IMAG **Interagency Modeling and Analysis Group**

2018 Futures Meeting

Moving Forward with the Multiscale Modeling Consortium

March 21-22, 2018 • Bethesda, Maryland

2018 IMAG Futures Meeting

Moving Forward with the MSM Consortium

With Gratitude to:

MSM Steering Committee

2017	*2017-2018*
Danny Bluestein	**Sylvia Blemker**
Jason Haugh	**Jeff Holmes**
Mike Henson	**Ellen Kuhl**
Jay Humphrey	**Bruce Lee**
Saleet Jafri	**Andrew McCulloch**
	Terry Sanger
2018-2019	*2019-2020*
Mark Alber	*Victor Barocas*
Gianluca Lazzi	*David Basanta*
Shayn Peirce-Cottler	*Mike Henson (2nd year)*
Steve Thomopoulos	*Guy Genin*
Tom Yankeelov	*Jim Bassingthwaighte*
	Bill Cannon

2018 IMAG Futures Planning Committee

NIH	*NSF*	*FDA*
Greg Bloss, NIAAA	Vipin Chaudhary, CISE/OAC	Donna Lochner
Regina Bures, NICHD	Michele Grimm, ENG/CBET	Tina Morrison
Wen Chen, NCCIH	Chi-Chi May, NSF/BIO	
Emily Conlan, NIBIB	Christy Payne, ENG/CBET	*ARL*
Jacklyn Ebiasah, NIBIB	Jim Powell, MPS/DMS	Liyi Dai
Michele Ferrante, NIMH	Junping Wang, MPS/DMS	Virginia Pasour
Liz Ginexi, OBSSR		
Tim Gondre-Lewis, NIAID	*NASA*	*DOE*
Orlando Lopez, NIDCR	Beth Lewandowski	Ramana Madupu
Dave Miller, NCI	Jerry Myers	
Grace Peng, NIBIB		*IARPA*
Haluk Resat, NIGMS	*AHRQ*	Jennifer Wang
Coryse St Hillaire-Clarke, NIA	Kerm Henriksen	
Xujing Wang, NIDDK	David Rodrick	*AFOSR*
Ken Wilkins, NIDDK		Fariba Fahroo

For extra support from:

The NIH National Institute of Biomedical Imaging and Bioengineering (NIBIB)
The National Science Foundation (NSF)
and The NIH The Office of Behavioral and Social Sciences Research (OBSSR)

Logistics

Welcome to the 2018 IMAG Futures Meeting -- Moving Forward with the Multiscale Modeling Consortium!

We are excited to have you here to participate in the second IMAG Futures meeting, where we plan the future for multiscale modeling and analysis of biomedical, biological and behavioral systems. The 2009 IMAG Futures Meeting was seminal in setting the stage for addressing modeling challenges that can make an impact on biomedical research through the IMAG Multiscale Modeling (MSM) Consortium. This year's 2018 IMAG Futures Meeting takes a look at how well the 2009 challenges have been addressed and sets next steps for the MSM. In particular we focus on new methods to bridge theory-driven models with data-driven models and determine how machine learning can play a role for future impact. We look forward to everyone's interactive participation throughout these two days. Enjoy the meeting!

Check-In
Check-in will begin at 8:00 AM on all meeting days.

Meeting Topics
This year the MSM PI project leaders will lead the Consortium in discussions on each of the 2009 challenges and introduce new challenges. Please use the interactive agenda on the IMAG wiki to follow along and add your comments and questions during each talk. Everyone is encouraged to contribute!

Working Groups – Breakout Sessions
The MSM Steering Committee members will lead the MSM Working Groups in grouped breakout sessions on Day 1 and 2. All notes will be posted in the interactive agenda as the discussions take place. The outcomes of the breakout sessions are expected to produce associated white papers and or journal articles after the meeting.

Posters
All posters should be displayed for the duration of the 2-day meeting. Poster board layouts and assignments begin on **page 14** of this meeting booklet. Please use the registration table to view the abstracts and final posters, https://msmmeeting.nibib.nih.gov/attendee-information-and-presentations. Presenters should stand by their posters during the dedicated poster presentation times for Group 1 or Group 2 on Day 1 and Day 2.

Wireless Access & IMAG wiki login
Wireless internet is free and can be accessed using the network **NIH-Guest**.
We strongly encourage you to interact with the IMAG wiki (**SEARCH: imag wiki**), https://www.imagwiki.nibib.nih.gov/ during the meeting (or just click on the links in the agenda!). To add your comments to the wiki please login using your **IMAG wiki username and password**. If you don't have an account or forgot your login, use the following: **Username: conference_guest; Password: 2018IMAGfutures!**

Videocast & Twitter
The meeting will be videocast on Day 1 to allow remote access attendees to participate and contribute feedback to the discussions (through Twitter and the IMAG wiki login). The videocast and future archive will be available on https://videocast.nih.gov/. Please use **#MSM2018** to contribute your questions and thoughts via Twitter.

