

## **NIMBioS Workshop: Scientific Collaboration Enabled by High Performance Computing**

**All sessions will be held in NIMBioS 205 & 206**

### **Monday morning:**

- 8:30 – 9:00 Breakfast, NIMBioS Breakroom (Room 104)
- 9:00 – 9:15 Introduction to NIMBioS (Lou Gross)
- 9:15 – 9:30 Participant Introductions
- 9:30 – 9:40 Overview and goals of the Workshop (Michela Taufer)
- 9:40 – 10:40 Tandy Warnow: Mathematics and Computer Science Aspects of Species Tree Estimation
- 10:40 – 11:00 **BREAK**
- 11:00 – 12:00 Jack Dongarra: High Performance Computing and Big Data: Challenges for the Future
- 12:00 – 1:20 **LUNCH**

### **Monday afternoon:**

- 1:30 – 2:30 Amanda Randles: Development and Applications of Massively Parallel Models of Human Hemodynamics
- 2:35 – 3:00 **BREAK**
- 3:00 – 4:15 Panel Discussion: Tales of Progress through Failure and Taking Risks  
Panelists: Kate Evans (Moderator), Shirley Moore, Anthony Danalis, and Hai An Nam
- 4:15 – 4:45 Discussion on Planning Breakout Groups
- 5:00 – 6:15 Reception and Poster Session, NIMBioS Breakroom (Room 104)

### **Tuesday morning:**

- 8:30 – 9:00 Breakfast, NIMBioS Breakroom (Room 104)
- 9:00 – 10:00 Miriam Leeser: High-performance Transformation of Protein Structure Representations Between Internal and Cartesian Coordinates
- 10:00 – 10:20 **BREAK and Group Photo**
- 10:20 – 11:20 Breakout Sessions
- 11:30 – 12:30 Tanzima Islam: Scalability challenges and opportunities for I/O bound applications
- 12:30 – 1:25 **LUNCH**

### **Tuesday afternoon:**

- 1:30 – 2:30 Hai Ah Nam: Navigating the Unknown: The Power of Collaboration in HPC
- 2:30 – 3:30 Cathy Wu: Data-Driven Discovery: Integrative Literature Mining and Semantic Computing for Drug Analytics and Precision Medicine
- 3:35 – 3:50 **BREAK**
- 3:50 – 4:40 Breakout Sessions

### **Wednesday morning:**

- 8:30 – 9:00 Breakfast, NIMBioS Breakroom (Room 104)
- 9:00 – 9:30 Discussion about promoting diversity in this research field, led by Lenhart
- 9:35 – 10:35 Srinivas Aluru: HPC-driven forays into genomics and systems biology
- 10:40 – 10:55 **BREAK**
- 11:00 – 11:50 Breakout Session
- 11:55 – 12:15 Summary, followed by **LUNCH**

## Posters Titles and Authors

The UMBC High Performance Computing Facility  
**Carlos Barajas**, Reetam Majumder, and Matthias Gobbert

Multidisciplinary Research and Education on Big Data + High-Performance Computing + Atmospheric Sciences  
Carlos Barajas, Pei Guo, Chamara Rajapakshe, Aryya Gangopadhyay, **Matthias Gobbert**, Jianwu Wang, and Zhibo Zhang

Parallel Algorithms for Updating Tree Like Properties of Dynamic Graphs  
**Sanjukta Bhowmick**, Boyana Norris, Sajal Das, Sriram Srinivasan, and Sara Riaz

Parallel MPI and Multi-Threaded Chromosome Matching Program for .BED Files  
Michael Porter, Nick Weiner, Victoria Van, and **Phil Bording**

Novel Sequence Alignment Algorithm for NGS Parallelized for HPC Systems  
**Sunita Chandrasekaran**, Sanhu Li, and Erin Crowgey

Challenges Deploying Stochastic Workloads on HPC Systems  
**Ana Gainaru**

A Blueprint for Designing and Simulating Whole-cell Models of Human Cells  
**Arthur Goldberg**, Balázs Szigeti, Yosef Roth, John Sekar, Yin Hoon Chew, and Jonathan Karr

Identifying Shifts in Forest Communities Using Machine Learning Techniques;  
Jonathan Knott, **Chathurangi Pathiravasan**, and Trenton Ford

Ultrastructural 3D Simulations of Neuronal Processes Using Highly Scalable Computational Algorithms  
**Gillian Queisser**

Moment Representation in the Lattice Boltzmann Method on Massively Parallel Hardware  
**Madhurima Vardhan**, John Gounley, Luiz Hegele, Erik Draeger, and Amanda Randles

A Parallel Workflow Framework for Data and Compute Intensive Application (openDIEL :  
cfdlab.utk.edu/opendiel + MAGMADNN : icl.utk.edu/magma)  
**Kwai Wong**, Frank Betancourt, Daniel Nichols, and Stanimire Tomov

A New Implementation of the Vortex Method  
**Ling Xu** and Robert Krasny

Better Feature Selection for Bacterial Movement by Machine Learning  
**Yue Ma**, Tian Hong, Gladys Alexandre, and Hong Guo