



INTEGRATING MACHINE LEARNING WITH MULTISCALE MODELING FOR BIOMEDICAL, BIOLOGICAL AND BEHAVIORAL SYSTEMS

OCTOBER 24-25, 2019



With Gratitude to:

<i>MSM Co-Chairs</i>	<i>IMAG</i>	<i>NIBIB</i>
<p>Suvranu De Ellen Kuhl</p> <p><i>MSM Session Chairs</i></p> <p>Mark Alber Bill Cannon Adrian Buganza Tepole Krishna Garikapti George Karniadakis Bill Lytton Paris Perdikaris Linda Petzold</p>	<p>Leonardo Angelone, NIDA Jennifer Couch, NCI Joshua Elliott, DARPA Fariba Fahroo, AFOSR Elizabeth Ginexi, OBSSR Susan Gregurick, NIH/OD Tony Kirilusha, NIAMS Laurel Kuxhaus, NSF Steven Lee, DOE Elebeoba (Chi-Chi) May, NSF David Miller, NCI Jerry Myers, NASA Virginia Pasour, ARL Grace Peng, NIBIB Rachel Slayton, CDC Junping Wang, NSF Xujing Wang, NIDDK Ken Wilkins, NIDDK</p>	<p>Jacklyn Ebiasah, Analyst Shirley Coney-Johnson, Planner Isabella Yoo, Graphic Designer Anuj Sharma, IMAG wiki Kolbi Harrison, IMAG wiki Mangala Manivannan, IMAG wiki Elaine Gibson, IMAG wiki Rosslyn Hart, Admin Shaun Simms, Admin Lavern Colclough, Tech Support</p>

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NVIDIA
Rensselaer Polytechnic Institute (RPI)
Organization for Computational Neuroscience (OCNS)
The National Science Foundation (NSF)

Logistics

Welcome to the 2019 IMAG ML- MSM Meeting -- Integrating Machine Learning with Multiscale Modeling for Biomedical, Biological, and Behavioral Systems. We look forward to everyone's interactive participation throughout these two days. Enjoy the meeting!

Check-In

7:30am NIH Gateway Center (Bldg. 66): Proceed through security to obtain a visitors badge, please bring a government-issued photo ID.

Walk directly from Bldg. 66 to **Natcher (Bldg. 45)** - see yellow highlight on  [NIH Visitor's Map.pdf](#)

8:00 AM Registration opens in the lower level outside the Ruth L. Kirschstein Auditorium. Obtain badge and meeting folder.

Posters

All posters should be displayed in the Atrium level for the duration of the 2-day meeting. Presenters should stand by their posters during the dedicated poster presentation times on Day 1 (see Poster Group # and schedule in [Agenda](#)).

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** (your registration login). If you don't have an account or forgot your login, use the following: **Username: conference_guest; Password: IMAG2019MLMSM!**

Videocast

The meeting will be videocast on both days to allow remote access attendees to participate and contribute feedback to the discussions. The videocast and future archive will be available on <https://videocast.nih.gov/>.

Breaks and Lunch

Refreshments will be located in the **Alcove area in the Natcher Lobby** (NOT in the Atrium).

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 be provided in the Lobby Alcove, during the morning and afternoon breaks. You may also buy snacks or lunch at the Natcher cafeteria, open from **6:30AM to 2:30PM**, and the Natcher concession stand, open from **7AM to 3:30PM**.

Dinner Information

Those who signed up for the dinner should plan to arrive at the **Curry Place Bethesda** in downtown Bethesda the evening of Day 1, October 24th, 2019 at **6:00pm**.

Curry Place Bethesda

7345-A Wisconsin Ave, Bethesda, MD 20814

Phone: 301-656-4444

<https://www.curryplacebethesda.com/>

Those attending the group dinner should meet at **Curry Place Bethesda** at 6:00pm on Day 1, Thursday October 24th.

