

# **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 surprisingly 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)

The screenshot shows a Firefox browser window with several tabs open, including Gmail, Reviewer Area, Google Calendar, and the current page: Multiscale Systems Biology Working Group. The address bar shows the URL: [http://www.imagwiki.nibib.nih.gov/mediawiki/index.php?title=Multiscale\\_Systems\\_Biology\\_Working\\_Group](http://www.imagwiki.nibib.nih.gov/mediawiki/index.php?title=Multiscale_Systems_Biology_Working_Group). The page features a search bar, a navigation menu, and a main content area with sections for 'Goals and Objectives', 'Participation in Working Group', 'Presentations and Recent Activity', and 'Relevant Infrastructure'. The IMAG logo is visible in the top left corner.

**IMAG**

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## Multiscale Systems Biology Working Group

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### Multiscale Systems Biology Working Group

Working Group leads: [Aleksander Popel](#), [Dan Beard](#), [Mike King](#)

#### Goals and Objectives:

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.

#### Participation in Working Group:

Participation in this working group (WG) is open to all who are interested; to join please contact one of the WG co-leads listed above. WG participants will be kept apprised of WG, Multiscale Modeling (MSM) Consortium, and IMAG discussions. Responsibilities of this working group include: (i) defining the WG title, goals and objectives, (ii) determining the current state of the art in multiscale systems biology, and identifying new challenges and opportunities, and (iii) suggesting and attending webinar presentations, contributing to WG white papers, workshops and publications. Participants will be expected to actively engage in WG activities, including managing content on the site, participating in online presentations, and other relevant activities (MSM participants are assigned IMAG wiki logins by IMAG staff). The activities of the WG should not reflect someone's personal agenda, but should represent the consensus of the group.

#### Presentations and Recent Activity

Tuesday May 31, 2011 11am-12pm ET: [The Cardiovascular System and Disease](#)

#### Relevant Infrastructure:

##### Simulation Tools

BISEN (Biochemical Simulation Environment) <http://www.biocoda.org/BISEN/>  
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/>  
CompuCell3D <http://www.compuCell3d.org/>  
Copasi <http://www.copasi.org/>  
DYNSTOC: a tool for simulating large-scale rule-based models <http://public.tgen.org/dynstoc/>  
E-cell Project <http://www.e-cell.org/ecell/>  
FLAME, Flexible Large-scale Agent Modelling Environment <http://www.flame.ac.uk/>  
Gepasi (Biochemical Kinetics Simulator) <http://www.gepasi.org/>  
JDesigner (Visual Network Design Tool) <http://www.sys-bio.org/>  
JSim <http://nsl.bioeng.washington.edu/jsim/>  
MASON (Multi-Agent Simulator Of Neighborhoods... or Networks: discrete-event multiagent simulation library core in Java) <http://cs.gmu.edu/~eclab/projects/mason/>

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# 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.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?)