Nicholas S. Flann, Department of Computer Science, Utah State University, Logan, UT 84322-4205, USA
Ahmadreza Ghaffarizadeh, Department of Computer Science, Utah State University, Logan, UT, USA
Gregory J. Podgorski, Department of Biology, Utah State University, Logan, UT, USA
Seunghwa Kang, Pacific Northwest National Laboratories, DOE, Pasco, WA, USA
Simon Kahan, Department of Computer Science, University of Washington, Seattle, WA, USA
Jason E. Mcdermott, Pacific Northwest National Laboratories, DOE, Pasco, WA, USA
Ilya Shmulevich, Institute for Systems Biology, Seattle, WA, USA

BioCellion: A High-performance Computing Framework for Multiscale Modeling and Simulation of Multicellular Biological Systems

Modeling and simulation of large-scale biological systems is becoming essential in the support of high-throughput experiments and the discovery and evaluation of therapies. As the need grows for higher fidelity models that couple micro, meso and macro scale subsystems, the computational resources required are emerging as the key limitation preventing advancement. This work describes a new modeling software framework specifically designed for rapid simulation of large scale biological models that span multiple embedded scales. BioCellion utilizes high-performance computing up to petascale supercomputers (10^{15} floating point operations per second) and can simulate complex systems of billions or more cells.

BioCellion is a hybrid multicellular modeling system where biomechanical mechanisms are represented through local spatial interactions of off-lattice particles, domain scale biomolecular interactions through PDEs and intracellular regulation through ODE and/or Boolean biomolecular networks. BioCellion supports alternative levels of cellular abstraction where a cell can be represented as a single spherical particle or as a contiguous cloud of interacting particles (the sub-cellular model).

BioCellion is currently being applied to investigate a diversity of prokaryotic and eukaryotic cellular systems: biofilm-like development of yeast colonies, breast cancer micro-tumor interactions between growth and extracellular matrix degradation, the formation and homeostasis of complex thermophilic bacterial colonies, and the morphodynamics of vascularization. To support diverse model specification, a set of generic cellular mechanisms has been implemented including regulated growth and division, differential adhesion, reaction and diffusion, contact mediated signaling, contact inhibition, extracellular secretion and degradation, and chemotaxis.

BioCellion is intended to be a resource for the biological modeling community. Specific biological systems are specified using a combination of XML when utilizing mechanisms previously implemented, combined with customized c-language plugins for new mechanisms. Specialized knowledge of high-performance computing is not necessary. XML instantiations support the definition of the model domain, initial conditions, and cell type physiology as intracellular regulatory networks coupled to configurations of cellular mechanisms. A public repository of models and mechanisms will be built to enable active collaboration among modelers.

The aim of this talk is to introduce BioCellion to the broader modeling community, demonstrate its capabilities using examples from a diversity of multicellular systems and invite researchers to be part of the project as it develops.