Answers from a user of advanced computing infrastructure

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I. RESEARCH NEEDS / OPPORTUNITIES

a. Ab-initio description (using realistic 2- and 3-body forces from effective field theory) of atomic nuclei and nuclear reactions; Accurate description of nuclear matrix elements needed for high-precision tests of the standard model; Comprehensive Energy Density Functional for the entire nuclear landscape.
   Will advance our understanding of nucleosynthesis, of the origin of the elements, of stellar burning and stellar evolution, of nuclear fision and nuclear fusion; may give us hints about physics beyond the standard model.
   All these problems deal with strongly correlated self-bound many-body quantum systems, with both repulsive and attractive forces, and both short-range and long-range interactions.

b. Not per se in my field of theoretical nuclear physics, but data-taking, -storage, and -analysis at current and future nuclear (FRIB, RHIC) and particle (LHC) experimental facilities does require data-intensive computing; in addition theoretical/computational problems that require large amount of memory could benefit from supercomputers designed for data-intensive computing.

c. yes, see e.g. DOE report 'SCIENTIFIC GRAND CHALLENGES: FOREFRONT QUESTIONS IN NUCLEAR SCIENCE AND THE ROLE OF COMPUTING AT THE EXTREME SCALE' (2010)
   http://extremecomputing.labworks.org/nuclearphysics/index.stm
   For low-energy nuclear physics, see in particular pages 153 - 165
   and NAS study 'NUCLEAR PHYSICS: EXPLORING THE HEART OF MATTER' (2013)
   http://www.nap.edu/catalog/13438/nuclear-physics-exploring-the-heart-of-matter
   For low-energy nuclear physics, see in particular pages 51 - 56

d. Storage of large data-sets (e.g. wavefunctions) , to be used for postprocessing at a later date, may become problematic (tens to hundreds of TBs / year).

II. ADVANCED COMPUTING CAPABILITIES, FACILITIES, REQUIREMENTS

e. Everything from laptops/desktops for data analysis to leadership-class facilities (Mira, Titan, Blue Waters, K, . . .) for large production runs. We do not use commercial cloud services. Both capacity computing at medium-sized facilities (up to petascale) and capability computing at leadership-class facilities are essential for our research.

f. Rely on repositories at supercomputing facilities (NERSC, ALCF, OLCF)

g. Support from computer scientists is essential for us to keep up with computer hardware developments: we have / had collaborations with computer scientists through DOE–SciDAC and NSF–PetaApps; I regularly go to training workshops; and we also get support through early-science projects.

h. I, or more general, theoretical nuclear physicists develop and maintain codes (in Fortran or C, with MPI plus OpenMP), with help from computer scientists as mentioned above.

i. Barely.

III. CHALLENGES AND SUGGESTIONS

j. Stability of the compute environments, as well as stability of support
(it takes time to explain the nuclear physics problems and our needs to a computer scientist and to have an effective collaboration going);
Rapid developments in hardware, which make it very hard to keep up with efficient codes for current and next-generation systems.

k. Support for software maintenance and development
(performance and efficiency improvements for current and future systems);
For our own computing needs: Access to large-scale systems with sufficient memory per core (aggregate memory is our biggest constraint); but if I look at the field in general, access to several different large-scale systems with different balance of capabilities.

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