Breaks and Lunch
The poster session will be located on the Natcher Atrium level. Pre-ordered lunch boxes will be ready for pick-up outside the Natcher Auditorium.

Food and drinks cannot be brought into the auditorium. ****Please note that refreshments will NOT be provided at the meeting this year. You can buy snacks or lunch at the Natcher cafeteria, which is open from **6:30AM to 2:30PM**, and the Natcher concession stand, open from **7AM to 3:30PM**.

Dinner
Those who signed up for the dinner should plan to arrive at the **Shangri-La** restaurant in downtown Bethesda the evening of Day 1, March 21, 2017 at **6:00pm**. All dinner spots are currently filled. You are welcome check at the registration desk if there are changes in availability. Location information is found on **page 4** of this meeting booklet.

Taxi information
Please allow 20-30 minutes for taxis or Uber or Lyft to arrive!

The conference is located in Building 45 at the NIH. **Please ask to be picked up at** the NIH Security Gate called the **GATEWAY VISITORS CENTER** next to the MEDICAL CENTER METRO STATION or in front of the Natcher Building. Picking up in front of Natcher will take significantly longer as the cars must go through security.

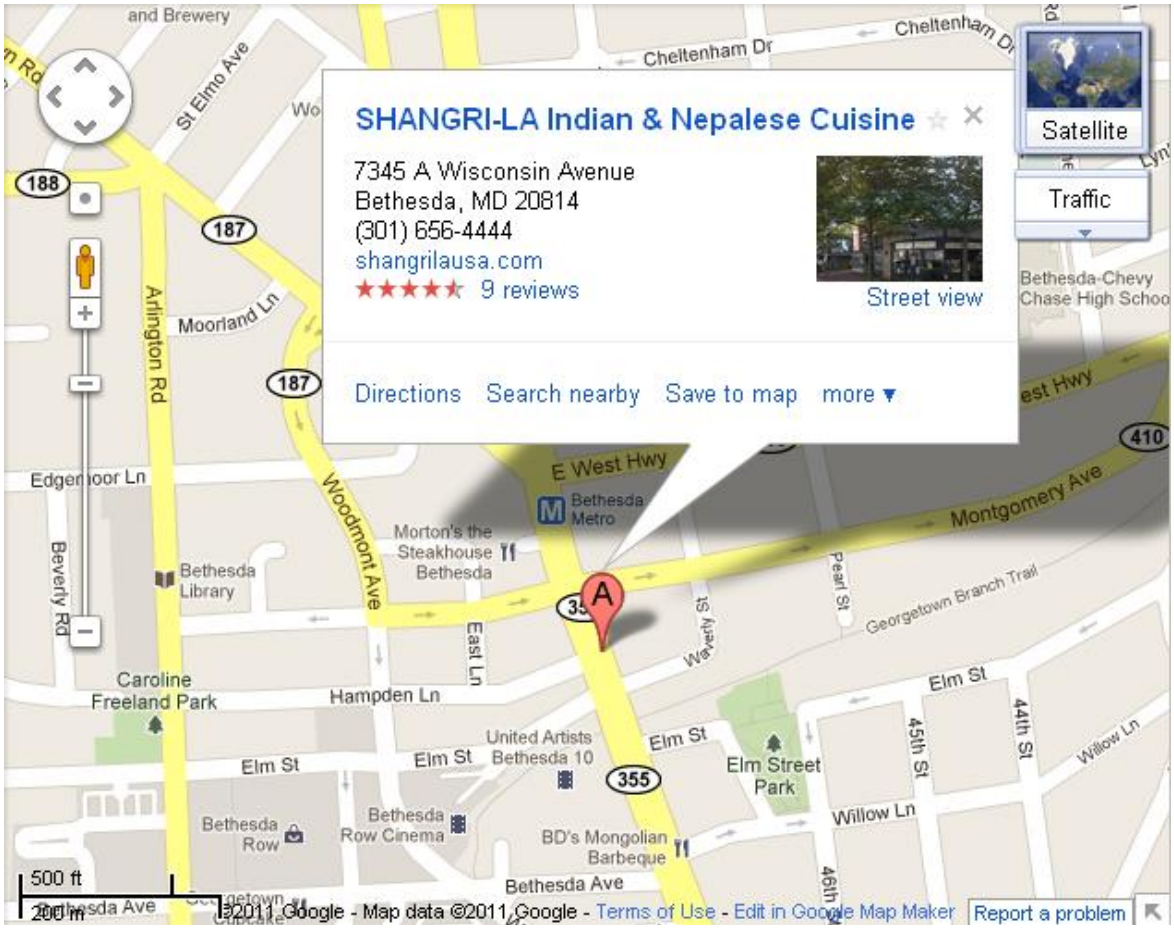
Barwood Taxi	301-984-1900
Regency Cab	301-990-9000
Action Taxi	301-840-1000
Super Shuttle	1-800-BLUE-VAN

Dinner Information

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

Those attending the group dinner should meet at Shangri-La Restaurant at 6:00pm on Day 1, Wednesday, March 21st.

