Computational Nuclear Physics and AI/ML Workshop

6-7 September, 2022 / SURA headquarters

Organized by:
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Schedule
Registration, schedule, and other information can be found at: https://indico.jlab.org/event/581/

Tuesday, 6 September
1:00 – 1:05 Welcome, David Dean and Sean Hearne
1:05 – 1:20 DOE remarks, Tim Hallman
1:20 – 2:00 QCD, William Detmold (JLab) and Swagato Mukherjee (BNL)
2:00 – 2:40 Quantum many-body problems, Thomas Papenbrock (UT/ORNL)
2:40 – 3:00 BREAK
3:00 – 3:40 Fundamental Symmetries,Emanuele Mereghetti (LANL)
3:40 – 4:20 Astrophysics, George Fuller (UCSD)
4:20 – 5:00 AI/ML, Amber Boehnlein (JLab)
5:00 – 5:40 Preliminary list of recommendations discussion (Peter Petreczky, lead)
5:40 – 7:30 Reception

Wednesday, 7 September
7:45 – 8:30 Continental Breakfast
8:30 – 10:00 Breakout Sessions
1. QCD (Phiala Shanahan, lead)
2. Nuclear Structure and fundamental symmetries (Alessandro Lovato, lead)
3. Astrophysics (Bronson Messer, lead)

10:00 – 10:30 Break
10:30 – 12:00 Breakout reports
12:00 – 1:00 Lunch
1:00 – 2:30 Recommendations discussion and next steps

Jefferson Lab
Thomas Jefferson National Accelerator Facility

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Outline of the white paper

1. Executive summary (use BLUF: bottom line up front)
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 (3 vignettes – scidac announcements…)
   a) What are the important scientific questions that need to be explored where computational physics, combined with AI/ML and UQ techniques can provide insights.
   b) What are the missing data sets that would significantly advance our modeling capabilities?
   c) 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
   a) What are the key algorithms that must be developed or improved in order to advance the field of nuclear physics?
   b) 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?
   c) What computational hardware capabilities are required to make progress in answering the questions posed in section 3?
5. Outline specific mechanisms/capabilities that would address requirements described in section 3.
6. Flow from 5 to a recommendation and conclusion.