*, Phys. Rev. D 101 no.1, 014506 (2020) [Corresponding author]

Domain Wall Fermion QCD with the Exact One Flavor Algorithm, C.Jung *et al*, Phys. Rev. D 97 no.5, 054503 (2018)

Accelerating HPC codes on Intel(R) Omni-Path Architecture networks: From particle physics to Machine Learning, arXiv:1711.04883 (2017)

Meifeng Lin, Computational Scientist and Group Leader
Computational Science Initiative office: (631) 344 4379
Brookhaven National Laboratory fax: (631) 344 5751
Upton, NY 11973-5000 email: mlin@bnl.gov

Education and Training
Ph.D. Theoretical Particle Physics, Columbia University, 2007
B.S. Physics, Peking University, Beijing, China, 2001

Professional Appointments
07/2019 - present, Group Leader, High Performance Computing, BNL
11/2018 - 05/2019, Acting Group Leader, Quantum Computing, BNL
10/2018 - present, Computational Scientist, Brookhaven National Laboratory
05/2017 - 05/2020, Adjunct Associate Professor, Stony Brook University
10/2016 - 09/2018, Associate Computational Scientist, Brookhaven National Laboratory
11/2013 - 09/2016, Assistant Computational Scientist, Brookhaven National Laboratory
03/2013 - 09/2013, Assistant Computational Scientist, Argonne National Laboratory
11/2012 - 03/2013, Research Scientist, Boston University
10/2009 - 09/2012, Postdoctoral Research Associate, Yale University
09/2007 - 09/2009, Postdoctoral Research Associate, Massachusetts Institute of Technology

Select Publications
1. Abramczyk Michael, Blum Thomas, Izubuchi Taku, Jung Chulwoo, Lin Meifeng, Lytle Andrew, Ohta Shigemi, Shintani Eigo, others. Nucleon mass and isovector couplings in 2+ 1-flavor dynamical domain-wall lattice QCD near physical mass. Physical Review D. 2020; 101(3):034510
2. Z. Dong, Y.-L.L. Fang, X. Huang, H. Yan, S. Ha, W. Xu, Y-S. Chu, S.I. Campbell, ..., M. Lin, High-performance multi-mode ptychography reconstruction on distributed GPUs, 2018 New York Scientific Data Summit (NYSDS), 1-5
3. P.A. Boyle, M.A. Clark, C. DeTar, M. Lin, V. Rana and A. Vaquero, Performance Portability Strategies for Grid C++ Expression Templates, Proceedings of the 35th International Symposium on Lattice Field Theory (Lattice 2017)
4. V. Rana, M. Lin and B. Chapman, A Scalable Task Parallelism Approach For LU Decomposition With Multicore CPUs, Proceedings of Second International Workshop on Extreme Scale Programming Models and Middleware, 2016.
5. E. Papenhausen et al., Polyhedral User Mapping and Assistant Visualizer Tool for the R-Stream Auto-Parallelizing Compiler, Proceedings of the 3rd IEEE Working Conference on Software Visualization (VISSOFT 2015).

Select Professional Activities
- Local Organizing Committee, Lattice 2021
- USQCD Scientific Program Committee, 2018 - present
- Technical Paper and Poster Program Committees, SC21

- Technical Papers Review Committee, PASC21

Swagato Mukherjee email: swagato@bnl.gov
Physics Department office: (631) 344 2115
Brookhaven National Laboratory
Bldg. 510, Upton, NY 11973-5000

Education and Training

Ph.D.: Theoretical physics, 2007, Tata Institute of Fundamental Research, Mumbai, India.
MS: Physics, 2001, Calcutta University, India.

Professional Appointments

2016–present: Physicist, with Tenure, Physics Department, Brookhaven National Laboratory.
2014–2016: Physicist, Physics Department, Brookhaven National Laboratory.
2012–2014: Associate Physicist, Physics Department, Brookhaven National Laboratory.
2010–2012: Assistant Physicist, Physics Department, Brookhaven National Laboratory.
2009–2010: Postdoctoral associate, Physics Department, Brookhaven National Laboratory.
2007–2009: Postdoctoral associate, Faculty for Physics, Bielefeld University, Germany.