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.**



Curry Place Bethesda

4.8 ★★★★★ (12)

Indian restaurant



Directions



Save



Nearby



Send to your phone



Share

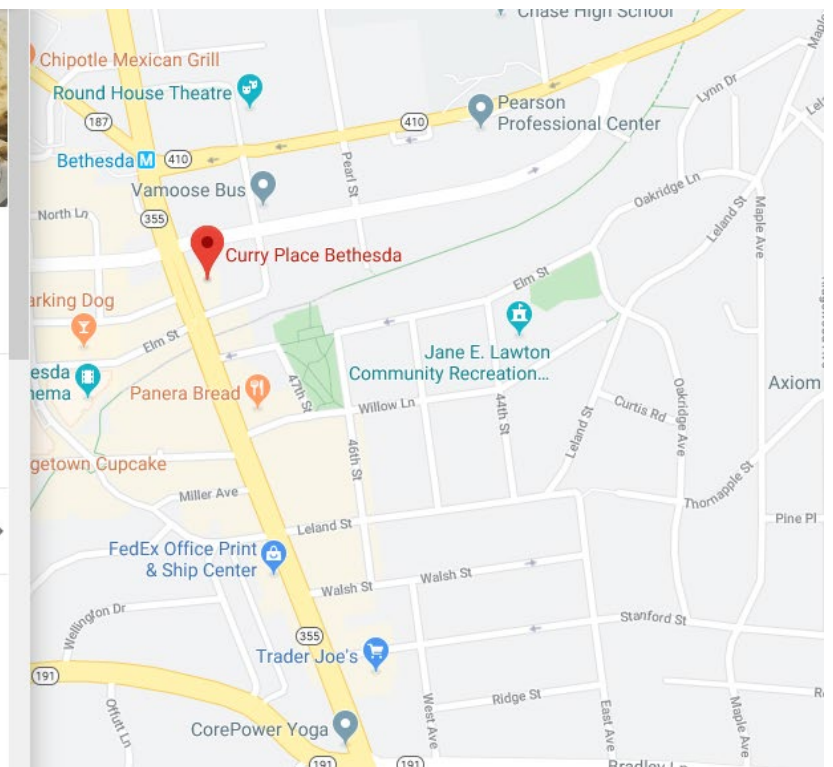
Comfort food · Casual · Vegetarian options

7345 Wisconsin Ave A, Bethesda, MD 20814

XWM4+7M Bethesda, 7, MD

[curryplacebethesda.com](https://www.curryplacebethesda.com)

(301) 656-4444



Agenda

DAY 1: Thursday October 24, 2019

**All sessions from 8:45AM to 12:30PM will be in the Auditorium --[Remote Access Instructions](#)*

****** Please review the [ML-MSM Background Information](#), [Perspectives Paper](#), and [Webinars](#) prior to the meeting!

7:30am - Arrive at NIH Security checkpoint. Use your registration Login to comment in these pages (Remote Access [Logistics](#))

8:00 - 8:45am: Check-in, Set up posters

8:45: Welcome from IMAG and MSM Co-Chairs: [Grace Peng](#), [Suvranu De](#) and [Ellen Kuhl](#) ([Perspectives Paper](#))

9:00-9:15am: Digital Twin Keynote: [Mark Palmer](#), Medtronic

9:15-9:30am: Human Safety Keynote: [Suvranu De](#), Rensselaer Polytechnic Institute

9:30 - 10:15am: Setting the stage: [Dr. Susan Gregurick](#), Associate Director for Data Science, NIH

[IMAG Government Panel](#) - Summary of [pre-meeting IMAG webinars](#)

10:15-10:30am: Overall Goals of 4 themes - Session Organizers

10:30 - 11:00am: Break - Poster Viewing- Group 1 presenters, refreshments - Atrium, Alcove

11:00am – 12:30pm THEME 1- Ordinary Differential Equations

Organizers: **Mark Alber** and **Krishna Garikipati**

12:30 – 1:30pm Lunch

- [Networking Lunch with IMAG program directors](#) - A/B
- [NVIDIA Informational Session](#) - E1/E2

1:30 – 3:00pm [THEME 2- Partial Differential Equations](#) - Auditorium

Organizers: **George Karniadakis** and **Adrian Buganza Tepole**

3:00 – 3:30pm Break - Poster Viewing - **Group 2 Presenters**, refreshments - **Atrium, Alcove**

3:30 – 4:15pm Breakout and group writing sessions for THEME 1 & THEME 2 -- **session 1**

4:15 – 5:00pm Breakout and group writing sessions for THEME 1 & THEME 2 -- **session 2**
(attendees rotate)

THEME 1: ODE & Human Safety - G1/G2	THEME 1: ODE & Digital Twin - E1/E2
THEME 2: PDE & Human Safety - C1/C2	THEME 2 PDE & Digital Twin - A/B

