Nuclear Science Long Range Plan and Computing

26th International Conference on Computing in High-Energy & Nuclear Physics (CHEP2023)

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Acknowledgment

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And

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Monday’s keynotes by David Dean and Markus Diefenthaler covered Computing and future trends in NP computing very well and thank you!

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1979 LRP (~30 people @ meeting, recommendations in table)
1983 LRP (J. Schiffer)
1989 LRP (P. Paul)
1996 LRP (E. Moniz/H. Robertson)
2002 LRP (J. Symons)
2007 LRP (R. Tribble)
2015 LRP (D. Geesaman)
2023 LRP ongoing (G. Dodge)
(town meetings: ~1300, ~600 (in person)
DOE/NSF Charge for NSAC

The new NSAC LRP should articulate the scope and the scientific challenges of nuclear physics today, what progress has been made since the last LRP, and the impacts of these accomplishments both within and outside the field. It should identify and prioritize the most compelling scientific opportunities for the U.S. nuclear physics program to pursue over the next decade (fiscal year (FY) 2023-2032) and articulate its potential scientific impact. Further, a nationally coordinated strategy for the use of existing and planned capabilities, both domestic and international, and the rationale for new investments should be articulated. To be most helpful, the LRP should indicate what resources and

Town Hall Meetings (led by Division of Nuclear Physics, APS) are part of the NSAC LRP exercise:

- Nuclear structure, reactions & astrophysics, ANL, Nov. 14-16, 2022
- Fundamental symmetries, neutrons, neutrinos, UNC Chapel Hill, Dec. 14-16, 2022
- Hot and Cold QCD, MIT, Sept. 23-25, 2022
Next decade intellectual challenges for nuclear structure, reactions and astrophysics captured in new questions

What is the nature of the nuclear force that binds protons and neutrons into stable nuclei and rare isotopes, and how do the rich phenomena of nuclear structure and reactions emerge?

How do single-nucleon, cluster, and collective degrees of freedom coexist and evolve with increasing proton-neutron imbalance and excitation energies?

What are the limits of nuclear existence, and what features arise near and beyond these limits?

What are the astrophysical origins of the elements and how did the associated chemical evolution proceed?

How do stars evolve, and what nuclear signatures do they leave behind?

What is the nature of neutron stars and dense matter?

How can the knowledge and technological progress provided by nuclear science best be used to benefit society?

https://indico.phy.anl.gov/event/22/attachments/72/393/TownMeeting_Whitepaper_StructureReactionsAstro.pdf
To answer these questions: research program in nuclear structure, reactions, astrophysics with experiment+theory working in concert

Arrive at a predictive understanding of atomic nuclei and their decays and reactions

Provide accessible, state-of-the-art, accredited nuclear data to advance nuclear science and its broad applications

Chart the limits of nuclear existence

Reveal the underlying nuclear physics of stars, stellar explosions, and element synthesis in the cosmos

Apply nuclear science for societal benefit

Leverage the properties of nuclei to enable precision tests of nature’s fundamental symmetries
Computing from Nuclear structure, reactions & astrophysics

HPC at the Exascale
Predictive capabilities:
• Structure & reactions of light nuclei
• Nuclear matrix elements
• Neutrino & electron int.
• Nuclear matter; Fission
• Nucleosynth., explosions

AI/ML
• UQ, extrap. in structure, reactions, astrophysics
• Fast, accurate emulators
• Experiment design
• Detect. design, particle id, beam tuning, upgrades
• ML for ‘multi-setup’ data
• Training of large models

QC
• Ideal for many-body syst.
• Solve NP problems with known ‘classical’ issues
• Algorithms & demos: state prep; time evol.; spectral density
• Guide QC hardware design

Needs
• Support for refactoring/optimizing codes
• Increased access: Capacity, HPC, many-core (GPUs, tensor proc. units) computer resources
• Interdisciplinary Collabs: Math, CS; AI/ML; QIS

For all your charged particle, neutron and photon detection needs
Define environments that can scale from simple desktop machines to HPC systems.

Compatibility with legacy software.

Ability to extend to any number and type of auxiliary detectors from different universities or national laboratories.

Ability to readout data in trigger-less mode to bypass issues as event pile-up or overlapping of signals from different events.

