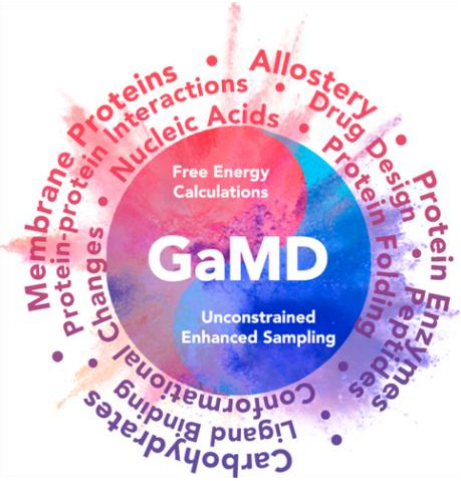
UNC SCHOOL OF MEDICINE

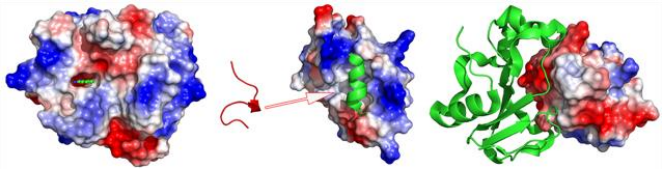
The Department of Pharmacology and the Computational Medicine Program

The Gaussian accelerated Molecular Dynamics (GaMD) Workshop 2024

Monday, October 28th, 2024
9 am - 5 pm

University of North Carolina at Chapel Hill





Welcome to the Gaussian accelerated Molecular Dynamics (GaMD) workshop at the University of North Carolina (UNC), Chapel Hill, on Monday, Oct 28, 2024. The workshop is designed for all students and researchers in Computational Chemistry, Biophysics, and Biomedicine in the areas of Molecular Dynamics, Enhanced Sampling, and Drug Design. The covered topics will include the latest developments and advanced application studies of the GaMD methodology.

The workshop will consist of invited talks in the morning and “hands-on” tutorial sessions on different GaMD algorithms in the afternoon. We greatly appreciate the support from the Department of Pharmacology, Computational Medicine Program, and Research Computing at UNC.

AGENDA

Monday, October 28, 2024.

Location: UNC-Chapel Hill-Bioinformatics 1131

9:00 AM	**Welcome Remark** *by Henrik Dohlman, PhD, UNC-Chapel Hill*
9:05 AM	**Introduction and Overview of GaMD** by *Yinglong Miao, PhD, UNC-Chapel Hill*
9:20 AM	**Investigation of Mechanism of Calcium Sensitivity Modulation of Cardiac Troponin C by Small Molecules** *Steffen Lindert, PhD. Ohio State University*
9:50 AM	**MDANCE: flexible and versatile n-ary clustering packag**e *Ramon Alain Miranda Quintana, PhD, University of Florida*
10:20 AM	*BREAK (group photo)*
10:30 AM	**Conformational Distributions of Glycans on Glycoproteins: NMR and GaMD** *by James Prestegard, PhD, University of Georgia*
11:05 AM	**Bridging timescales in protein simulations using Parallelized Gaussian Accelerated Molecular Dynamics (ParGaMD)** *Surl-Hee (Shirley) Ahn, PhD, University of California, Davis*
11:35 AM	**Running Gaussian Accelerated Molecular Dynamics for Customized Regions in OpenMM** *Pengfei Li, PhD, Loyola University Chicago*

Location: UNC-Chapel Hill-Mary Ellen Jones 3112

NOON	*LUNCH*
1:00 PM	**Hands-on tutorial: GaMD** *by Victor Adediwura, UNC-Chapel Hill*
2:15 PM	**Hands-on tutorial: Ligand GaMD (LiGaMD)** *by Jinan Wang, PhD, UNC-Chapel Hill*
3:30 PM	*BREAK*
3:45 PM	**Hands-on tutorial: Protein-Protein Interaction GaMD (PPI-GaMD)** *by Keya Joshi, UNC-Chapel Hill*
5:00 PM	**END**

Steffen Lindert, PhD. Ohio State

Dr. Lindert received his M.Sc. in Physics from the University of Leipzig in 2006 and his Ph.D. in Chemical and Physical Biology (Molecular Biophysics track) from Vanderbilt University in 2011. Co-advised by Prof. Jens Meiler and Prof. Phoebe Stewart, he worked on a combined experimental and computational project developing a program – EM-Fold – which folds proteins into medium-resolution cryo-EM density maps. After finishing his Ph.D., he joined the laboratory of Prof. Andy McCammon at the University of California, San Diego, as a postdoctoral fellow. His research focused on macromolecular simulations of proteins involved in cardiomyocyte contraction and computer-aided drug discovery. He was awarded a prestigious postdoctoral fellowship from the American Heart Association. He started his research group at Ohio State University in August of 2015. Research in the lab focuses on the development and application of computational techniques for modeling biological systems, intending to gain a deeper understanding of biomolecular processes, predicting protein structure with the use of sparse experimental data, and discovering new drugs. Dr. Lindert will move to UCLA in July 2025.

