Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Twelfth Round

Committee

James C. Gumbart

Chair

James C. “J.C.” Gumbart, PhD, is an Associate Professor of Physics at the Georgia Institute of Technology in Atlanta, Georgia. He obtained his B.S. from Western Illinois University and his Ph.D. in Physics from the University of Illinois, Urbana-Champaign in 2009 under the mentorship of Klaus Schulten, focusing on the area of computational biophysics. After two years as a postdoctoral fellow at Argonne National Lab working with Benoit Roux, he started his lab at Georgia Tech in early 2013. His lab carries out molecular dynamics simulations aimed primarily at understanding the composition, construction, and function of the Gram-negative bacterial cell envelope. Dr. Gumbart has served on previous molecular dynamics review committees convened by the National Academies.

Ravinder Abrol

Member

Ravinder “Ravi” Abrol, PhD, is an Associate Professor of Biochemistry at California State University, Northridge (CSUN). Dr. Abrol’s research lab is focused on developing and using computational methods to probe how protein structure and biochemical (protein-ligand and protein-protein) interactions of G protein-coupled receptors (GPCRs) determine cellular signaling and physiology, as well as how this knowledge can be used for the rational design of drugs targeting GPCR signaling pathways. GPCRs are integral membrane proteins that form the largest superfamily in the human genome. The activation of these receptors by a variety of bioactive molecules regulates key physiological processes (e.g., neurotransmission, cellular metabolism, secretion, cell growth, immunity, differentiation), through a balance of G protein-coupled and beta-arrestin-coupled signaling pathways. This has made them targets for ~50% drugs in the clinic. A molecular and structural understanding of these GPCR signaling pathways will have a broad impact on our understanding of cellular signaling and on drug discovery efforts targeting GPCRs. Research in the Abrol Lab lies at the interface of Chemistry and Biology, where they are also combining computational biophysics and structural bioinformatics based methods to gain mechanistic insights into the biochemistry of GPCR signaling along with membrane protein folding mechanisms. Dr. Abrol received a BS in 1994 from the University of Delhi, an MS in 1995 from Indian Institute of Technology, and a PhD in 2003 from California Institute of Technology, Pasadena.

Jerome Baudry

Member

Jerome Baudry, Ph.D. is the Pei-Ling Chan Professor of Biological Sciences in the Department of Biological Sciences at the University of Alabama, Huntsville (UAH). Dr. Baudry obtained his PhD in Molecular Biophysics from the University of Paris, UPMC/Sorbonne Universities, France. He subsequently joined the group of Klaus Schulten at the University of Illinois at Urbana-Champaign as a post-doc. After his post-doctoral work, Dr. Baudry worked in the pharmaceutical industry as a Research Scientist, and then accepted a Senior Research Scientist position back in Illinois on a non-tenure track research faculty position. Dr. Baudry joined the University of Tennessee, Knoxville and the UT/ORNL Center for Molecular Biophysics as a tenure track Assistant Professor in 2008. In 2014, he was promoted to Associate Professor with tenure. In August 2017, Dr. Baudry joined UAH as the Pei-Ling Chan Professor. At UAH, Dr. Baudry's group develops and applies methods and protocols for computational drug discovery, both on small-molecules and biologicals, within academic, national laboratories and industrial collaborations.

James Briggs

Member

James Briggs, Ph.D. is a Professor within the Biology and Biochemistry Department at the University of Houston. Dr. Briggs received his Ph.D. in Chemistry from Purdue University in 1990. His research focuses on computational studies of protein structure and function, inhibitor design, investigations of possible inhibitor resistance pathways, and development of methods for the above areas. Targets for these studies include those important in the treatment of AIDS, cancer, bacterial infections, and other disease states. In addition, Dr. Briggs has worked on inhibitors to aid in biowarfare defense (botulinum neurotoxins, anthrax toxin, cholera toxin). Dr. James Briggs' research is focused in the highly interdisciplinary and collaborative area of computational chemistry/biochemistry. He develops and applies computational methods to problems of chemical and biochemical interest. His research falls into two general categories: computer-aided inhibitor design/discovery and computational biophysics. His main target areas in the inhibitor/ligand area are Rho kinase 1 (heart disease), PTEN (cancer), PTEN/5HTC2C (addiction control), BCL2 (cancer), gluconeogenesis and glucose uptake (cancer); those for the computational biophysics area include cholera toxin, biofilm control, RNA structure prediction, protein electrostatics and pKa predictions, and identification of protein/enzyme function from structure only. Dr. Briggs has served on previous Molecular Dynamics review committees convened by the National Academies, including serving as Committee Chair in 2019 for the 10th round of proposal evaluations.

