IMAG

Interagency Modeling and Analysis Group

September 8 – 9, 2015, Bethesda, MD

Satellite Session September 10, 2015

2015 Multiscale Modeling Consortium Meeting

Logistics

Welcome to the 2015 MSM Consortium Meeting!

We are excited to have you here for our annual meeting of the IMAG Multiscale Modeling (MSM) Consortium. This year's meeting will incorporate presentations on three themes with breakout sessions to further discuss the topics. The meeting also includes a satellite session to further discuss topics of interest. We look forward to everyone's interactive participation throughout these three days. Enjoy the meeting!

Check-In

Check-in will begin at 8:00 AM on both of the main meeting days.

Meeting Themes

Portions of this year's meeting are dedicated to discussing pressing topics of interest to the Consortium. Each theme includes a link to a wiki page that contains a comment box for the audience to provide real-time feedback. Please go to the IMAG Wiki, www.imagwiki.org to participate (no log-in required). Everyone is encouraged to contribute!

Working Groups

Working group breakouts will occur on Day 1 with summaries of the discussions presented on Day 2. All notes should be posted on the wiki at the end of Day 1 to present on Day 2.

Wireless Access

Wireless is free at the NIH and can be accessed using the NIH-Guest-Network.

We strongly encourage you to monitor the IMAG Wiki (www.imagwiki.org) during the meeting. Attendees are welcome to post their notes on the IMAG Wiki and questions will be taken from the comments section on the event pages of the wiki during the Q&A sessions (Please identify yourself with your comment).

Webcast

Please see the IMAG Wiki, www.imagwiki.org, for instructions.

~Special Thanks to the National Institute of Biomedical Imaging and Bioengineering (NIBIB) and EMBS for their support of this year's meeting. ~

Breaks and Lunch

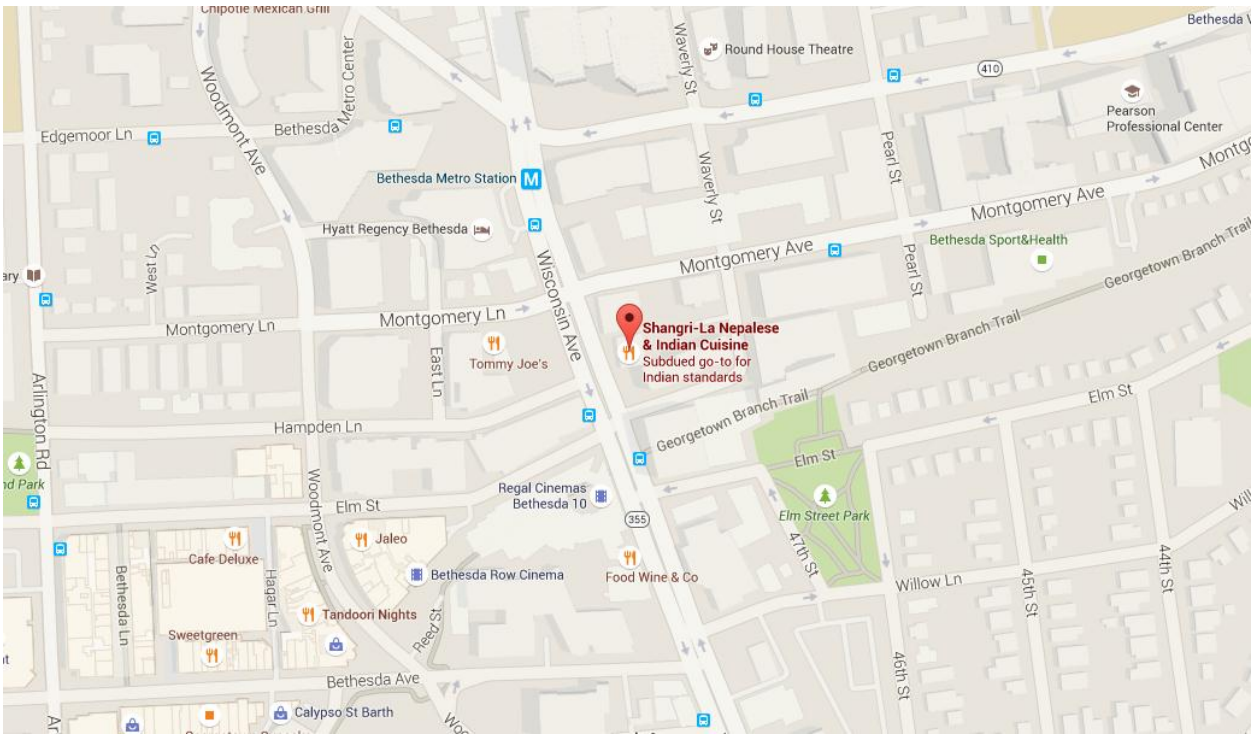
The poster session viewings and breaks will have refreshments sponsored by the IEEE Engineering in Medicine and Biology Society (EMBS). Coffee and food items are also available for purchase on the lower level of Lister Hill and in the cafeteria at Natcher (Bldg 45). **Please note that food and drinks cannot be brought into the auditorium.**

