Keynote Lecture

KN12

Neutrons and supercomputing for Complex Biological Systems

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Frontier challenges in biological research increasingly require gaining a predictive understanding of complex dynamic and flexible multi-component systems. Gaining that understanding can come from combining several experimental approaches to inform multi-scale computer models and simulations. Complementary experimental approaches used include electron microscopy, mass spectrometry, X-ray scattering, and NMR, but outstanding challenges remain. Neutron scattering has great potential to address the remaining challenges by providing elusive information that cannot be obtained otherwise. Researchers are now gaining access to new instrumentation on intense neutron beam lines at the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL). An unprecedented opportunity exists that we are exploiting by developing and broadening the use of neutrons in biological research by leveraging deuterium labeling and high performance computing. In order to develop this innovative integrated approach, and to take full advantage of the increase in availability and capability of neutron beam lines, further technological advances are required. In this talk I will present an overview of neutron facilities at ORNL, and give examples of their growing application in biological research. I will then discuss how the future challenges in biology are driving further technological developments that will lead to new understanding in the emerging areas of dynamic functional assemblies, disorder and flexibility, biological membranes and associated complexes, and biomolecular function and ligand binding. Neutrons can provide unique information that will transform these areas of research, opening up new lines of biological inquiry.

Keywords: Neutrons, High Performace Computing, Biological complexes