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 Riazi

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