The restaurant is a short walk away from the **Bethesda Metro Station** and the **Hyatt Regency Bethesda**. Parking is available in public garages nearby. The buffet price is $30 and includes one meal per person with a glass of wine or beer (includes tax and tip). **Please bring cash, if possible.**



Agenda

DAY 1: Wednesday March 21, 2018

*All sessions from 8:00AM to 12:00PM will occur in the Auditorium

8:00 - 8:15 am: Check-in, Set up posters

8:15 - 8:25 am: Welcome from IMAG Leadership

- **Dr. Jill Heemskerk, Acting Director, NIBIB**
- **Dr. David Shurtleff, Acting Director, NCCIH**

8:25 – 8:30am: Addressing 2009 IMAG Futures Challenges - Grace Peng, IMAG Chair

8:30 - 9:00 am: Method integration from multiple domains and environments

Challenges #1, 2 PI Leads: David Kaplan, Bill Lytton, Silvia Blemker, Carlos Figueroa

9:00 - 9:30 am: Fusing data, processes and mechanisms across scales

Challenges #3, 4 PI Leads: Michael Henson, David Zawieja, Ross Carlson, Jeff Holmes

9:30 - 10:00 am: Building reuseable, standardized models

Challenges #5, 6 PI Leads: Jim Bassingthwaighte, Raj Vadigepalli, Jon Lederer, Eric Sobie

10:00 – 10:30 am: Break / Poster viewing (Group 1)

10:30 – 11:00 am: Models to predict and test outcomes

Challenges #7, 9, 10, 18 PI Leads: Colleen Clancy, Tom Yankeelov, Dan Beard, Scott Diamond, Bill Cannon, James Glazier, Tim Corcoran, Gianluca Lazzi

11:00 – 11:30 am: Population level models for behavioral and social sciences

Challenge #11-17 PI Leads: David Basanta, Bruce Lee, Ching-Long Lin

11:30 – 12:00 pm: HPC models & Machine Learning

Challenge #8 **and** Machine Learning PI Leads: Julius Guccione, Denise Kirschner, Guy Genin, Xiaobo Zhou

12:00 - 1:00 pm: Lunch with IMAG and WGs (See lunch room assignments, p10-11)

1:00 – 2:30 pm: Special Session: Bridging Mechanistic, Causal and Predictive Models – what can machine learning do for the MSM? (Auditorium)

2:30 - 3:00 pm: Break / Poster viewing (Group 2)

3:00 – 5:00 Concurrent Breakout Sessions:

Auditorium: New Methods Challenges – MSM **Methods, Integrating Machine Learning and AI**

Balcony A: New Applications Challenges - MSM **Applications, Clinical translation**

Balcony B: Dissemination – **Tutorials, Papers, Social Media**

6:00 - 9:00 pm: Group Dinner

DAY 2: Thursday March 22, 2018

*All sessions from 8:00AM to 11:00AM will occur in the Auditorium

8:00 - 8:20am: Check-in

8:20 - 8:30am: Welcome back - Grace Peng, IMAG Chair

8:30 – 9:30am: Model Credibility and Model Reusability

9:30 – 10:10am: Model Credibility Plan – Lightning Talks (19 projects)

10:10 - 11:00am: Break / Poster viewing – visit Model Credibility Posters

11:00 – 12:00pm Breakout Sessions – Finalize White Papers

Auditorium: New Methods Challenges – MSM **Methods, Integrating Machine Learning and AI**

Balcony A: New Applications Challenges - MSM **Applications, Clinical translation**

Balcony B: Dissemination – **Tutorials, Papers, Social Media**

12:00 - 1:00 pm: Lunch with IMAG and WGs (See lunch room assignments, p10-11)

1:00 – 2:00pm Poster viewing (Group 1 & Group 2, switch at 1:30 pm)

1:00 - 2:00pm: MSM Steering Committee Meeting (Closed Session, Room D)

2:00 – 2:30pm: MSM Steering Committee Panel (Auditorium)

2:30 – 3:00pm: MSM Initiative Discussion (Auditorium)

- Feedback on MSM Initiative goals
- Feedback on MSM Review process
- Feedback on MSM Consortium

3:00pm: Final Thoughts, Adjourn

Special Speakers

Dr. Olaf Dammann, Tufts University

"Nested Boxes" - Causal-Mechanical Explanation in Multi-Scale Modeling of Disease Occurrence