Ability to analyze data at 100x incoming rate to support decision making in real time.

Taking advantage of AI/ML for tasks such as automatic beam tuning, particle identification, event reconstruction and classification…
Report from the “Fundamental Symmetries, Neutrons and Neutrinos” Town Hall

Vincenzo Cirigliano
University of Washington

Co-Conveners:
Leah Broussard (ORNL), Jon Engel (UNC), Lindley Winslow (MIT)

275 participants, of which ~ 180 in person
December 13-15, 2022

APS April Meeting
April 16-23, Minneapolis
Nuclear Science FSNN portfolio

- Three classes of low-energy probes, pushing the boundary of BSM sensitivity in qualitatively different ways and at different mass scales

1. **Searches for rare or SM-forbidden processes** that probe approximate or exact symmetries of the SM (L, B, CP, Lα):
   - $0\nu\beta\beta$ decay, EDMs, n-nbar oscillations, $\mu \rightarrow e$ conversion, $ep \rightarrow \tau X$, …

2. **Precision tests** of SM-allowed processes: $\beta$-decays (mesons, neutron, nuclei), muon $g$-2, PV electron scattering, HPV, …

3. **Searches / characterization of light and weakly coupled particles**: active $\nu$'s, sterile $\nu$'s, dark sector particles and mediators, axions, …
Shedding light on big questions

FSNN probes cluster around four interconnected questions

1. Rare / forbidden processes
2. Precision tests
3. Light & weakly coupled

Origin of neutrino mass
- $0\nu\beta\beta$
- Absolute $\nu$ mass, $\nu$ scattering, sterile $\nu$, ...

Nature of dark matter
- PV electron scattering, Muon g-2, $\beta$-decays, ...
- Searches for dark bosons (e-scattering), neutron interferometry ...

Baryon asymmetry (violation of B, L, CP)
- EDMs, ..., $n-\bar{n}$ oscillations

Are there new forces, weaker than the weak force?
Key Computational Challenges for FSNN

- Exposure-limited sensitivity: precious data
  - All data on disk
  - Optimization → reprocessing
  - Remote access
- Few groups make use of massive parallelism at present
- Many groups not associated with a major facility
- If anyone sees a BSM signal, theorists are suddenly going to need a lot more computing.

- **Project 8**: Cyclotron Radiation Emission Spectroscopy
  - RF time series recorded at 100 MB/s per receiver (~3 PB/yr)
  - Locate tracks and measure energy, pitch, other topology info (FFT, DBSCAN, Consensus Thresholding, KD-Trees, Hough Transforms…)
  - Current: 1 receiver, short runs: TB of data, hundreds of kCPU-hrs processing, little parallelism.
  - Future: 60 receivers, longer runs → ~200 PB/yr, millions of CPU-hrs. Data reduction and GPU methods under investigation.
LQCD + neutron decay now places tightest constraints on right-handed BSM currents

Adapted from: Alioli, S., Cirigliano, V., Dekens, W., de Vries, J., and Mereghetti, E. JHEP 05, 086 (2017)
Hot and Cold QCD Town Meeting, September 23-25, 2022, MIT

Ian Cloët (ANL)
Or Hen (MIT)
David Lawrence (JLab)
Wei Li (Rice)
Swagato Mukherjee (BNL)
Bjoern Schenke (BNL)
Anne Sickles (Illinois)
Ramona Vogt (LLNL & UCD)
Feng Yuan (LBNL)
Xiaochao Zheng (UVA)

https://indico.mit.edu/event/538/

422 registered participants, ~ 200 in-person
Probing the hot QCD

Hard: Jet, heavy flavor, …
Soft: anisotropy ($v_n$), correlations, fluctuations, …
EM: photon, dilepton, …

Experiments:
Relativistic Heavy Ion Collider (RHIC) @ BNL; Large Hadron Collider (LHC) @ CERN
CBM@FAIR
Cold QCD: from quark to cosmos

How do the spin and orbital degrees of freedom of quarks and gluons within the nucleon combine to make up its total spin?

What is the origin of the mass of the nucleon and other hadrons?

Do gravitational form factors inform us about the origin of mass and can they be extracted from measurements?

Where are the quarks and gluons located within the nucleon?