Select Publications

1) X. Gao *et. al*., “Origin and Resummation of Threshold Logarithms in the Lattice QCD Calculations of PDFs,” Phys. Rev. D 103, 094504 (2021).
2) X. Gao *et. al*., “Towards studying the structural differences between the pion and its radial excitation,” Phys. Rev. D 103, 094510 (2021).
3) Z. Fan *et. al.,* “Isovector Parton Distribution Functions of Proton on a Superfine Lattice,” Phys. Rev. D 102, 074504 (2020).
4) X. Gao *et. al.,* “Valence parton distribution of the pion from lattice QCD: Approaching the continuum limit,” Phys. Rev. 102, no.9, 094513 (2020).
5) T. Izubuchi *et al*., “Valence parton distribution function of pion from fine lattice,” Phys. Rev. D 100, no.3, 034516 (2019).

Select Professional Activities

- Co-convener of the “QCD and strong interactions: Heavy Ions” Topical Group of the Snowmass 2021.
- Co-principal investigator of the “Scientific Discovery through Advanced Computing (SciDAC- 4) project Computing the Properties of Matter with Leadership Computing Resources, 2017-.
- Project Director of the Beam Energy Scan Theory (BEST) Topical Collaboration, 2016-.
- Member of the Executive Committee of the USQCD collaboration: 2018-.
- Member of the Program Committee of American Physical Society’s Division of Computational Physics: 2018-.
- Member of the Hardware Advisory Committee of Jefferson Laboratory: 2018-2020.
- Member of the Supervisory Board of the European Training Networks EuroPLEx: 2018-.

Nathan Urban (Computational Scientist)

Brookhaven National Laboratory Tel: (631) 504-0024
Computational Science Initiative (CSI), Bldg. 725
Upton, NY 11973 E-mail: nurban@bnl.gov

Biographical Sketch

Dr. Urban is a physicist and group leader for Applied Mathematics in CSI. His Ph.D. is in statistical mechanics (Monte Carlo methods), and his research career has focused on developing and applying computational statistics and machine learning methods, such as hybrid/Hamiltonian Monte Carlo, variational Bayes, normalizing flows to uncertainty quantification (UQ) problems in the applied physical sciences. He is an DOE Office of Science Early Career Award recipient for research into multi-model UQ, has been a co-organizer of the leading SIAM Conference on Uncertainty Quantification, and has served as a thematic lead and whitepaper author for DOE's "AI for Science" strategic initiative.

Education and Training

2006	Ph.D./M.Ed., Physics, Penn State
1997	B.S., Physics, Computer Science, Mathematics, Virginia Tech

Professional Experience

2020 – Present	Group Leader and Computational Scientist, Brookhaven National Laboratory
2011 – 2020	Scientist, Los Alamos National Laboratory
2010 – 2011	Postdoc, Princeton University, Princeton School of Public and International Affairs
2007 – 2010	Postdoc, Penn State, Geosciences

Leadership Activities

- PI for >$8M (Co-PI for additional >$10M) in DOE projects on climate and uncertainty quantification
- Co-organizer of SIAM Conference on Uncertainty Quantification (2018)
- Contributor to DOE strategy (e.g. ASCR "AI for Science", other ASCR and BER planning activities) at program manager invitation in many workshops and whitepapers

Selected Peer-Reviewed Publications

P. Melland, E.J. Albright, and **N.M. Urban**, "Differentiable programming for online training of a neural artificial viscosity function within a staggered grid Lagrangian hydrodynamics scheme", *Machine Learning: Science and Technology* **2**, 025015 (2021).

A. DeGennaro, **N.M. Urban**, B.T. Nadiga, and T. Haut, "Model structural inference using local dynamic operators", *International Journal of Uncertainty Quantification* **9**, 59 (2019).

A. DeGennaro and **N.M. Urban**, "Scalable extended dynamic mode decomposition using random kernel approximation", *SIAM Journal on Scientific Computing* **41**, A1482 (2019).

A.K. Jonko, **N.M. Urban**, and B. Nadiga, "Towards Bayesian hierarchical inference of equilibrium climate sensitivity from a combination of CMIP5 climate models and observational data", *Climatic Change* **149**, 247 (2018).

T.E. Fricker, J.E. Oakley, and **N.M. Urban**, "Multivariate emulators with nonseparable covariance structures", *Technometrics* **55**, 47 (2013).

C.M. Little, M. Oppenheimer, and **N.M. Urban**, "Upper bounds on twenty-first-century Antarctic ice loss assessed using a probabilistic framework", *Nature Climate Change* **3**, 654 (2013).

A. Schmittner, **N.M. Urban**, J.D. Shakun, N.M. Mahowald, P.U. Clark, P.J. Bartlein, A.C. Mix, and A. Rosell-Melé, "Climate sensitivity estimated from temperature reconstructions of the Last Glacial Maximum", *Science* **334**, 1385 (2011).