Multiscale modeling (MSM) is a research technique of growing importance in biology and medicine. The goal of MSM is to explain differences among patients regarding disease occurrence and/or therapy by opening the "black box of disease." Causal inference and mechanistic reasoning are at the core of systems medicine. Therefore, one of the major questions in this field is: how should one transition from mechanistic to causal and ultimately to predictive models in MSM? Writing from my personal perspective as perinatal neuroepidemiologist, I will briefly review recent developments in philosophy of the health sciences. Most pertinent to the question at hand is the debate unleashed by what has come to be called the Russo-Williamson Thesis (RWT), which states that the health sciences make claims based on evidence of both physical mechanisms and probabilistic dependencies. The scales (i.e. levels of evidence generated in support of causal hypotheses) in the health sciences range from molecular to societal. As an epidemiologist interested in population modelling, I suggest taking the etiological stance, which calls for association-based mechanistic evidence to be explained by some sort of mechanistic hypothesis that in turn explains overall causal claims, as per W. Salmon's causal-mechanical explanation, (1984). I suggest using the biostatistical model of capturing the strength of an association between two phenomena by calculating odds ratios (ORs), which are dimensionless, do not refer to a time frame, and can be adjusted for confounders. These ORs can be used to capture, in a single number, association-based mechanistic evidence. As such, they can be incorporated as co-variables in nested regression models, depicting nested black boxes. They may also be used in mediation analysis, designed to identify mediators between cause and effect. The concept will need to be in explanatory coherentist frameworks, for which Paul Thagard's ECHO system appears to be a reasonable candidate.

Dr. Olaf Dammann is Professor of Public Health and Community Medicine at Tufts University and Editor-in-Chief of the journal PEDIATRIC RESEARCH (more in special session agenda).

Dr. Todd Coleman, UCSD

Dr. Todd P. Coleman is currently Professor of Bioengineering and ECE Affiliate Professor of Electrical and Computer Engineering at the University of California, San Diego. He joined the

Jacobs School of Engineering in 2011 as an associate professor in the Department of Bioengineering. He received bachelor's degrees in electrical engineering (summa cum laude), as well as computer engineering (summa cum laude) from the University of Michigan, Ann Arbor, in 2000, along with master's and doctoral degrees in electrical engineering from the Massachusetts Institute of Technology, Cambridge, in 2002, and 2005. During the 2005-06 academic year, he was a postdoctoral scholar in computational neuroscience at MIT and Massachusetts General Hospital. From fall 2006 until June 2011, he was an assistant professor of Electrical & Computer Engineering and Neuroscience at the University of Illinois, Urbana, Champaign.

Professor Coleman's research is multi-disciplinary at its core. His main goal is to use tools from information theory, neuroscience, machine learning and bioelectronics to understand – and control – interacting systems with biological and computer parts. His research in developing multi-functional, flexible bio-electronics are enabling wireless health applications that are minimally observable to the user. His brain-machine interface research uses information theory, control theory and neuroscience to interpret – and design – systems from the viewpoint of multiple agents cooperating to achieve a common goal. The benefits of this research include helping subjects with disabilities as well as enabling all members of society to enhance capabilities in many daily activities. His research on causal inference uses information theory and machine learning to understand causal relationships in time series of data. Within the context of neuroscience, it is being used to understand dynamical aspects of brain function. The approach is applicable to arbitrary modalities and to a variety of applications, including financial networks, social networks and network security.

Dr. Timothy Lillicrap, Google DeepMind

Dr. Timothy Lillicrap is currently a Staff Research Scientist at Google DeepMind and an Adjunct Professor at University College London. He received an Hon. B.Sc. in Cognitive Science & Artificial Intelligence from the University of Toronto and a Ph.D. in Systems Neuroscience from Queen's University in Canada. He moved to the University of Oxford in 2012 where he worked as a Postdoctoral Research Fellow. In 2014 he joined Google DeepMind as a Research Scientist and became a Senior Research Scientist in 2015. His research focuses on machine learning for optimal control and decision making, as well as using these mathematical frameworks to understand how the brain learns. He has developed new algorithms for exploiting deep neural networks in the context of reinforcement learning, and new recurrent memory architectures for one-shot learning problems. His recent projects have included applications of deep learning to robotics and solving games such as Go.

Day 1 and Day 2 Lunch Sessions

Working Groups (Room E1/E2)

Biomechanics Working Group

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Clinical and Translational Issues Working Group

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Terry Sanger tsanger@usc.edu

Committee on Credible Practice of Modeling & Simulation in Healthcare

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Computational Neuroscience Working Group

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Raj Vadigepalli, (Thomas Jefferson University): (rajanikanth.vadigepalli@jefferson.edu)

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Alison Galvani (alison.galvani@gmail.com)

Public Dissemination and Education (PDE) Working Group

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Theoretical and Computational Methods Working Group

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Brian Drawert (bdrawert@cs.ucsb.edu)

