

## MODELING

# New institute will explore complex biological interactions

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Homewood

Supported by a three-year \$2.7 million grant from the U.S. Department of Energy, Johns Hopkins and two partner institutions, the University of Delaware and Los Alamos National Laboratory, have established a new advanced institute dedicated to computational biology research and education.

The Institute for Multi-Scale Modeling of Biological Interactions will draw on a variety of scientific disciplines to study biological systems across multiple scales of time and length, ranging from protein interactions at the molecular level to the behavior of complex biochemical networks in entire organisms.

“Applications of mathematical modeling and simulations to describe biological interactions have become increasingly important in recent years as a complement to traditional laboratory research,” said Michael Paulaitis, a Johns Hopkins professor of chemical and biomolecular engineering, who will serve as director of the new institute. “However, in recognizing the growing acceptance of the computational methods themselves, this new institute will focus on applying combinations of computational methods as a general and clearly powerful approach to unraveling the hierarchical nature of complex biological interactions.”

The institute is unique in that it will involve more than 20 faculty members from three divisions within Johns Hopkins—the Whiting School of Engineering, the Krieger School of Arts and Sciences and the School of Medicine—as well as faculty from Delaware and researchers from Los Alamos.

The participants come from such diverse disciplines as biophysics, chemistry, physiology, chemical and biomolecular engineering, biomedical engineering, mechanical engineering, and electrical and computer engineering.

Three faculty members will serve as institute co-directors: Bertrand Garcia-Moreno, professor of biophysics at Johns Hopkins; Pablo Iglesias, professor of electrical and computer engineering at Johns Hopkins; and Abraham Lenhoff, professor of chemical engineering at the University of Delaware.

William R. Brody, president of Johns Hopkins, said, “The new institute, which will help train the next generation of researchers in the emerging field of computational biology, is an outstanding example of the type of multidisciplinary collaboration that is so important in the advancement of science and technology.”



**Structure prediction of the complex formed between a prion protein and an antibody fragment made using computer models created in the laboratory of Jeff Gray, faculty member in the Institute for Multi-Scale Modeling of Biological Interactions.**

The institute builds on the Program in Computational Biology at Johns Hopkins supported by a Burroughs Wellcome Fund “Interfaces” seed grant. Awarded in 1999, that five-year initiative supported interdisciplinary training in computational biology at the interface between the biological sciences and the physical, chemical and computational sciences at Johns Hopkins. According to Paulaitis, “The Institute for Multi-Scale Modeling of Biological Interactions represents our next step in an integrated, multidisciplinary approach to computational biology.”

The federal grant will allow the new institute to support doctoral students and postdoctoral fellows. Each will choose two faculty mentors and select research projects that involve modeling or computer simulation of biological interactions on different time/length scales.

To complement the research, the institute will also offer courses on such topics as the modeling of biological macromolecules, properties of macromolecular solutions, membrane biology and systems biology.

About 10 graduate students and postdoctoral fellows are expected to participate in the institute’s training program at any one time. Several postdoctoral fellows have already entered the program at Johns Hopkins, Paulaitis said, and the first doctoral students are expected to enroll next fall; in addition, two doctoral students have begun the program at the University of Delaware. Researchers at Los Alamos will be available to serve as co-mentors.