Dinner

Those who signed up for dinner should plan to arrive at Shangri-La Nepalese & Indian Cuisine on Tuesday September 8, 2015 from 6:30 – 9:30pm. If you did not sign up, and would like to attend dinner, please check at the registration if there is availability.

Shangri-La Nepalese & Indian Cuisine
7345-A Wisconsin Ave
Bethesda, MD 20814
Phone: (301) 656-4444
http://www.shangrilabethesda.com/

Those attending the group dinner should meet at Shangri-La Nepalese & Indian Cuisine at 6:30pm on Tuesday September 8, 2015. The restaurant is near the Bethesda Metro Station and the Hyatt Regency Hotel. The price per person is $30.00 including taxes and one drink. Payment will be collected at the door, upon entry, to expedite checkout.



Agenda

Tuesday September 8, 2015
8:00 – 8:30am **Check-In, Set up Posters**
8:30 – 8:50am **Welcome** 2015 MSM Co-chairs - David Eckmann and Marc Garbey IMAG - Grace Peng NIBIB - William Heetderks
8:50 –10:20am **THEME 1: Part A - Bio-medical Multiscale Modeling Success Stories and Lessons Learned** Moderator: Mark Alber Theme 1 Goal and Charge to Speakers
8:50-9:30am **Keynote** Fifteen years experience modeling fish population response to river management: Lessons learned and strategies for success Steve Railsback
9:30-10:00am The power of coupled multiscale imaging and modeling - How good is good enough? Melissa Knothe-Tate
10:00-10:30am An in vivo systems biology approach to understanding and treating tuberculosis Jennifer Linderman
10:30 – 10:50am **Refreshments* and Poster Viewing**
10:50 – 12:20pm **THEME 1: Part B - Bio-medical Multiscale Modeling Success Stories and Lessons Learned** Moderator: Lealem Mulugeta Theme 1 Goal and Charge to Speakers
10:50-11:20am Multiscale and Multi-physics Modelling of Degenerative Disc Disease and in silico Clinical Trials for Disc Repair Weiyong Gu
11:20-11:50am Responding to the Ebola Outbreak: Computational Epidemiology in the age of big data and high performance computing Madhav Marathe
11:50 – 12:20pm Theme 1 Panel discussion
12:20 – 1:20pm **Lunch on your own (Lister Hill or Natcher, Bldg. 45)**

1:20 – 2:10pm Working Group Breakout Session A	
Working Group (WG)	**Meeting Location (See Floor Plan)**
Biomechanics	Auditorium Area 1
Multiscale Systems Biology	Auditorium Area 2
Computational Neuroscience	Lobby Area 1
Theoretical and Computational Methods	Lobby Area 2
Model and Data Sharing	Alcove Area 1
Committee on Credible Practice of Modeling & Simulation in Healthcare	Alcove Area 2
2:10 – 3:00pm **Working Group Breakout Session B**	
Working Group (WG)	**Meeting Location (See Floor Plan)**
Biomechanics	Auditorium Area 1
Cell-to-Macroscale	Auditorium Area 2
Population Modeling	Lobby Area 1
Integrated Multiscale Biomaterials Experiment and Modeling Group (ImuBEAM)	Lobby Area 2
Clinical and Translational Issues	Alcove Area 1
High Performance Computing	Alcove Area 2
3:00 – 4:30pm **Refreshments* and Poster Presentations (See Floor Plan and Poster Abstracts)**	
3:00 – 3:45pm **Poster Presenters in Group 1 stand by their posters**	
3:45 – 4:30pm **Poster Presenters in Group 2 stand by their posters**	
4:30 –5:30pm **New U01 Awardee Presentations (10 minutes each)** **Microconnectomics of primary motor cortex: a multiscale computer model - Bill Lytton** **Multiscale studies of mitochondrial calcium cycling - Saleet Jafri and Jon Lederer** **Multiscale modeling and empirical study of a mechanism limiting blood clot growth - Mark Alber** **Fluid Pumping and Mass Transfer in the Lymphatic System - James Moore** **Predictive Multiscale Modeling of Microbial Consortia Biofilms - Ross Carlson** **Multiscale modeling of wound healing - Jason Haugh**	
6:30 - 9:30pm **Group Dinner: Shangri-La Nepalese & Indian Cuisine, 7345 Wisconsin Ave, Bethesda, MD 20814**	

