Multiscale Modeling (MSM) Consortium Meeting & NHLBI Systems Biology Grantee Meeting
October 5, 2011

Multiscale Systems Biology Working Group

- This working group is devoted to multiple-scale analysis and simulation of biological systems, with a special emphasis on cellular phenomena.

- Our first goal is to establish on this site a clearinghouse of up-to-date information on available tools, novel concepts, and major relevant review papers in the field. This resource will aim to capture the state of the art in significant research, for purposes of advancing research, education, and training.

- Secondary goals include identifying and articulating current challenges and opportunities in the field, as well as fostering scientific collaborations.

Overview of WG Activities 2010-2011

1. Webinars

   – May 31, 2011 11am-12pm ET: The Cardiovascular System and Disease

     Translating multi-scale modelling to the Heart of the clinic: developing personalised cardiac models. Nicolas Smith, Kings College London

     Multiscale model of platelet adhesion and thrombus formation: validation with the humanized mouse. Michael King, Cornell University

   – October 28, 2011: Multiscale Modeling of Cancer

     Lance Munn, Harvard University and MGH

     Kasia A. Rejniak, H. Lee Moffitt Cancer Center & Research Institute

Upcoming Webinar

October 28, 2011: Multiscale Modeling of Cancer. 1-2pm ET

Lance Munn. "Imaging vascular dynamics"

Although therapies targeting the vasculature have had growing popularity in the past decade, we still know surprisinlgy little about how vasculature is formed or remodeled in plastic tissues such as wound beds or tumors. Intravital microscopy in transparent windows has the potential to reveal how cells organize and cooperate to accomplish critical processes such as morphogenesis and anastomosis. Facilitated by the recent availability of in vivo reporters and time-lapse imaging which allow tracking of specific cell populations, intravital microscopy is a powerful tool for determining cellular mechanisms of vascularization and tumor growth.

Kasia A. Rejniak. "Computational Bridging of Epithelial Morphogenesis and Tumor Mutations"

A major challenge in biology is the mapping of genotypic changes to phenotypic outcomes. I will present how a computational model of epithelial morphogenesis (IBCell) can address this problem by linking molecular alterations to epithelial morphology through cellular core traits. In particular, I will show an example in which IBCell interrogated with 3-dimensional experimental acinar morphologies of breast epithelial cells expressing a mutant HER2 receptor leads to identification of previously unknown core trait alterations, i.e., loss of negative feedback from autocrine secreted ECM. I will also briefly show other applications of the IBCell model.

Wiki Portal (accessed 5,469 times as of Oct 1, 2011)

Overview of WG Activities 2010-2011

Wiki Portal

Content posted in three main areas:

I. Relevant Infrastructure

Simulation Tools (e.g., Virtual Cell http://www.nrcam.uchc.edu/)

Sensitivity and Uncertainty Analysis Tools

Databases

Imaging/Visualization

Markup Languages

Ontologies

Relevant Project Portals

Standards

Disease- and Organ-Specific Resources

Education Simulation Resources

II. References: List of recent relevant publications (largely reviews and tutorials)

III. List of Participants

Simulation Tools

Biochemical Network Modeling

BISEN (Biochemical Simulation Environment) http://www.biocoda.org/BISEN/

Copasi http://www.copasi.org/

E-cell Project http://www.e-cell.org/ecell/

Gepasi (Biochemical Kinetics Simulator) http://www.gepasi.org/

JDesigner (Visual Network Design Tool) http://www.sys-bio.org

SimBiology http://www.mathworks.com/products/simbiology/index.html

Systems Biology Workbench http://www.sys-bio.org

TinkerCell (Visual Network Design Tool) http://www.tinkercell.com

Spatial Modeling

CompuCell3D http://www.compucell3d.org/

COMSOL Multiphysics http://www.comsol.com/

JSim http://nsr.bioeng.washington.edu/jsim/

Virtual Cell http://www.nrcam.uchc.edu/

Agent-based Modeling

CellSys, a modular software tool for simulation of growth and organization processes in multicellular systems in 2D and 3D implementing agent-based modeling http://msysbio.com/software/cellsys/

Chaste (Cancer, Heart and Soft Tissue Environment), a general purpose multi-scale simulation package http://web.comlab.ox.ac.uk/chaste/

DYNSTOC: a tool for simulating large-scale rule-based models http://public.tgen.org/dynstoc/

FLAME (Flexible Large-scale Agent Modelling Environment) http://www.flame.ac.uk/

MASON (Multi-Agent Simulator Of Neighborhoods… or Networks; discrete-event multiagent simulation library core in Java) http://cs.gmu.edu/~eclab/projects/mason/

NetLogo (Multi-Agent Modeling) http://ccl.northwestern.edu/netlogo/

RULEMONKEY: a tool for simulating large-scale rule-based models http://public.tgen.org/rulemonkey/

Stochastic Modeling

MCell and DReAMM (Center for Quantitative Biological Simulation Microphysiology Gateway) http://www.mcell.psc.edu/

NFsim (the network-free stochastic simulator, an open-source, modeling and simulation platform for biology) http://emonet.biology.yale.edu/nfsim/

Imaging/Visualization Tools

Cytoscape (An Open Source Platform for Complex-Network Analysis and Visualization)
http://www.cytoscape.org/

MCV (Multiscale Spatiotemporal Visualisation, Development of an Open-Source Software Library
for the Interactive Visualisation of Multiscale Biomedical Data) http://www.msv-project.eu/

NA-MIC (National Alliance for Medical Image Computing) http://www.na-mic.org/

NIfTI (Neuroimaging Informatics Technology Initiative) http://nifti.nimh.nih.gov/

3D Slicer (An open source software platform for visualization and medical image computing)
http://www.slicer.org/

V3D (3D/4D/5D Image Visualization & Analysis System for Bioimages & Surface Objects)
http://penglab.janelia.org/proj/v3d/V3D/

Disease- and Organ-Specific Resources

Human Body Simulator (Integrated Human Physiology):
HumMod http://hummod.org/

Cancer:
caBIG https://cabig.nci.nih.gov/
NCI thesaurus http://ncit.nci.nih.gov/

Cardiovascular:
The Cardiac Atlas Project http://www.cardiacatlas.org/
SimVascular Cardiovascular Modeling and Simulation Application https://simtk.org/home/simvascular/

Renal:
The Quantitative Kidney Database http://physiome.ibisc.fr/qkdb/

Overview of WG Activities 2010-2011

Special Issue of Annals of Biomedical Engineering
on "Multiscale Systems Biology"

Publication Date: Summer 2012

Editors: Scott Diamond and Michael King

What is needed?

– Is the material posted on our Portal useful for researchers and trainees?

– To make the tool list most comprehensive and up-to-date with the help of the group members

– Q: Is it possible to introduce comments on the different tools?

– Extend the coverage, e.g. Disease- and Organ-Specific Resources (Immune System, Respiratory System, Infectious Diseases)

– What should we focus on in 2012? (Suggested webinar topics, other suggestions?)