Low-Energy Nuclear Theory Working Group Summary

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A.I. for Nuclear Physics Workshop
Jefferson Laboratory
March 4-6, 2020

Participants:

Wednesday: 9 local and 4 remote participants
Thursday: 7 local and 4 remote participants + joint session with LQCD WG

Presentations:

Dean Lee (MSU)
Eigenvector continuation and machine learning

Sarah Wesolowski (Salisbury U)
Bayesian methods in nuclear effective field theories

Samuel A. Giuliani (MSU)
Beyond the proton drip line with Bayesian analysis

Rahul Jain (MSU)
Extrapolating Nuclear Masses using Bayesian GPR

1. Where are we?

What is the current level of understanding of AI/ML within the low-energy nuclear theory community? We introduce the following classification:

Non-user: does not use ML tools.

User: applies off-the-shelf tools.

Informed user: understands the ML glossary and makes educated choices.

Well informed user: makes informed choices about modern ML tools and considers uncertainty quantification to be an essential part of the answer.

Innovator: considers the full feedback between ML and physics problems, adapting the ML applications depending on physics outcomes.

Workshop questionnaire statistics: 38% new to AI, 70% would like to apply techniques from this workshop, 42% actively working on projects using AI.

Conclusion:

Considering the work performed so far, more sophistication is needed. Our community does not fully understand the depth of the AI/ML universe. The starting point is good. Nuclear theorists have good technical backgrounds and are used to problem-driven approaches to tool selection. This helps in choosing the best/right tools for our problems. One has to remember, however, that the newest ML tools are often untested. It takes some experience to know which tools to use. Understanding this will help nuclear theorists avoid dangerous pitfalls.

2. Need for collaborations

Long-term access to experts in AI/ML/data science is essential as it takes time for all parties involved to learn the language and methods.

Working remotely with AI/ML/data science consultants is often not effective.

Considering the low level of AI-literacy, local collaborations are better than remote.

The best solution is to hire an AI/ML/data science expert as a joint faculty member or postdoc.

Oftentimes, financial incentives are needed. SCIDAC-like programs help by facilitating connections to computer science.

How can we interface with the new DOE Office of Artificial Intelligence and Technology to create SCIDAC-like programs in AI/ML?

Conclusion:

Considering the low level of AI literacy, access to AI/ML/data science experts is essential. Establish funding mechanisms to support local and national collaborations in NP and ML/AI/data science.

3. How can we break down silos?

Inter-disciplinary research is popular. But making it succeed is difficult.

Formal mechanisms must address the issues of how people's scholarship is assessed and how their teaching is assigned and evaluated, particularly before tenure.

Conclusion:

DOE-funded bridge positions at universities would help to create joint faculty appointments at many institutions.

4. Education is key

Exciting research programs and curricula in AI/ML help to attract the best students, who can then compete for jobs in the workforce.

Establishing vigorous research efforts in AI/ML are essential to being competitive in student recruitment.

The current educational efforts in AI/ML in nuclear physics are patchwork. A coherent inter-departmental approach is needed.

Establishing graduate fellowships in the area of AI/ML/data science applied to nuclear-physics problems would help.

Dual Ph.D. programs would also help, allowing students to work across two different graduate programs.

These mechanisms incentivize data scientists to work on nuclear physics.

Online courses are better than nothing, but regular courses are preferred.

Conclusion:

Establish university-wide courses in AI/ML/data science. Establish dual Ph.D. programs in AI/ML/data science. Establish graduate fellowships in AI/ML/data science applied to nuclear physics problems.

5. Case studies

The following case studies are examples of high-impact science that will be facilitated by AI/ML applications.

5.1 Microscopic description of fission
ML can help on several levels: production of potential energy surfaces and related quantities, action minimization, dissipative dynamics, etc.

5.2 Origin of heavy elements
ML can help by providing nuclear physics input (masses, capture and decay rates, fission observables) with full uncertainty quantification.

5.3 Quantified calculation of ^{208}Pb using realistic inter-nucleon forces
Quantified predictions for heavy nuclei based on NN and NNN interactions using pseudo-data from microscopic calculations with supervised ML.

5.4 Development of a spectroscopic-quality nuclear energy density functional

A massive inverse problem that can involve a variety of ML tools. Crucial for understanding of rare isotopes.

5.5 Discovering nucleonic correlations and emergent phenomena

Unsupervised learning can be used to discover correlations in calculations of nuclear wave functions that use underlying forces. There are terabytes of data from calculations with nucleonic degrees of freedom that can be data mined to discover clustering and emergent phenomena such as superfluidity, nuclear rotation, etc.

5.6 Neutron star and dense matter equation of state

Data from intermediate-energy heavy-ion collisions can be explored to deduce the nuclear matter equation of state using ML. ML classification tools can also be used in conjunction with sophisticated simulations of the system to discover phases and associated order parameters.