Wednesday September 9, 2015
8:00 – 8:15am **Check-In**
8:15 – 8:20am **Welcome Back – Plans for Today**
8:20 – 9:00am **IMAG Initiative Updates** **IMAG MSM U01 (PAR-15-085) -** Grace Peng, Manana Sukhareva **NCI Cancer Systems Biology Consortium Initiative -** Dan Gallahan and Shannon Hughes **BRAIN Theories R01 (RFA-EB-15-006) -** Grace Peng **DoD Medical Simulation and Training initiatives -** Kevin Kunkler
9:00 – 10:30am **THEME 2: Multiscale Modeling Implementation into Medical Simulators/Trainers** Moderator: Marc Garbey Theme 2 Goal and Charge to Speakers
9:00-9:20am Modeling approaches for simulations of tissue deformations during robotic surgery Iwona Jasiuk
9:20-9:40am Design Approach to a Working Virtual Conversational Patient for Medical Education Thomas Talbot
9:40-10:00am MSM algorithms for medical simulator design Suvranu De
10:00-10:05am **COSINE5 meeting recap** Marc Garbey
10:05-10:30am Theme 2 Panel Discussion
10:30 – 11:00am **Refreshments* and Poster Viewing (See Floor Plan and Poster Abstracts)**
11:00 – 12:30am **THEME 3: Multiscale Modeling for Optimal Disease Diagnosis/Treatment Applications** Moderator: David Eckmann Theme 3 Goal and Charge to Speakers
11:00-11:10am Virtual-tissue computer simulations Maciej Swat
11:10-11:20am Coarse graining data-driven cellular models in multiscale simulations Scott L. Diamond
11:20-11:30am The meaning of parameter space in the context of clinical populations: lessons from the simulation of 80 million sepsis patients Gary An

11:30-11:40am From proteins, viruses and cells to patient Populations: simulations of potential HIV cures Feilim Mac Gabhann
11:40-11:50am From biomolecular events to neuronal network dynamics: Efficient scale-linking enables higher levels of integration Jean-Marie C Bouteiller
11:50-12:00pm Value of computational modeling in understanding human pulmonary defensive reflexes Don Bolser
12:00-12:30pm Theme 3 Panel Discussion
12:30 – 1:30pm **Lunch on your own (Lister Hill or Natcher, Bldg. 45)**
1:30 – 2:00pm **IMAG Representatives Grant Process Overview / Lightning Presentations**
2:05 – 3:10pm **Refreshments* and Table Chats with IMAG Representatives (See Floor Plan)**
3:10 – 3:30pm Annals of BMES Special Issue on MSM - Tom Yankeelov
3:30 – 3:45pm IEEE EMBS TBME Special Issue on Model Reproducibility - Ahmet Erdemir & Herbert Sauro
3:45 – 5:00pm **MSM Consortium Discussion** MSM Consortium Goals and Structure—*IMAG* Plans for 2016 Consortium meeting—*All* Highlights from Working Group breakouts—*WG leads* Accomplishments from 2015 Biomechanics Working Group Cell-to-Macroscale Working Group Clinical and Translational Issues Working Group Committee on Credible Practice of Modeling & Simulation in Healthcare Computational Neuroscience Working Group High Performance Computing Working Group Integrated multiscale biomaterials experiment and modeling group (ImuBEAM) Model and Data Sharing Working Group Multiscale Systems Biology Population Modeling Working Group Theoretical and Computational Methods Transitioning WGs and WG co-leads, Proposals for New WGs
5:00pm **Meeting Adjourn** **Refreshments courtesy of the IEEE Engineering in Medicine and Biology Society – Thank You!*

