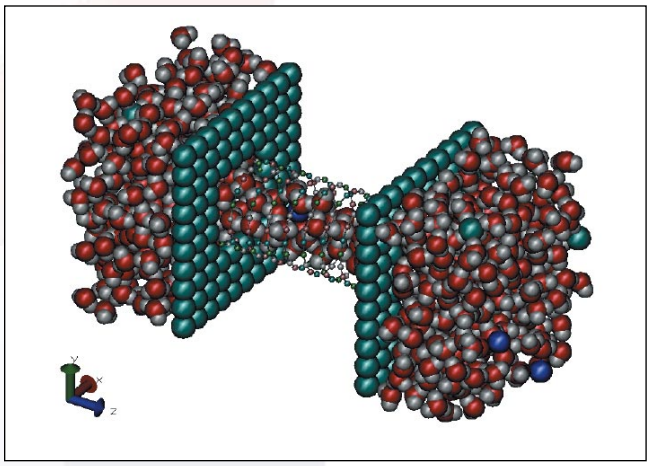
BIOTECHNOLOGY
CAPABILITIES

Sandia National Laboratories

BIOINFORMATICS & COMPUTING

Computational Science

Sandia is employing its world-class computing and computational science capabilities on computational biology problems. Such applications include computational tools for analyzing and understanding data from high-throughput experimental methods (bioinformatics), relating protein molecular structure to function (molecular biophysics and chemistry), and modeling cellular behavior



Snapshot of a molecular dynamics model where the selectivity of different ions in an ion channel was studied.

as a whole (complex system modeling). Many of the computational capabilities developed for Sandia's historical missions (e.g., parallel I/O, massively parallel computing architectures, algorithms and enabling technologies, molecular physics and chemistry, and complex system modeling) have found immediate applicability to life science and computing for life science problems. Sandia works with a wide variety of universities and nonprofit institutions and are funded primarily through DOE and other federal agencies.

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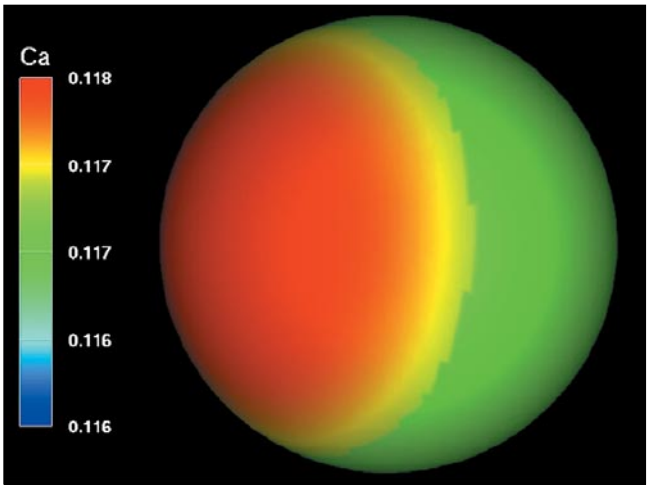
Modeling and Simulation

Modeling and simulation will have a significant impact on advances in biotechnology and medicine. It can extend from instrument and device design to modeling of complex biological systems such as entire cells to gain understanding of biomolecular processes to predict likely behaviors of organisms under varying conditions.

Sandia offers a broad range of expertise and a variety of modeling and simulation tools that can analyze complex biological systems. For example, Sandia's GOMA code, with its capability to treat moving boundaries, capillary and electrostatic forces, can simulate multi-species transport within the human body. The MPSalsa code has been used for micro-chem-lab design, analyte gaseous transport, and other biomedical areas of interest.



Density plot of calcium ions in a Xenopus Laevis frog egg immediately after fertilization.

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Scientific Data Discovery

The pattern recognition technique of "ensemble classifiers" is generally recognized as the best means of applying parallel processing to mining scientific data. Sandia is a leader in applying this technique to scientific data, which generally presents a unique combination of challenges. The data we handle is huge, noisy, and the regions of interest in the data are comparatively tiny; the problem is much like looking for a needle in a wind-swept hayfield.

As a result, the practical and analytical tools provided by ensemble classification are essential. In our computational modeling of molecular recognition, for instance, ensemble classifiers improved our overall sensitivity and specificity, allowed us to select the sensitivity specificity trade-offs we wanted, and provided confidence intervals.

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Computational Docking

Sandia has an active effort in computational docking calculations. These calculations simulate the interactions of biological molecules at the atomistic level and provide the fundamental basis for understanding important biological processes such as how a protein binds to its receptor, how an antibody interacts with an antigen, or how a drug molecule interacts with its target protein. Docking can further be used to predict which molecules will bind to a target biological molecule. For example in the pharmaceutical industry, docking calculations are used to identify new potential drugs to bind (and block) a particular target macromolecule. We are developing new docking tools that take advantage of the massively parallel computing capabilities at Sandia to add more realistic physics to our calculations. Our current focus is in biodefense, where we are applying these calculations to identify small molecule ligands that bind and recognize known biowarfare agents, and can be used in affinity-based detection systems.

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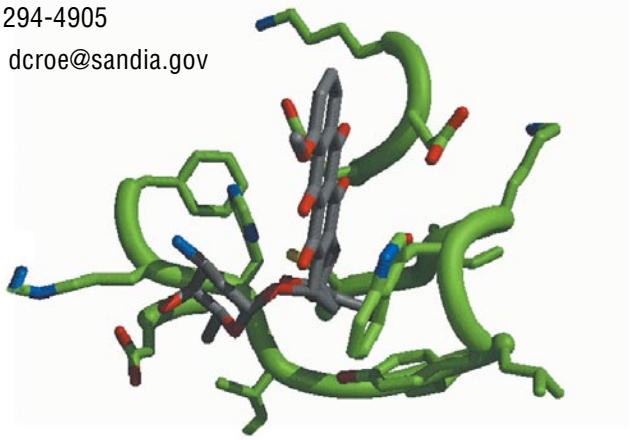

Small molecular (gray) bound to tetanus toxin (green), identified using docking calculations.

LOCKHEED MARTIN

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