5:00 - 5:30pm [Report out](#) - THEMES 1 & 2

6:00-9:00pm: [Group Dinner](#)

DAY 2: Friday October 25, 2019

**All sessions from 8:45AM to 12:30PM will be in the Auditorium --[Remote Access Instructions](#)*

*** Please review the [ML-MSM Background Information](#), [Perspectives Paper](#), and [Webinars](#) prior to the meeting!*

7:30am - Arrive at NIH Security checkpoint. Use your registration Login to comment in these pages (Remote Access [Logistics](#))

8:00 - 8:45am: Check-in

8:45 - 9:00am: [Bruce Tromberg](#), Director National Institute of Biomedical Imaging and Bioengineering (NIBIB)

Integration Keynote: [Gunnar Cedersund](#), Linköping University

9:00– 10:30am **THEME 3- Data-Driven Approaches**

Organizers: **Bill Lytton** and **Linda Petzold**

10:30 – 11:00am **Break - Poster Viewing, refreshments - Atrium, Alcove**

11:00am – 12:30pm **THEME 4- Theory-Driven Approaches**

Organizers: **Bill Cannon** and **Paris Perdikaris**

12:30-12:45pm [Lunch](#) pick-up

(Working Lunch)

12:45 – 1:30pm Breakout and group writing sessions for THEME 3 & THEME 4 -- **session 1**

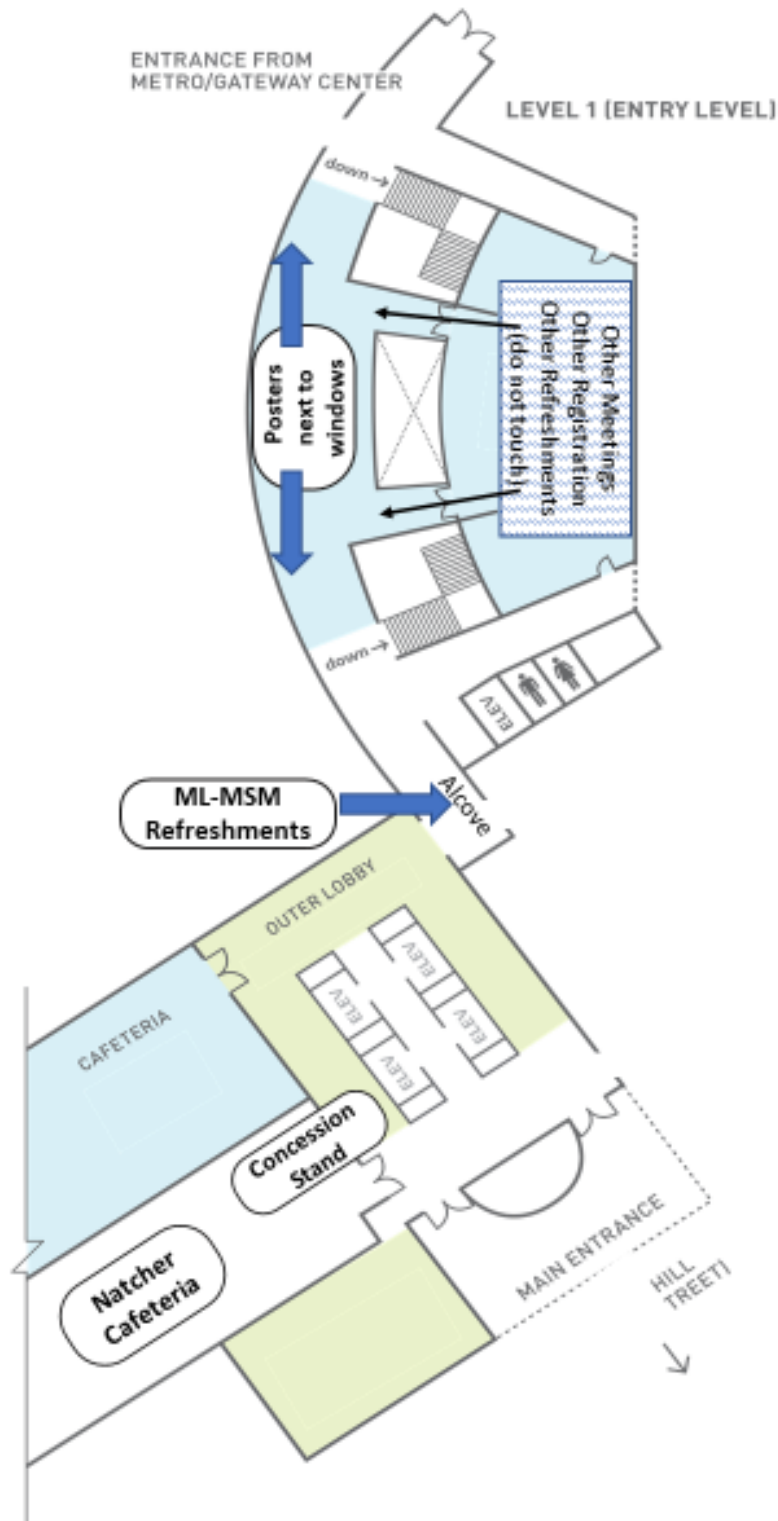
1:30 – 2:15pm Breakout and group writing sessions for THEME 3 & THEME 4 -- **session 2**
(attendees rotate)