How does the quark-gluon structure of the nucleon change when it is bound in the nucleus?

What is the spectrum and structure of conventional and exotic hadrons?
Current major DOE QCD facilities

Enhanced capabilities in existing Halls

2022: Joint effort from both hot and cold QCD

QCD White Paper
Project Design Goals

- High Luminosity: \( L = 10^{33} - 10^{34} \text{cm}^{-2}\text{sec}^{-1}, \) 10–100 fb\(^{-1}\)/year
- Highly Polarized Beams: \( \sim 70\% \)
- Large Center of Mass Energy Range: \( E_{\text{cm}} = 20–140 \text{ GeV} \)
- Large Ion Species Range: protons – Uranium
- Large Detector Acceptance and Good Background Conditions
- Accommodate a Second Interaction Region (IR)

Conceptual design scope and expected performance meet or exceed NSAC Long Range Plan (2015) and the EIC White Paper requirements endorsed by NAS (2018)
Complete RHIC Science Mission in 2015 NSAC LRP

- sPHENIX will use energetic probes (jets, heavy quarks) to study quark-gluon plasma with unprecedented precision
- How the structureless "perfect" fluid emerges from the underlying interactions of quarks and gluons at high temperature

RHIC data taking scheduled for 2023–2025
sPHENIX upgrade and STAR with forward upgrade will fully utilize the enhanced (~50 times Au+Au design) luminosity of RHIC

Most demanding in the next decade prior to EIC full luminosity
RHIC computing evolution

4-6 increase over the next 3 years

- ~70k CPU cores
- >700 PB on Tape
- Lustre 100 PB
sPHENIX Data Streaming and nearline processing

Trigger readout
- FEM
- DCM2
- SEB
- Buffer Box

Streaming readout
- FEE
- FELIX
- EBDC
- Buffer Box

FEM/FEE: Front-End Module / Electronics
DCM2 - Data collection Module (v2)
FELIX - ATLAS-developed readout card
SEB - SubEvent Buffer
EBDC - Event Buffer and Data Compressor

100+ Gigabit Crossbar Switch

10 GB/s

Processing
Archive

Calorimeters, MBD
TPC, MVTX, INTT
sPHENIX
Data Streaming and nearline processing

Events are distributed over 60 files
Nearline reconstruction

- 1st pass tracking
- 2nd pass tracking
- Calorimeters

Offline Event writing / reading

We are storing individual files at the SEB/EBDC level on central servers

This makes our operations a lot less risky, less moving parts, simpler software

For the reconstruction, one would need to combine about 60 files with the pieces of a given event

Online, we would do that for a fraction of event (like 10-50Hz worth) for onl. monitoring

Demonstrated
- Data streaming: 90 Gbps writing into Tape system
- Sustained concurrent Write & Read to/from Lustre around 1Tbps

Particle Flow/Jet Reconstruction

Orchestrated by PanDA

2023: 65 PB

10 GB/s

Tape

Buffer boxes

60 files

Tape Buffer

RAW 20PB (2 weeks)

DST

Reconstruction

Data streaming: 90 Gbps writing into Tape system

Sustained concurrent Write & Read to/from Lustre around 1Tbps
Lattice QCD calculations will impact all of US Nuclear Physics Program

Essential for progress:

- Access to Leadership Class Computing Facilities, e.g. ALCF, OLCF through programs like ALCC and INCITE as well as NERSC and dedicated computing resources of USQCD

USQCD provides test bed of new hardware 21g cluster first cluster with AMD GPUs

⇒ Frontier at OLCF equipped with AMD GPUs

- Development of highly specialized and optimized software for lattice QCD

SiCDAC-3: 2012-2017
SciDAC-4: 2017-2022
SciDAC-5: 2023-2028
???: 2028-
Hot lattice QCD long range plan

- **sPHENIX, LHC**: state-of-the-art lattice QCD results for heavy quarks in quark gluon plasma
  - heavy quark diffusion coefficient
  - thermal masses, widths of quarkonia
  - complex static quark potential

These quantities are encoded in spectral functions
⇒ difficult inverse problem
⇒ very small lattice spacings

- Theory support for RHIC BES-2 program and CBM: extend the reach of lattice QCD calculations to larger $\mu_B$
Cold QCD: hadron structure

how properties of existing matter arise from QCD?