Ramon Alain Miranda Quintana, PhD, University of Florida

Ramon Alain Miranda-Quintana majored in Radiochemistry at the Higher Institute of Technologies and Applied Sciences in 2011 and obtained his Ph.D. in Chemistry from the University of Havana. After a research appointment at McMaster University, he won a York Science Fellowship to work at York University as a Postdoctoral Scholar (where he received the 2019 Polanyi Prize in Chemistry). He then joined the Department of Chemistry at the University of Florida as an Assistant Professor in 2020, where he is also a member of the Quantum Theory Project. His research interests include the development of ab initio electronic structure methods to study strongly correlated systems, understanding how charge and spin transfer processes shape chemical reactivity and solvation processes, and developing efficient extended similarity-based tools for data science applications in chemistry and the biomedical sciences. At UF, he received an Oak Ridge Ralph E. Powe Junior Faculty Enhancement Award, the OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award in Computational Chemistry, and an NIH R35 grant.

James Prestegard, PhD, University of Georgia

Dr. Prestegard received his B.S. in chemistry in 1966 from the University of Minnesota and his Ph.D. in chemistry from the California Institute of Technology in 1971. Before joining the CCRC in January 1998, Dr. Prestegard spent 27 years in the Chemistry Department at Yale University, where he held positions of assistant professor, associate professor, and professor. In addition to his normal professorial duties, he now directs the regional NMR facilities at the University of Georgia. Dr. Prestegard serves on the editorial boards of several journals, including the Journal of Magnetic Resonance and the Journal of Biomolecular NMR, and is a frequent member of advisory and review panels. Dr. Prestegard's group is applying nuclear magnetic resonance (NMR) spectroscopy to the study of the structure and function of biologically important macromolecular assemblies involving carbohydrates, proteins, and membranes. Research in the Prestegard laboratory focuses on NMR methods development, membrane proteins, cell-surface carbohydrates, protein structure, and protein-protein interactions.

Surl-Hee (Shirley) Ahn, PhD, University of California, Davis

Surl-Hee (Shirley) Ahn is an assistant professor in the Department of Chemical Engineering at the University of California, Davis. She received her B.A. in Biochemistry and Mathematics, her M.A. in Mathematics, and her M.S. in Chemistry from the University of Pennsylvania in 2012, and her Ph.D. in Chemistry (Chemical Physics) from Stanford University, advised by Prof. Eric Darve, in 2018. Subsequently, she worked as a postdoctoral scholar in the Department of Chemistry and Biochemistry at the University of California, San Diego (UCSD), advised by Prof. J. Andrew McCammon and Prof. Rommie Amaro for four years before starting her independent career at the University of California, Davis, in July 2022. Shirley is interested in developing enhanced sampling methods for molecular dynamics simulations and applying those methods to study important biophysical phenomena. She was selected to participate in the 2018 MIT Rising Stars in Mechanical Engineering Workshop, was awarded the 2021 ACS PHYS Division Young Investigator Award, and was a finalist for the 2021 Chancellor's Outstanding Postdoctoral Scholar Award at UCSD.

Pengfei Li, PhD, Loyola University Chicago

Dr. Pengfei Li received his B.S. degree in Chemistry from Xiamen University in 2011, followed by a Ph.D. degree in Chemistry under the mentorship of Dr. Kenneth M. Merz Jr. at Michigan State University in 2016. He then pursued postdoctoral research in Dr. Sharon Hammes-Schiffer's lab at the University of Illinois, Urbana-Champaign, and Yale University. In 2020, Dr. Li began his independent career as an Assistant Professor at Loyola University Chicago. His research group focuses on developing metal ion models, studying the mechanisms of metalloproteins, and designing molecules related to metalloproteins. To date, Dr. Li has published 37 peer-reviewed journal articles and two book chapters, with his work amassing thousands of citations. Since 2015, he has also contributed as a developer for the AMBER software package.

SPECIAL THANKS

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