Thursday, September 10, 2015
Satellite Meeting Overview and Use of Standards and Formats Relevant to MSM (Michael Hucka)
8:30-8:35am **Welcome: Satellite Meeting**
8:35-8:50am **Overview of popular modeling formalisms and representation approaches** Michael Hucka
8:50-9:20am **SBML and SBML Packages: summary of coverage and capabilities** Michael Hucka
9:20-9:35am **Integration of SBML in NEURON** Anna Bulanova
9:35-10:00am (TBD)
10:00-10:30am **Break**
10:30-11:00am **Using standards to enable model reproducibility: Software demonstrations** Herbert Sauro
11:00-11:30am **Multiscale models in CompuCell3D** James Sluka
11:30-12:00pm **Models and simulations as a service using Galaxy** Mark Walker
12:00-12:15pm **A brief overview of BioModels Database** Michael Hucka
12:15-12:30pm **Discussion**
12:30-2:00pm **Lunch on your own (Lister Hill or Natcher, Bldg. 45)**
2:00-3:00pm **Annotating models: practical experiences and approaches** James Sluka
3:00-3:15pm **Break**
3:15-4:00pm **Discussion and software demos of model reuse and reproducibility**

Keynote Speaker

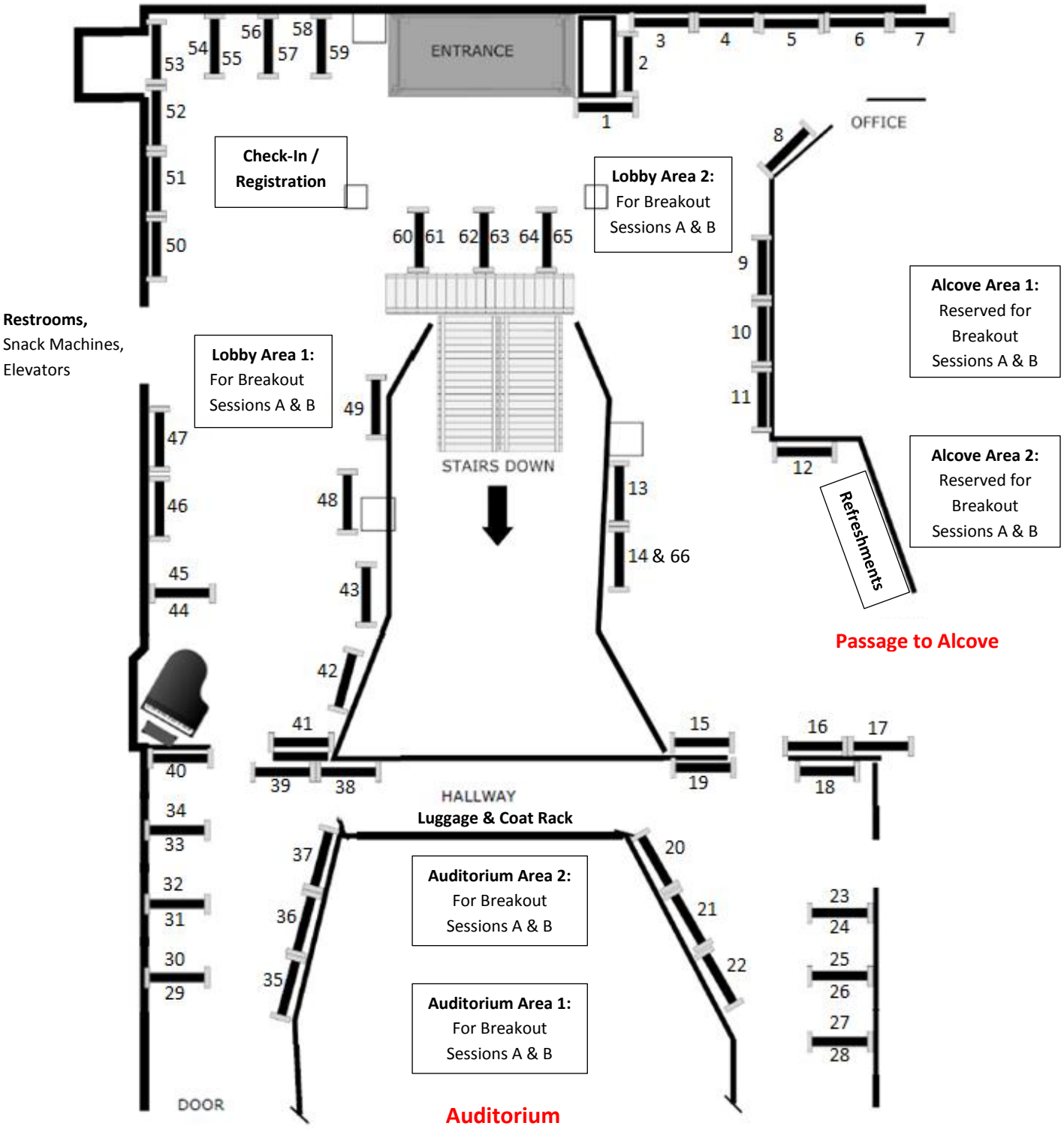
Steve Railsback, Ph.D.

