

Assess the current status and future prospects of computational nuclear physics, including all the subfields (QCD, nuclear structure and reactions, fundamental symmetries and nuclear astrophysics, as well as its impact on experimental program

Discuss the potential impacts of AI/ML on nuclear theory and problems that will require quantum computing

Make preliminary recommendation on investments in computational nuclear physics that are needed to make impact on the experimental program  $\Rightarrow$  Workshop summary

Discuss the findings of this workshop at the DNP Town Hall Meetings on Hot and Cold QCD, Nuclear Structure and Astrophysics, and Fundamental Symmetries

Computational Nuclear Physics and AI/ML Workshop, SURA, Washington D.C., September 6, 2022

## Possible outline of the workshop summary

1. Executive summary

2.Progress that has been made in computational nuclear physics since 2015 (drawn from the talks)

3.Connecting to the scientific case for nuclear physics

- What are the important scientific questions that need to be explored where computational physics, combined with AI/ML can provide insights.
- What are the missing data sets that would significantly advance our modeling capabilities?
- How do current and future planned experimental capabilities within Nuclear Physics enable advances in computational nuclear physics, and how will computational nuclear physics be utilized to guide and interpret the next generation of experiments.

4.Connecting computational nuclear physics to DOE computing and applied math resources

- What are the key algorithms that must be developed or improved in order to advance the field of nuclear physics ?
- What are the key computational hurdles to be overcome in the next 5-10 years that will enable more precise comparisons of theory and experiment?
- What computational hardware capabilities are required to answer and make progress on the questions posed in section 3 ?

5.Outline specific mechanisms/capabilities that would address requirements described in section 3.

6. Conclusion.

To facilitate breakthroughs in nuclear theory and provide adequate theoretical support for the nuclear physics experimental program, investments in computational nuclear physics should be made, which include:

- 1) Strengthen and expand programs and partnerships dedicated to computational excellence in Nuclear Physics, such as SciDAC. These include continued support and development for HPC to exploit evolving hardware, support for the development of novel algorithmic approaches including as AI/ML, and the development of emerging technologies such as quantum computing.
- 2) Expand access to computational resources which are essential for progress. These include a mix of hardware resources including traditional HPC and GPU computing and disk storage, programmatic resources (such as USQCD), and DOE and NSF HPC allocations.
- 3) Establish programs to support the development of a multi-disciplinary workforce in high-performance computing including and AI/ML-based research;
- 4) Build the literacy of the NP community, enhance the educational activities in highperformance computing, quantum computing, and AI/ML.