THEME 3: Data-Driven & Human Safety- G1/G2	THEME 3: Data-Driven & Digital Twin- E1/E2
THEME 4: Theory-Driven & Human Safety- C1/C2	THEME 4 Theory-Driven & Digital Twin - A/B

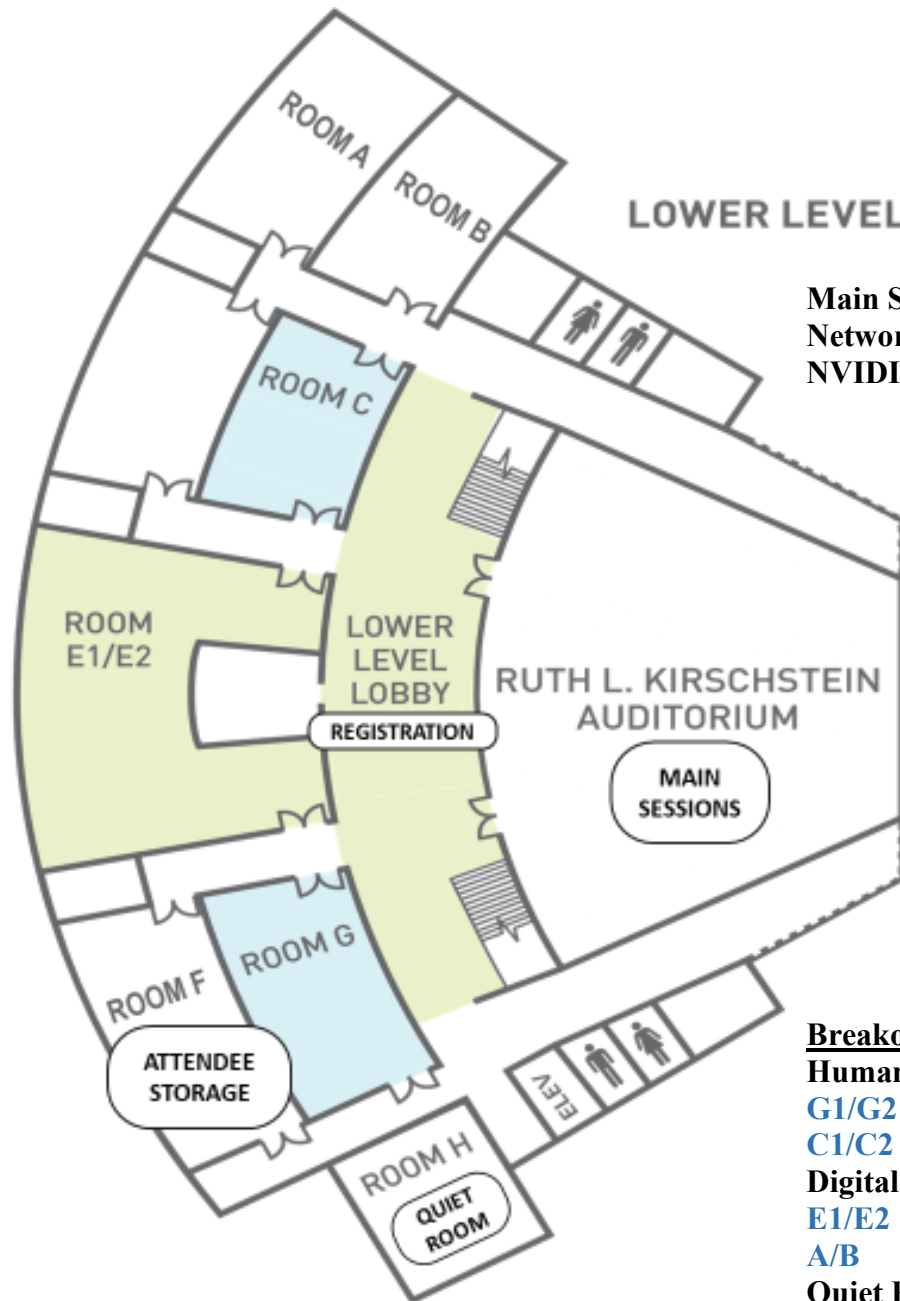
2:30 - 3:00pm [Report out](#) - THEME LEADS 3 & 4