Steve Railsback is an environmental engineer and ecologist who specializes in the use of individual-based (or 'agent-based') models to address ecological management problems. His experience includes an MS in environmental engineering (University of Illinois, 1981), five years as a staff scientist at Oak Ridge National Laboratory, a PhD in biology (University of Bergen, Norway, 2004), over 20 years experience as a consulting ecological modeler, and supervising students in the Environmental Modeling Graduate Program at Humboldt State University. Steve's interest in river management led to involvement in some of the earliest applications of individual-based models in applied ecology. This experience resulted in concern about general issues of across-level simulation modeling. With Volker Grimm, Steve authored the first full monograph on individual-based modeling in ecology (2005) and the first textbook on individual- and agent-based modeling (2012). He is an author of more than 40 publications on specific model applications and modeling methods.

Abstract

My colleagues and I produced the first version of "inSTREAM", an individual-based stream trout model, in 1999. The model is complex, representing how population ecology emerges from habitat conditions that vary over space and time, the behavior and physiology of individual fish, and competition among the fish for food and habitat. Yet this model has been successful, at least because we still adapt and apply it to a wide range of basic and applied research questions. Lessons learned from this experience include recognizing the importance of (a) close collaboration between modelers and empirical researchers, (b) professionalism in software development, and (c) building models around multiple observed patterns that guide model design and evaluation. Strategies for success include use of widely used standards (e.g., for model descriptions, software platforms), and "pattern-oriented modeling" as a way to design models that are just complex enough and have a strong theoretical basis

Floor Plan


ENTRANCE
OFFICE
Check-In / Registration
Lobby Area 2: For Breakout Sessions A & B
Lobby Area 1: For Breakout Sessions A & B
Alcove Area 1: Reserved for Breakout Sessions A & B
Alcove Area 2: Reserved for Breakout Sessions A & B
Restrooms, Snack Machines, Elevators
STAIRS DOWN
Refreshments
Passage to Alcove
HALLWAY
Luggage & Coat Rack
Auditorium Area 2: For Breakout Sessions A & B
Auditorium Area 1: For Breakout Sessions A & B
DOOR
Auditorium

Poster Abstracts

Category	Poster #	Presenter	Abstract Title	Group
Biomaterials	14	Ebrahimi, Davoud	Biomaterials: Predictive Design, Synthesis and Material Properties	2
Cancer	4	Barnes, Stephanie	Incorporating Patient-Specific Imaging Data and Therapeutic Regimens to Predict Eventual Response in Locally Advanced Breast Cancer via a Multi-Scale Model	1
Cancer	39	McKenna, Matthew	Multi-scale Treatment Response Model for Triple Negative Breast Cancer Linking Drug Administration Schedules to Tumor Cell Population Dynamics	1
Cancer	44	Paudel, Bishal	Understanding complex drug response behavior of BRAF-mutated melanoma cells treated with targeted therapies	1
Cancer	52	Searfoss, Abigail	A Controllable and Imaging Compatible 3D Tumor Environment to Experimentally Test and Refine Tumor Growth Models	1
Cancer	60	Weis, Jared	A Numerically Efficient Mechanically Coupled Reaction-Diffusion Model to Predict the Response of Breast Cancer to Neoadjuvant Therapy	1
Cardiovascular	1	Alber, Mark	Multi-scale Models of Fibrin Networks and Blood Clots	2
Cardiovascular	3	Barbee, Kenneth	Regulation of Store-Operated Calcium Entry in Endothelial Flow-Induced Nitric Oxide Production	2
Cardiovascular	6	Bluestein, Danny	A Predictive Multiscale Model for Simulating Platelets Activation in Shear Flows	1
Cardiovascular	7	Buerk, Donald	In vivo studies of NO and ATP-induced arteriolar vasodilation during hypoxia	1
Cardiovascular	17	Garbey, Marc	VASCULAR ADAPTATION: CLOSING THE LOOP BETWEEN GENE EXPRESSION AND MORPHOLOGICAL CHANGE	2