N.M. Urban, S.M. Gatica, M.W. Cole, and J.L. Riccardo, "Thermodynamic properties and correlation functions of Ar films on the surface of a bundle of nanotubes", *Phys. Rev. B* **71**, 245410 (2005).

BROOKHAVEN NATIONAL LABORATORY
PROPOSAL INFORMATION QUESTIONNAIRE
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT PROGRAM

EQUIPMENT (Reference: DOE Order 413.2C for guidance on equipment restrictions)

Will LDRD funding be used to purchase equipment? Y/N No_____

If "Yes," provide cost and description of equipment

Year 1 - $

Year 2 - $

Year 3 - $

Description:

2. HUMAN SUBJECTS (Reference: DOE Order 443.1)

Are human subjects involved from BNL or a collaborating institution? Human Subjects is defined as "A living individual from whom an investigator obtains either (1) data about that individual through intervention or interaction with the individual, or (2) identifiable, private information about that individual".

If **yes**, attach copy of the current Institutional Review Board Approval and Informed Consent Form from BNL and/or collaborating institution.

Y/N No

3. VERTEBRATE ANIMALS

Are live, vertebrate animals involved?

If **yes**, attach copy of approval from BNL's Institutional Animal Care and Use Committee. Y/N No

Y/N No

4. NEPA REVIEW

Are the activities proposed similar to those now carried out in the Department/Division which have been previously reviewed for potential environmental impacts and compliance with federal, state, local rules and regulations, and BNL's Environment, Safety, and Health Standards? (Therefore, if funded, proposed activities would require no additional environmental evaluation.) Yes

If **no**, has a NEPA review been completed in accordance with the National Environmental Policy Act (NEPA) and Cultural Resources Evaluations Subject Area and the results documented? Y/N

(**Note:** If a NEPA review has not been completed, submit a copy of the work proposal to the BNL NEPA Coordinator for review. No work may commence until the review is completed and documented.)

5. ES&H CONSIDERATIONS

Does the proposal provide sufficient funding for appropriate decommissioning of the research space when the experiment is complete?	Y/N	Yes
Is there an available waste disposal path for project wastes throughout the course of the experiment?	Y/N	Yes
Is funding available to properly dispose of project wastes throughout the course of the experiment?	Y/N	Yes
Are biohazards involved in the proposed work? If yes, attach a current copy of approval from the Institutional Biosafety Committee.	Y/N	No
Can the proposed work be carried out within the existing safety envelope of the facility (Facility Use Agreement, Nuclear Facility Authorization Agreement, Accelerator Safety Envelope, etc.) in which it will be performed?	Y/N	Yes

If **no**, attach a statement indicating what has to be done and how modifications will be funded to prepare the facility to accept the work.

6. TYPE OF WORK

Select Basic, Applied or Development Basic

7. ALIGNMENT WITH THE LABORATORY PRIORITIES

Type A proposals need to be clearly aligned with BNL's priority programs and initiatives. For FY22, the highest priorities for Type A proposals (not in priority order) are: Accelerator Science and Technology; Atmospheric and Climate Science; Clean Energy; Discovery Science Driven by Human-AI-Facility Integration; Isotope Production and R&D Capabilities; and Quantum Information Science and Technology. The Appendix that accompanies the solicitation clarifies the types of R&D covered in each of these areas.

The Laboratory Initiatives are in the areas of: 1. Nuclear Physics; 2. Clean Energy and Climate; 3. Quantum Information Science and Technology; 4. Artificial Intelligence and Data Science; 5. High Energy Physics; and 6. Isotope Production.

Please identify which area(s) the proposal supports.

The application supports 1, 4, and 5 Nuclear Physics (EIC) and AI and Data Science and High Energy Physics.

With regard to the Appendix, the application has considerable elements of "Discovery Science Driven by Human-AI-Facility Integration" with human, AI and theoretical input to facilities and flagship DOE experiments.