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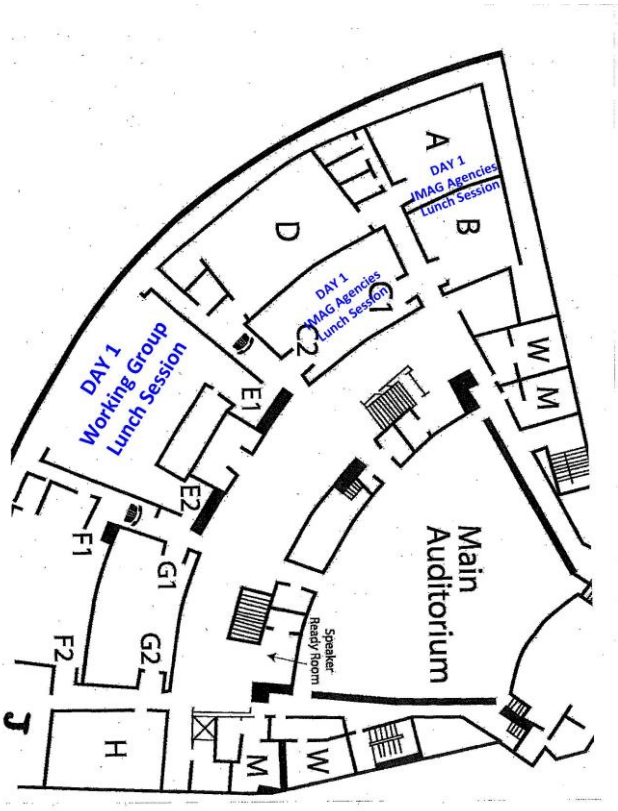
Natcher Building Meeting Rooms

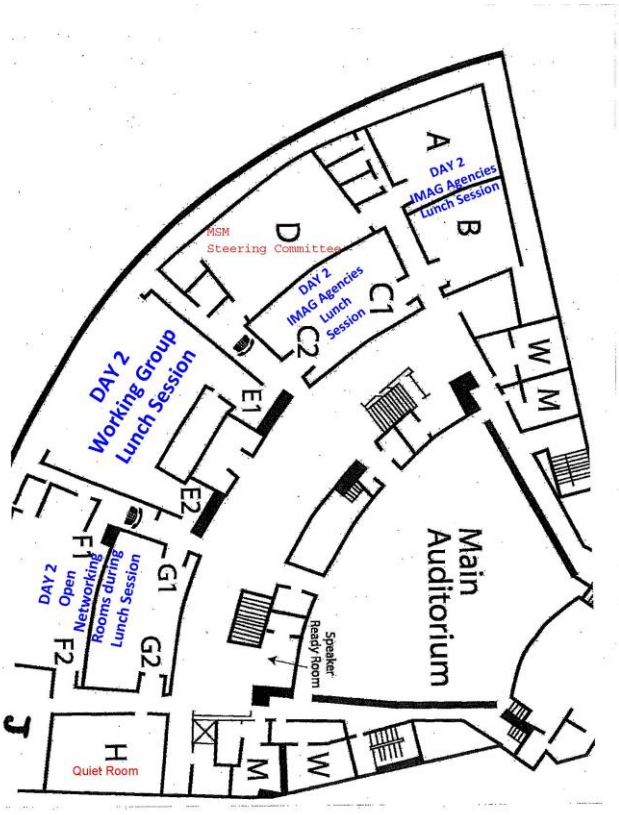
Basement Level:

Ruth Kirschstein Auditorium /
C1-C2 / E1-E2 / F1-F2 / G1-G2 / H / J / B

Day 1 Lunch



Day 2 Lunch



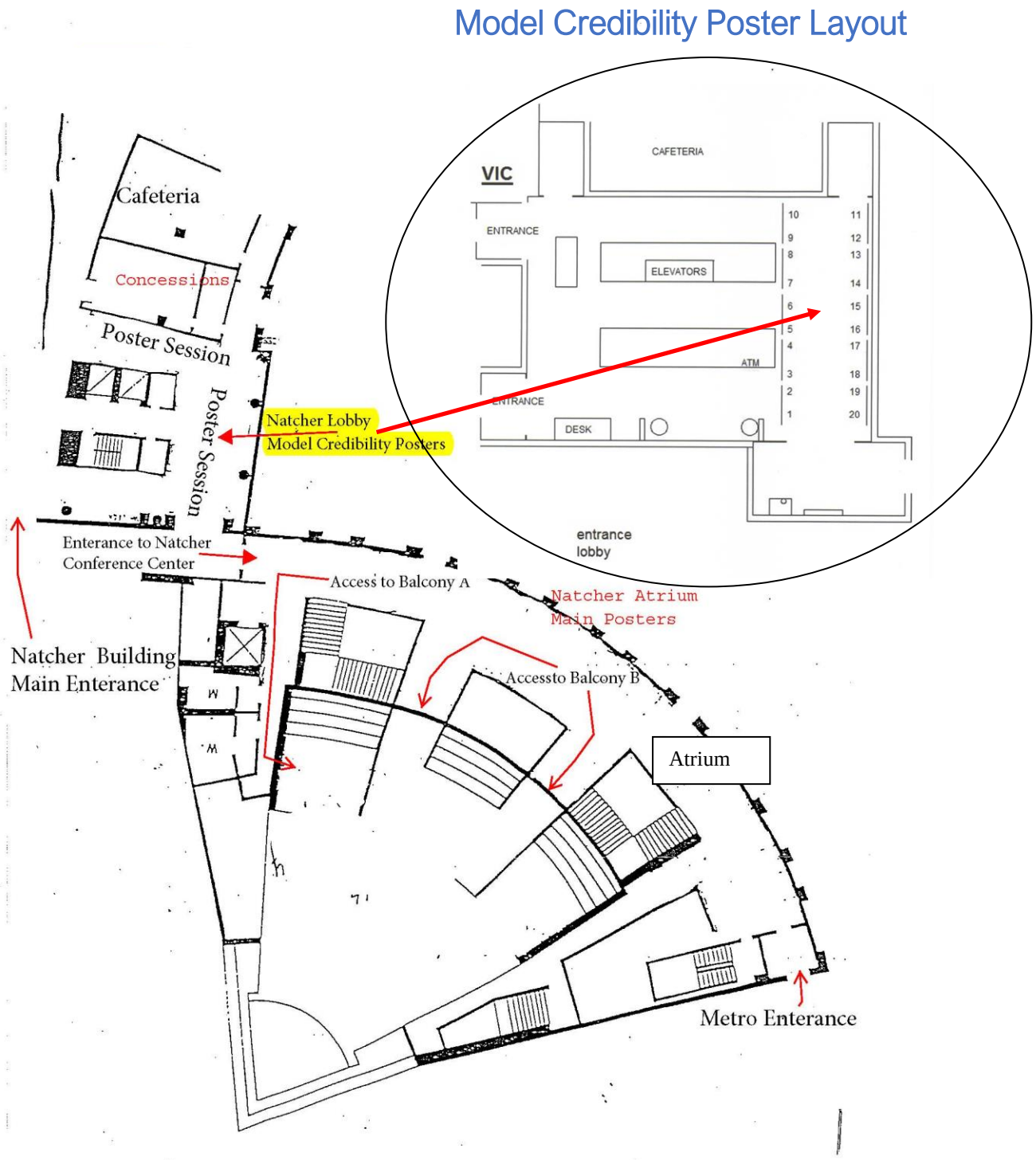
*****Elevator Service Notice**

The elevators to/from the Natcher Auditorium level are not working. Should you need assistance with an elevator, please call 301-435-2208 and someone will come to assist you.