3:00pm: Final Thoughts, Adjourn - Ellen Kuhl, Suvranu De, Grace Peng

Natcher Meeting Rooms



Natcher Meeting Rooms



Main Sessions: Auditorium
Networking lunch w/ IMAG: A/B
NVIDIA Information Session: E1/E2

Breakout Sessions Themes 1-4:
Human Safety
 G1/G2
 C1/C2
Digital Twin
 E1/E2
 A/B
Quiet Room: Room H
Attendee Storage: Room F1/F2

Background

Multiscale modeling has advanced to one of the most successful strategies to integrate data across the scales and offer mechanistic insights; yet, multiscale modeling alone often fails to efficiently combine large data sets from several different sources. **Machine learning** is a powerful technique that can guide model building, accelerate multiscale and multiphysics computational algorithms, train models to learn from data, identify patterns, and inform decision making. While traditional machine learning tools perform these tasks with minimal human intervention, this meeting focuses on integrating machine learning methods with multiscale modeling methods guided by the fundamental principles of mathematics and physics. **The objective of this meeting is to identify the perspectives, challenges, and opportunities of integrating machine learning with multiscale modeling (ML-MSM) in biomedical, biological, and behavioral systems.** Specifically, we will address four approaches within ML-MSM modeling: ordinary differential equation based, partial differential equation based, theory-driven, and purely data-driven approaches. **Attendees will discuss these approaches in the context of developing [Digital Twins](#) and addressing [Human Safety](#).**

A **digital twin** is a digital replica of a living or non-living physical entity, such as a manufacturing process, medical device, piece of medical equipment, and even a person. Utilizing sensor data, digital twins combine simulation and analytics to gain insight into present and future operational states of each physical twin. The resulting digital twin can be wrapped with artificial intelligence, combined with ensembles of similar twins, or used in tandem with other predictive tools to analyze and diagnose operational states and to optimize performance under real-world operating conditions. This enables companies to make predictions about future performance, improve operations and productivity, and reduce the risk of unplanned downtime. Essential to the digital twin concept is a two-way connection between the physical asset and its virtual representation through the Internet of Things (IoT). This connection ensures that the virtual twin remains a faithful representation of the physical asset and provides a platform to predict the physical assets immediate future.

Issues surrounding **human safety** encompasses multiple spatial and temporal scales in various environments; including occupational, operational, recreational, medical and surgical environments. **The Human Safety framework** includes the following levels of behaviors for consideration:

- 1) **Individual patient/operator/user** - human biology, physiology, EHR's, health history, expertise, experience
- 2) **Provider** – biopsies/procedures/processes, surgical/environmental safety checklists, adherence to behavioral interventions
- 3) **Tools, Smart Instrumentation** - wearable devices, development data, technology considerations for safety and economic benefits
- 4) **Team** - observational studies, training, communication, medical advocate benefit to patient
- 5) **System level** – hospitals, nursing homes, research facilities, centers of excellence for different health care issues, methods to select an excellent hospital, factories, schools, gyms/fields
- 6) **Population scale** – geographic location, analytics of low and high safety records, interactions occurring outside the healthcare system, public health, non-health related influences on safety
- 7) **Disease level/injury level** - Influence of changing State (and Federal) laws on public health, pathophysiology observed, disease or patient models
- 8) **Data and information sharing** – data quality, data analysis, performance measures, lessons learned, sharing mechanisms, linking with existing medical specialty groups