Although not perfectly aligned, our optimisation of dataflow in GPU-GPU communication over advanced networks - with significant interest from industry (Mellanox, Intel, Nvidia) and supercomputing centres [Boyle gave a plenary talk at Nvidia's 2021 GTC conference, an invited talk at the 2020 HPC Advisory Council, and an invited talk at the 2021 Exascale Computing Project all hands meeting] has significant technical overlap with the technical elements of **AI enhanced Detectors, Accelerators and Sensors.**

Specifically: "Against the backdrop of exponentially increasing data rates, sustainable data management will require increasingly powerful, lower-level processing capabilities to produce the best possible value of information per available power as a critical figure of merit." describes the technical challenges we address daily, while "These pipelines will require careful design, management, and optimization, in terms of placement of compute power, storage, algorithms (including AI), and network connectivity in accelerators" overlaps with our hardware aware algorithms proposal. We have forced multiple vendors (Atos, Intel) to revise software stacks to deliver wirespeed capability and have a coherent proposal for "smart" algorithms on modern hardware. We believe the technological sophistication of our proposal can be useful more widely within BNL with sharing of know-how and techniques. In fact our approach to programming these devices is near-real-time. Boyle was invited to give a plenary talk at the IEEE "Real Time" conference in 2018, largely because of the deep connection between advanced HPC optimisation and dependable real time execution.

The ML element of our proposal also aligns well with "**Optimal experimental design and steering**". Specifically, "continued development of algorithms for end-to-end automation, uncertainty propagation, and optimal design under uncertainty for multi-stage, multi-fidelity, multi- modal workflows" matches our aim for algorithms that self-learn the optimisation of multi-length-scale physics and collective degrees of freedom. Regarding multi-fidelity, the key is to embed these approximations in an exact algorithm (the Metropolis algorithm is a good example) that "self heals" the black box that machine learning represents. Markov chain monte carlo is a natural fit for this, and we hope that lessons learned from our proposal will be transferable to other domains.

We emphasize that MCMC for High Energy Physics has a long history of developing transferable techniques that have been applied in a broad range of areas. The downstream science enabled by this proposal will enable a decadal program of theoretical calculation providing input to important DOE experiments including EIC, g-2 and Belle II.

8. POTENTIAL FUTURE FUNDING

Identify below the Agencies and the specific program/office, which may be interested in supplying future funding. Give some indication of time frame. This information is required.

The potential for future funding and attracting science to Brookhaven is both short term and long term, and we can look at appropriations for the next five years and identify opportunities.

https://science.osti.gov/-/media/budget/pdf/sc-budget-request-to-congress/fy-2022/FY_2022_SC_HEP_Cong_Budget.pdf

In the short term and for conventional algorithms, we anticipate applying for funding from the next SciDAC recompete, with the aim of producing BNL leadership in an EIC focused SciDAC-NP (at $1M per year) and to lead rebuilding SciDAC-HEP (which was subsumed into ECP at $2M per year in the last 5 year cycle). The next cycle of funding is expected to start in 2024, and this LDRD will place us in a strong position as more science becomes enabled by Brookhaven software and algorithms.

The $35.8M AI/ML budget may admit further proposals for ML based acceleration of LQCD sampling based on the second strand of this proposal.

ASCAC foresees a decade of DOE science powered by AI. In the longer term this LDRD proposal seeks to create an opportunity for BNL to lead the application of AI to Lattice Gauge theory. The US will want to continue to dominate world scientific computing, and with AI emerging as a powerful tool it is very likely that DOE will produce funding rounds that enable science to exploit ML in a transformative way. The ML powered algorithm direction we wish to explore is a foundational seed that would position us to attract and exploit the scientific and funding opportunities.

https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202004/Transition_Report_202004-ASCAC.pdf

https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202009/AI4Sci-ASCAC_202009.pdf

Finally, the science this proposal can bring to Brookhaven is very significant. Both HET and NT groups seek to embark on a decade of research based on the capabilities this LDRD would develop.

9. BUDGET JUSTIFICATION

Include a description of all costs requested in your budget. You do not need to describe the Lab burdens.

The work in DD-HMC is initially being carried out in a grass-roots collaboration between Boyle and Kelly. Kelly is partially funded by the DOE Exascale Computing Project while Boyle is unfunded. Once the basic software development is complete we hope that the LDRD will fund a **postdoc-1** for 3 years to research the algorithmic development and performance research, along with the simulation work needed to prove algorithmic performance and select simulation discretisations and parameters for a decadal programme of research. The postdoc will also test this algorithm in combination with open boundary conditions (loosely speaking to make "introducing hurricanes easier") and Fourier accelerated algorithms such as RMHMC and the ML work of postdoc-2.

The work in ML based FT-HMC has also started in a grass-roots fashion with weekly meetings of the investigators. This work is initially led by (unfunded) investigator Luchang Jin, and subsequently (years 0.5/1.0/0.5) by **postdoc-2**. This is appropriate since the work requires focused effort in development of the basic framework followed by a ramp in searching over (large) space of possible neural network structures for both a fast-to-train and a fast-in-operation algorithm. Given the worldwide level of effort being thrown at ML directions in LQCD, our request for support is modest, but we believe our ideas are sound and being based on a change of variables under the established best-practice HMC are more likely to work. This does seem very much a level of work appropriate to the staff effort and a full post-doctoral position.