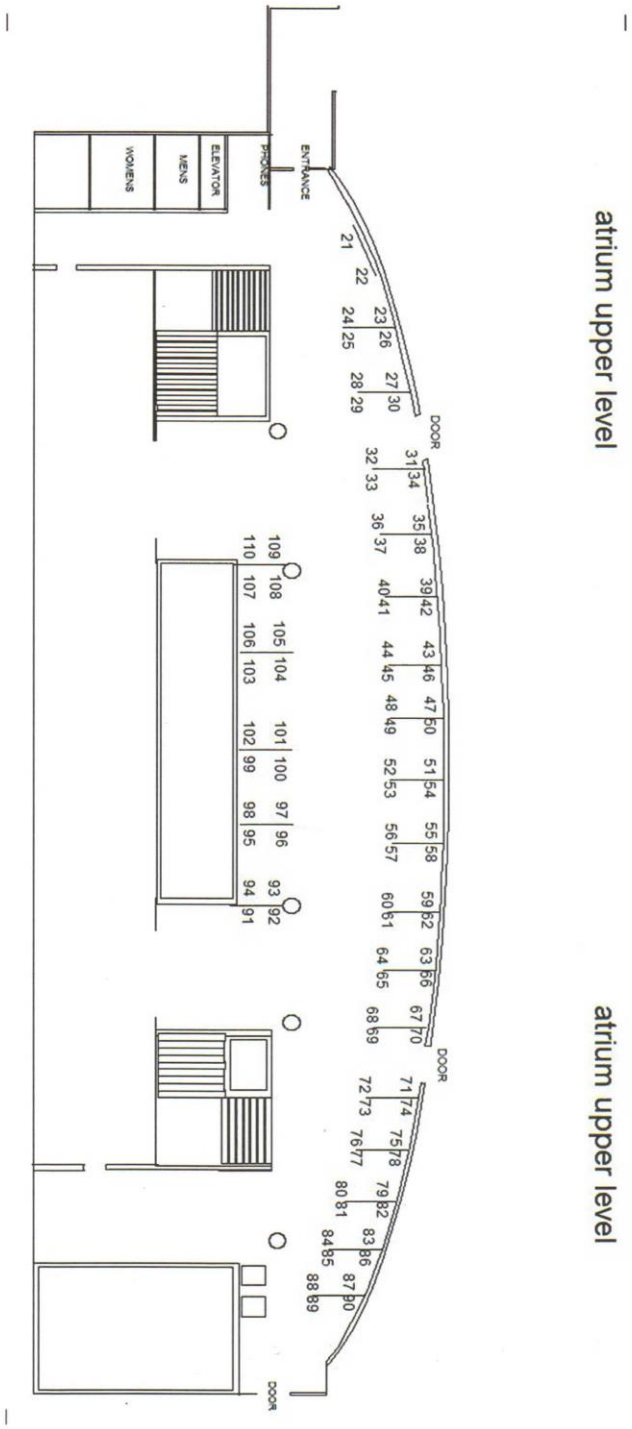
Natcher Building Meeting Rooms

Ground Floor:

Balcony A / Balcony B / Balcony C / Atrium



Main Poster Layout



Poster Numbers & Group Assignments

Author Name	Affiliation	Contact PI name	Poster Title	Group #	Poster #
Raquel Adams	George Mason University		Segmentation and Modeling of Mitochondria with Densely Convoluted Inner Membranes	2	64
Parya Aghasafari	University of Georgia		Developing an Linear-Parameter Varying Model for Thymocyte Development with Age	1	49
Mark Alber	University of California Riverside	Mark Alber	Modeling Deformation, Embolization and Permeability of Blood Clots under Shear Flow	1	105
Gary An	University of Chicago		Examining control of a multi-scale system: Using Deep Reinforcement Learning to control an agent-based model of sepsis	2	80
Jacob Barhak	Barhak, Jacob		The Reference Model Visualizes Gaps in Computational Understanding of Clinical Trials	2	72
David Basanta	H. Lee Moffitt Cancer Center & Research Institute		Computational modeling of macrophage polarization dynamics in skeletal malignancies. An integrated in	1	77

			silico and in vivo approach		
James Bassingthwaighte	University of Washington	James Bassingthwaighte	U01 HL199122 The Cardiac Energy Grid: Modeling Metabolism to Fuel Ion Fluxes and Contraction	2	40
Clayton Bingham	University of Southern California	Theodore Berger	Multi-Scale Modeling of the Hippocampus: Integration and Validation of Microelectrode, Neural Network, and Volume Conductor Models	2	48
Danny Bluestein	Stony Brook University	Danny Bluestein	Multiscale Modeling of Blood Flow and Platelet Mediated Thrombosis	1	67
Walter Boron	Department of Physiology & Biophysics, Case Western Reserve University School of Medicine	Walter F. Boron	MULTI-SCALE MODELING OF GAS TRANSPORT THROUGH CHANNELS IN LIVING CELLS	1	103
William Cannon	Pacific Northwest National Laboratory	Willaim R. Cannon	Multi-scale Modeling of Circadian Rhythms: From Metabolism to Regulation and Back	2	68
Ross Carlson	Montana State University - Boseman	Ross Carlson	Predictive Multiscale Modeling of Microbial Consortia Biofilms	1	109
Tim Corcoran	University of Pittsburgh	Corcoran	Multi-scale Models of	2	82

			Therapeutic Response in Cystic Fibrosis		
Yasin Dhaher	Northwestern University/Sheirly Ryan AbilityLab (formally RIC)	Yasin Dhaher	Computational modeling of sex hormone effects on tissue degradation after ACL injury	1	91
Scott Diamond	University of Pennsylvania	Scott L. Diamond	Multiscale Analysis of Trauma	2	36
Thomas Dick	Case Western Reserve University	Thomas E. Dick	Ventilatory pattern variability decreases and becomes more deterministic during sepsis in rodents.	2	54
Salvador Dura-Bernal	SUNY Downstate		Data-driven multiscale model of primary motor cortex microcircuits	2	74
David Eckmann	University of Pennsylvania	David M. Eckmann	Impact of deformability of cross-linked lysozyme-core/dextran-shell nanocarriers on vascular targeting: a combined experimental and multiscale modeling study	2	98
Aiyana Emigh	UC Davis		Structural Modeling of hERG Channel Interactions with Drugs Using Rosetta	1	81
Ahmet Erdemir	Cleveland Clinic		A collaborative pathway to establish credible	1	73

