Scheraga receives supercomputer processor hours

Cornell University
By Lauren Gold [1]

The U.S. Department of Energy (DOE) has awarded 6 million supercomputer processor hours at the Argonne National Laboratory to Harold A. Scheraga, Cornell's George W. and Grace L. Todd Professor of Chemistry Emeritus, Adam Liwo, Cornell senior research associate and professor of chemistry at the University of Gdansk, Poland, and colleagues to study the mechanism behind protein folding.

Scheraga, Liwo and colleagues at Cornell and the University of Gdansk will use the IBM Blue Gene supercomputer to study the dynamics of the interactions of proteins with HSP70, which plays a crucial role in helping amino acid chains fold into the correct three-dimensional structure of a protein inside human cells.

The shape a protein molecule takes when it folds determines its biological activity. Proteins that fold incorrectly or aggregate with other molecules are associated with a variety of diseases, including Parkinson's disease, Alzheimer's and cancer.

When a protein is synthesized, "it has two choices: it can fold properly, or it can aggregate," said Scheraga. Understanding the mechanism behind proper folding could lead to new ways of treating such diseases.

In human cells, HSP70 acts as a so-called chaperone molecule, binding with other protein chains to help them fold correctly or even refold those that are misfolded. The chaperone also plays a role in preventing aggregation and programmed cell death.

The researchers will use the supercomputer's thousands of parallel processors over one year to simulate the dynamics of the interactions of proteins with HSP70 as they transition from their inactive to active form, and as they bind to the chaperone, which controls the folding process.

By calculating the potential energy of interaction between each amino acid of the protein and the chaperone, the simulations will provide a better understanding of the role chaperone molecules play in the process.

The DOE awarded the grant through its Innovative and Novel Computational Impact on Theory and Experiment program, which supports computationally intensive large-scale research projects with the potential to significantly advance key areas in science and engineering. This year the program awarded 1.6 billion supercomputer hours at Argonne and Oak Ridge National Laboratory to 67 projects, chosen based on peer review and computational readiness.

SOURCE [2]

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