The **visiting PhD** student will work with Post-doc 1, Mukherjee and Boyle to implement Milestone 3 in the GPT framework and prepare BNL to translate the opportunity created into scientific input to the EIC.

The remaining **staff time** is required to both supervise the postdoctoral and PhD effort, and to contribute to the effort at around the 10% level. As indicated, initial software development to kickstart these programmes is *already* being invested without funding, to kickstart this programme. We think it is a significant strength of this proposal that CSI, HET and NT already view it as so important that there are cross-division grass roots activities with weekly meetings working on these topics. This is already truly interdisciplinary.

Access to GPU computing resources has been offered by CSI. Laptop and desktop computers for the postdocs and PhD student are requested ($10k) and annual travel for conference presentation of work ($10k p.a.) is requested. $15k is budgeted for post-doc relocation.

10. NAME OF SUGGESTED BNL REVIEWERS

Provide the name of two BNL subject matter experts who may be contacted as potential reviewers of your proposal. Their reviews will be in addition to those conducted by the Associate Lab Directors and Directors of the Computational Science Initiative and Advanced Technology Research Office, Members of the Brookhaven Council, and Scientists not associated with the research.

Hubertus Van Dam (CSI)
Peter Petreczky (NT)
Rob Pisarski (NT)

APPROVALS (NPP)

Business Operations Manager Susan M. Pankowski
Susan M. Pankowski

Department Chair/Division Manager Hong Ma
Hong Ma

Associate Laboratory Director
for Nuclear and Particle Physics
Haiyan Gao

APPROVALS (CSI)

Business Operations Manager

Department Chair/Division Manager Francis J Alexander

Computational Science
Initiative Director
Kerstin Kleese van Dam

NEED TITLE
(FY22 Call TYPE A)
P. Boyle

Resource Category DESCRIPTION	FY22	FY23	FY24	
050 Salary - Scientific	51,608	24,875	58,888	
051 Salary - Research Assoc	99,950	103,015	106,249	
050 Salary - Professional	0	0	0	
050 Salary -Technical	0	0	0	
050 Salary - Management & Admin.	0	0	0	
Total FTEs	1.87	2.18	1.90	
TOTAL SALARY/WAGE & FRINGE	151,558	127,891	165,137	
180/185 Consultants/Research Collab	40,000	40,000	40,000	
201 RECHARGE LABOR - CSI	118,400	167,504	125,915	
TOTAL PURCHASED LABOR	158,400	207,504	165,915	
280 Foreign Travel				
290 Domestic Travel	10,000	10,000	10,000	
various Material Purchases	10,000		0	
TOTAL MSTC	20,000	10,000	10,000	
170 Relocation Expense	15,000			
240 Registration Fees	0	0	0	
271 Communications				
TOTAL COM/MISC	15,000	0	0	
480 Space				
TOTAL SPACE	0	0	0	
TOTAL DIRECT COSTS	344,958	345,395	341,053	
251 Electric Distributed (Electric Power Burden)	1,212	1,023	1,321	
700/701/481 Organizational Burden	16,823	14,196	18,330	
TOTAL ORGANIZATIONAL BURDEN	18,035	15,219	19,651	
745 Procurement (Material Handling)	1,400	700	700	
710 G&A Burden	0	0	0	
720 Common Support	135,607	138,686	138,596	
722 Safeguards & Security Assess	0	0	0	
TOTAL LABORATORY BURDEN	137,007	139,386	139,296	
705 LDRD Burden	0	0	0	
TOTAL PROGRAM COSTS	500,000	500,000	500,000	1,500,000

Labor Band	Name	FY22		FY23		FY24	
		FTE	Amount	FTE	Amount	FTE	Amount
RA2	Post Doc	1.00	99,950	1.00	103,015	1.00	106,249
RA3	Post Doc (CSI) See CAT 201	0.50	0	1.00	0	0.50	0
SCI1	Kelly, C. (CSI) See CAT 201	0.09	0	0.04	0	0.10	0
SCI2	Lin, Meifeng (CSI) See CAT 201	0.09	0	0.04	0	0.10	0
SCI3	Izubuchi, T.	0.09	23,416	0.04	11,287	0.10	26,719
SCI4	Boyle, P.	0.09	28,192	0.04	13,589	0.10	32,169
	Total	1.87	151,558	2.18	127,891	1.90	165,137