			practice of modeling and simulation in knee biomechanics in conformance with community recommendations		
Xinzeng Feng	University of Texas at Austin, Institute for Computational Sciences and Engineering		Deep neural network as a surrogate model: applications on a hybrid multiscale model of avascular tumor development	1	43
Marie Ferguson	Global Obesity Prevention Center at Johns Hopkins	Bruce Y. Lee	Modeling the Impact of Crime on African-American Women's Physical Activity and Obesity in Washington, D.C.	2	50
Vasilina Filonova	University of Michigan		Multiscale modeling of pulmonary hypertension using Fluid-Solid-Growth formulations	1	45
Guy Genin	NSF Science and Technology Center for Engineering MechanoBiology, Washington University	Guy Genin	Cross-scale interactions between mineral and collagen for tendon-bone attachment	2	56
Elizabeth Ginexi	National Institutes of Health		Challenge #11-17: Population level models for behavioral and social sciences	1	65
Simon Giszter	Drexel University College of Medicine	Terence D Sanger	Connectivity analysis of multielectrode	1	47

			neural recordings using a stochastic dynamic operator framework		
Rudy Gleason	Georgia Institute of Technology		Multi-scale modeling of lymphatic vasculature growth and adaptation	1	69
Matthew Guay	NIH/NIBIB		Bottom-up Multi-scale Modeling of Biological Structures with High-Throughput Electron Microscopy	1	33
Julius Guccione	UCSF	Julius Guccione	Multi-Scale Laws of Myocardial Growth and Remodeling	2	66
joon Ha	National Institutes of Health		Predicting Future Glycemic Trajectories with a Mathematical Model	1	25
Jason Haugh	North Carolina State University	Haugh, Jason M.	Multiscale Modeling of Wound Healing	2	108
Michael Henson	University of Massachusetts	Michael Henson	Multiscale Modeling of the Mammalian Circadian Clock: The Role of GABA Signaling	1	95
Jeff Holmes	University of Virginia	Jeffery Holmes	Comparison of Predicted Cardiac Growth Using a Hypertrophy Signaling Network vs. Phenomenologic Models	1	87

Eric Hu	University of Southern California	Theodore W. Berger	Multi-Scale Modeling of the Hippocampus: Nonlinear Synapse Models using Volterra Network Filters for Large-Scale Simulations.	2	58
Jay Humphrey	Yale University	Humphrey	Multiscale Multiphysics Model of Thrombus Biomechanics in Aortic Dissection	2	90
Mohsin Jafri	George Mason University	W. Jonathan Lederer	Multiscale modeling of Mitochondrial Crista Structure on Metabolic Function	2	92
Angela Jarrett	University of Texas at Austin		Towards a multi-scale model of combination targeted and cytotoxic therapy to evaluate treatment response in HER2+ breast cancer	2	28
Zhiwei Ji	UTHealth		Systematically understanding the immunity leading to CRPC progression	2	62
Brian Jones	University of Virginia	Sylvia Blemker	A computational model for predictions of skeletal muscle adaption to disuse and exercise	1	23
Olufemi Kadri	New Jersey Institute of Technology		Numerical Accuracy	2	88

			Comparison of Two Boundary Conditions Commonly used for Approximating Shear Stress Distributions in Tissue Engineering Scaffolds Cultured under Flow Perfusion		
David Kaplan	Tufts University	David Kaplan	MODELS TO PREDICT PROTEIN BIOMATERIAL PERFORMANCE	2	34
Oleg Kim	University of Pennsylvania/University of California Riverside	Mark Alber	STRUCTURAL AND BIOMECHANICAL ALTERATIONS ASSOCIATED WITH PLATELET-DRIVEN CLOT CONTRACTION	1	79
Pragya Kosta	University of Utah	Gianluca Lazzi and Theodore Berger	Increasing retinal prosthetic stimulation efficiency in degenerated retina through characterization of the electrical stimulus waveform	1	61
Reuben Kraft	Penn State University		Multiscale Modeling of the Brain: New Approaches to Model Axonal Bundle Physics for Injury, Rehabilitation and Beyond	1	29
Reinhard Laubenbacher	UConn Health/Jackson Lab for Genomic Medicine	Reinhard Laubenbacher	Modular design of multiscale models, with an	2	94

			application to the innate immune response to fungal respiratory pathogens		
Gianluca Lazzi	University of Southern California	Gianluca Lazzi	Multi-Scale Modeling of the Hippocampus: Neuron-Admittance Method for Estimating Endogenous Local Field Potentials	2	52
Jaeho Lee	NIH/Clinical Center		Tumor and organ uptake of Cu-64 labeled amatuximab, an anti-mesothelin antibody, in a nude mouse model bearing a shed antigen tumor by mathematical model simulation	2	76
Xuejin Li	Brown University	George Em Karniadakis	Multiscale Modeling of Sickle Cell Anemia: Methods and Validation	2	100
Ernesto Lima	The University of Texas at Austin	Thomas E. Yankeelov	Development and Calibration of a Hybrid Multiscale Model of Vascular Tumor Growth	2	70
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Igor Vorobyov	University of California, Davis, Department of Physiology and Membrane Biology	Colleen E. Clancy	Elucidating sex dependence of cardiac arrhythmias via multiscale modeling and simulations	1	55
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