- how are partons inside the nucleon distributed in both momentum and position space?
- how do the nucleonic properties such as mass and spin emerge from partons and their underlying interactions?
- how do the confined hadronic states, including QCD Goldstone bosons, emerge from these quarks and gluons?

Lattice calculations of GPDs, TMDs and high momentum form-factors
⇒ Highly boosted hadrons on the lattice
⇒ Challenges: small lattice spacing, noise problem

"The scientific challenges that would unfold with EIC require a robust theory program, not simply to design and interpret experiments, but also to develop the broad implications in an understanding of the quantum world, both through analytic theory as well as through lattice QCD simulations on large-scale computers."

Algorithmic developments Exa-scale computing resources are needed
Cold QCD: hadron spectroscopy, nuclei and tests of fundamental symmetries

What is the spectrum the confined hadronic states?
How do the quark-gluon interactions create nuclear binding?
What are the short distance properties of nuclei?

Lattice calculations of light nuclei with unphysical quark masses:
• Magnetic moments and polarizabilities
• Quenching of axial charge
• Nuclear PDF, EMC effect
• Lattice calculation of $nn \rightarrow ppee$ process (A. Grebe, Z. Fu, Lattice 2022)
  input for EFT: important for neutrinoless double beta decay
  (Algorithmic progress tracking complicated contractions of two electroweak current insertions)

Hadron spectroscopy:
First ever study of full decay of exotic: $\pi_1$ is a broad resonance
(new search strategies for GlueX), Woss et al. (HadSpec), Phys. Rev. D 2021
New frontier: 3-particle amplitude calculations on the lattice
Blanton et al, JHEP 2021, Hansen et al. PRL 2021
Will allow to study more complex resonances, $a_1$, Roper etc. Challenge: Contractions cost increase rapidly

Algorithmic developments exa-scale computing resources are needed to perform calculations for physical quark mass
Exascale Computing Project (ECP)

- LQCD is a major ASCR project to develop software and applications for exascale machines at Aurora at ANL & Frontier at ORNL.
- Lattice QCD is one of the 11 applications selected to compose one of the KPPs of the project.

NEW COMPUTATIONS ON SCATTERING AMPLITUDES ILLUMINATE QUARK AND GLUON PARTICLE INTERACTIONS

July 6, 2021

A transatlantic team of researchers has provided the first calculation of the full relativistic scattering amplitude for a three-hadron system of particles, which lies at the core of outstanding questions in quantum chromodynamics. The analytical and computational methods developed in this work pave the way for future calculations in more complicated systems involving multiparticle and nuclear systems. The researchers’ findings, which support the GlueX experiment at Thomas Jefferson National Accelerator Laboratory and other programs around the world, were published in the January 2021 issue of Physical Review Letters as an Editor’s Suggestion.

The majority of visible matter in the universe is composed of quarks and gluons. Experiments at particle and nuclear physics labs around the world investigate the mass, spin, and structure of single hadrons—particles composed of quarks and gluons—as well as multihadron systems using scattering amplitudes to reconstruct and discern the internal structure of hadrons. The determination of scattering amplitudes involving two particles is fairly well established, but challenges remain for three-particle systems. The team’s work addresses challenges associated with constructing amplitudes that obey fundamental properties and symmetries consistent with relativity and quantum mechanics.

Recently in Physical Review D, the team presented the first computation of the decays of an exotic meson, a state in which the gluon degrees of freedom are manifest. This additional research predicts the existence of such a state and provides the rates for decay particle pairs. Future calculations will probe the internal structure of states of quarks and gluons through the computation of matrix
Computational Nuclear Physics and AI/ML Workshop
Priorities for the next decade

We recommend investments in computational nuclear physics to accelerate discoveries and maintain U.S. leadership by:

• Strengthening programs and partnerships to ensure the efficient utilization of new HPC hardware and new capabilities and approaches offered by AI/ML and quantum computing (QC);

• Establishing programs that support the education and training of a diverse and multidisciplinary workforce with cross-disciplinary collaborations in HPC, AI/ML, and QC;

• Expanding access to dedicated hardware and resources for HPC and new emerging computational technologies.

https://indico.jlab.org/event/581/timetable/