Category	Poster #	Presenter	Abstract Title	Group
Cardiovascular	19	Guccione, Julius	Multi-Scale Laws of Myocardial Growth and Remodeling	2
Cardiovascular	22	Holmes, Jeffrey	Coupling an Agent-Based Model of Scar Formation to a Finite-Element Model of Tissue Mechanics	1
Cardiovascular	25	Humphrey, Jay	MSM of Thrombus Biomechanics in Aortic Aneurysms	2
Cardiovascular	31	Li, Ruizhi	High-throughput evaluation of platelet function under flow following trauma reveals platelet function defects & Recapitulation of mechanisms during trauma-induced coagulopathy in whole blood microfluidic assays	2
Cardiovascular	32	Li, Xuejin	Patient-specific modeling and analysis of hemodynamic behavior of individual sickle red blood cells under hypoxic conditions	1
Cardiovascular	34	Liang, Jie	Multiscale Spatial and Temporal Signaling and Patterning of Cells and Tissues: Stochastic Control Networks and Tissue Wound Healing	2
Cardiovascular	35	Lu, Yichen	Multiscale flow modelling of cell ensembles and reactive species transport with data-driven cellular activation models	2
Cardiovascular	63	Yazdani, Alireza	Multiscale Modeling of Blood Clotting: Coagulation Cascade and Platelets Aggregation	2
Cardiovascular	65	Zhang, Katherine	A Multi-Scale Mechanobiological Model Considering the Structure and Interrelation of ECM Constituents in Aorta	2
Cellular Physiology	8	Buerk, Donald	Shear Stress-Dependent NO, ATP and ADP Production from Endothelial Cells – a Modeling Approach	2
Cellular Physiology	10	Calvetti, Daniela	Modeling of the microenvironment around a pH electrode tip	1
Cellular Physiology	27	Jafri, Mohsin	Multiscale studies of mitochondrial calcium cycling	1

Category	Poster #	Presenter	Abstract Title	Group
Cellular Physiology	40	Mofrad, Mohammad	Multiscale Models of the Nuclear Pore Complex	1
Cellular Physiology	49	Sander, Edward	Image-Based Multi-scale Mechanical Models for Predicting In Vitro Remodeling in Fibrin Gels	2
Cellular Physiology	56	Spill, Fabian	Effects of 3D Geometries on Cellular Gradient Sensing and Polarization	1
Cellular Physiology	62	Xiaobo, Zhou	Glomerular intercellular cross talk elaborately regulates podocyte injury and repair: insights from a 3D multiscale modeling study	1
Genetics	36	Marjoram, Paul	Multi-scale modeling of genetic variation in a developmental network	1
Imaging	29	Knothe Tate, Melissa	The power of coupled multiscale imaging and modeling - How good is good enough?	1
Imaging	33	Lin, Ching-Long	Toward Imaging-based Asthma Sub-Grouping: Cluster Analysis with Multiscale Structural and Functional Variables in Asthma Populations	1
Imaging	45	Pereira, Andre	Paired, seamless multiscale imaging and modeling as a springboard to bridge the gap between nano- and macroscale models	1
Immunology	41	Moore, James	Fluid Pumping and Mass Transfer in the Lymphatic System	1
Immunology or Musculoskeletal	21	Henson, Michael	Spatiotemporal Metabolic Modeling of Chronic Wound Biofilm Consortia	1
Infectious Disease	12	Carlson, Ross	Predictive Multiscale Modeling of Microbial Consortia Biofilms	1
Infectious Disease	37	May, Elebeoba	Bacterial Adaptation to Host-Induced Environmental Stress	1
Infectious Disease	46	Kirschner, Denise	A hybrid multi-scale model of tuberculosis maps bacterial metabolic scale dynamics to host tissue scale infection outcomes	1
Metabolism	11	Cannon, William	Simulating Metabolism with Statistical Thermodynamics	1

