Challenges in Creating an Infrastructure for Physics-Based Simulation of Biological Structures

Russ B. Altman
Department of Genetics
Stanford University Medical Center
300 Pasteur Drive
Stanford, CA 94305-5120
russ.altman@stanford.edu

Physics-based simulation provides a powerful framework for understanding biological form and function. Physical simulations may be used by biologists to study macromolecular assemblies and by clinicians to examine disease mechanisms. Simulations help biomedical researchers understand the physical constraints on biological systems as they engineer novel drugs, drug delivery systems, synthetic tissues, medical devices, and surgical interventions. Although individual investigators have made elegant contributions to physics-based modeling in biomedicine, the field is fragmented. Modeling applications are typically limited to a single physical scale, and individual investigators frequently must create their own software. These conditions create a major barrier to advancing simulation capabilities, and its general availability to biomedical researchers working on problems critical to health. We have established a National Center for Physics-Based Simulation of Biological Structures (Simbios, http://simbios.stanford.edu/) to help integrate the field and accelerate future research.

Simbios is developing, disseminating, and supporting a simulation tool kit, SimTK, (http://www.simtk.org/) that will enable biomedical scientists to develop and share accurate models and simulations of biological structures from molecules to organisms. The challenges to this effort include (1) the creation of an open-source, extensible, object-oriented framework for manipulating data, models, and simulations, (2) encouraging a culture of sharing among scientists who develop innovative methods for physics-based simulation, (3) balancing the needs of biomedical researchers who want end-to-end applications, with tool builders who want access only to key algorithms, and (4) ensuring that our models, methods, and applications are disseminated and applied to important problems in biomedicine, thus accelerating progress in understanding and fighting disease.

In order to guarantee that real biomedical problems inform the creation of SimTK, the first set of driving biological problems for Simbios have been selected across physical scales and include RNA folding & dynamics, myosin dynamics, biomechanics, and cardiovascular fluid dynamics. The software we create is built by teams working to innovate and push the frontiers of science in these four areas, but will be applicable to a much wider range of application areas. We have an active set of additional collaborations to ensure generality.