Category	Poster #	Presenter	Abstract Title	Group
Modeling Methodology	43	Paluh, Janet	Nanoscale and Molecular Framework for Modeling and Applying Communication at the Bottom	2
Modeling tools and methods	66	Barhak, Jacob	The Reference Model Uses Modular Population Generation	2
Modeling tools and methods	13	Drawert, Brian	StochSS: An Integrated Development Environment for Simulation and Analysis of Discrete Stochastic Biochemical Models	2
Modeling tools and methods	16	Fleming, Ronan	Computing non-equilibrium steady states for a biochemical network	1
Modeling tools and methods	50	Saunders, Michael	Accurate solution of FBA models using large-scale optimization in quadruple precision	2
Modeling tools and methods	51	Sauro, Herbert	Fully Integrated Python Tools for Modeling, Analysis and Reproducibility	1
Modeling tools and methods	55	Somersalo, Erkki	Multi-scale inverse problems: Beyond the modeling limit	1
Modeling tools and methods	59	Walker, Mark	Delivering Models and Simulations as a Service (MaSS) with Galaxy	2
Musculoskeletal	18	Gu, Weiyong	Multiscale and Multi-physics Modeling of Degenerative Disc Disease and in silico Clinical Trials for Disc Regeneration	2
Musculoskeletal	20	Haugh, Jason	Multiscale Modeling of Wound Healing	2
Musculoskeletal	28	Jasiuk, Iwona	Multiscale Modeling of Bone	2
Musculoskeletal	53	Shelburne, Kevin	Multi-scale Muscle-Driven Simulation of Human Subjects: Muscle and Joint Mechanics in TKR	1
Musculoskeletal	57	Tan, Hua	Modeling bone MSC lineage progression in a growth factor – loaded CaP scaffold subjected to mechanical stress	2
Musculoskeletal	58	Boyle, John	Multi-scale mechanics of the tendon-to-bone attachment	2
Musculoskeletal	61	Winkelstein, Beth	Multiscale Modeling of Facet Capsule Biology	2

Category	Poster #	Presenter	Abstract Title	Group
Neuroscience	9	Bulanova, Anna	Integrating Systems Biology Markup Language (SBML) in the NEURON simulator	2
Neuroscience	23	Hormuth, David	Biophysical models of C6 glioma growth in rats	1
Neuroscience	24	Hu, Eric	The Volterra Functional Series is a Viable Alternative to Kinetic Models for Synaptic Modeling -Calibration and Benchmarking	2
Neuroscience	30	Lazzi, Gianluca	Towards an accurate multi-scale computational model for studying retinal prosthetic electrode design	2
Neuroscience	38	McDougal, Robert	Coupling 1D and 3D domains in neuroscience simulations	2
Neuroscience	42	Neymotin, Samuel	Optimizing computer models of layer 5 motor cortex pyramidal neurons using somatic whole cell recordings	1
Neuroscience	64	Yu, Gene	Estimation of Local Field Potentials in a Three-Dimensional, Computational Model of the Hippocampal Dentate Gyrus: A Multiscale, Multimodal Framework	2
Pharmacology	2	Ayyaswamy, Portonovo	Multiscale Modeling of Functionalized Nanocarriers in Targeted Drug Delivery: Effects of Blood Cell Interactions and Temporal Hydrodynamic Correlations	2
Pharmacology	15	Eckmann, David	Multiscale Modeling of Functionalized Nanocarriers in Targeted Drug Delivery: Effects of Blood Cell Interactions and Temporal Hydrodynamic Correlations	2
Pharmacology	26	Hunt, C. Anthony	Virtual Experiments Falsify a Prevailing Mechanistic Explanation for Acetaminophen Induced Liver Injury and Enable Discovery of Plausible Alternative Hypotheses	1

Category	Poster #	Presenter	Abstract Title	Group
Pharmacology	48	Radhakrishnan, Ravi	Next-Generation Pharmacodynamic Models for Targeted Drug Delivery: Multiscale Model for Nanocarrier Adhesion at the Live Cell Interface and Comparison to In Vivo Experiments	2
Pharmacology	54	Sluka, Jim	Tightly Coupled In Vivo Studies to Inform an In Silico Model of Acetaminophen Toxicity	1
Population Modeling	5	Bisset, Keith	A cyberinfrastructure supporting transdisciplinary research into population modeling at multiple scales	1
Population Modeling	47	Pruett, William	Accurate rapid estimation of physics based model outputs with surrogate techniques	2

Attendee List

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