David A. Case

Member

David A. Case, Ph.D. is Professor of Chemistry and Chemical Biology at Rutgers University. His research involves simulations of proteins and nucleic acids, and analysis of results from biomolecular NMR and crystallography. He is the lead developer for the Amber suite of biomolecular simluation software. He received a Ph.D. from Harvard University in 1977 in Chemical Physics. He received the President's Award from the International Society for Quantum Biology and Pharmacology in 2014, and the American Chemical Society Award for Computers in Chemical and Pharmaceutical Research in 2015.

Xiaolin Cheng

Member

Xiaolin Cheng, Ph.D. received his B.S. from Nanjing University in China, and his Ph.D. from the Stony Brook University. After a postdoctoral fellowship at University of California, San Diego, he joined the Center for Molecular Biophysics (CMB) at Oak Ridge National Laboratory (ORNL) as an Associate R&D Staff Scientist. After leaving his position as a Senior R&D Staff Scientist at ORNL, he became an Associate Professor in College of Pharmacy at The Ohio State University (OSU) in 2017. He is also a core faculty of OSU’s Translation Data Analytics Institute (TDAI). His research is focused on employing a myriad of computational and data analytics methods to elucidate molecular basis of drug action and to rationally design new drug molecules. Additionally, he is engaged in developing and applying advanced molecular modeling & simulation techniques to integrate experimental data, specifically from cryo-electron microscopy, into structural models of dynamic biological assemblies. His research has been continuously funded by NIH, NSF and DOE.

Brian Dominy

Member

"Brian Dominy, Ph.D. is an Associate Professor in the Department of Chemistry and Associate Dean of the Graduate School at Clemson University. Dr. Dominy earned his B.S. degree from Carnegie Mellon University in the Biological Sciences and Computer Science tracks with a minor in Chemistry. He then joined the Scripps Research Institute as a Ralph M. Parsons Foundation predoctoral fellow, earning his Ph.D. under the direction of Dr. Charles L. Brooks III. Following this, he worked as an NIH NRSA postdoctoral fellow at Harvard University with Dr. Eugene Shakhnovich in the Department of Chemistry and Chemical Biology. Dr. Dominy joined the faculty of the Department of Chemistry at Clemson in 2005 and received an NSF CAREER award in 2010 for his research in the development and application of computational models to study the physical chemistry driving biomolecular evolution. His service responsibilities over the years have focused significantly on the development and assessment of academic programs at the departmental, college, and university levels at Clemson. Dr. Dominy served as the interim associate dean of academic affairs for the newly formed College of Science from 2016-2018, and since 2018 has served as the associate dean of the Graduate School at Clemson University. This is Dr. Dominy’s third year serving on this recurring NASEM Committee.
"

Ellinor Haglund

Member

Ellinor Haglund, Ph.D. is currently an Assistant Professor in the Department of Chemistry at the University of Hawaii in Manoa. Dr. Haglund received her Masters in Molecular Biology and Chemistry from Umeå University, her Ph.D. at Stockholm University, and completed her post-doctoral work at Rice University and the University of California, San Diego, with the Center for Theoretical Biological Physics. Her research is focused on the folding event in proteins, utilizing both computational and experimental techniques to understand the molecular details of how proteins fold into biologically active molecules. She is inspired by how nature works and utilizes her multidisciplinary training to answer questions at the interface of chemistry, biology, and physics.

Yu-ming M. Huang

Member

Dr. Y. Mindy Huang received her Ph.D. degree in computational chemistry from the University of California, Riverside, in 2014. She is currently an assistant professor in the Department of Physics and Astronomy at Wayne State University (WSU). Since joining WSU, she has established a vibrant Computational Biophysics Group. The central goal of her research work is to understand the fundamental mechanism of biomolecular recognition and diffusion processes by using theoretical and classical mechanical models. Her research involves the development and application of computational methods to address biologically and medically important problems. Dr. Huang has established an excellent track record of 22 published articles, including 12 first-author papers and 8 corresponding or co-corresponding author papers. Her pioneering work on the diffusion study has been honored with the NVIDIA GPU award, Best Paper Award from Protein Science publications, and Wiley Computers in Chemistry Outstanding Postdoc Award. She has also been awarded computational time on the specialized architecture ANTON machine for hundreds of μs MD and also received the computational allocation award of CPU hours on the XSEDE supercomputer.

Margaret Johnson

Member

Margaret Johnson, Ph.D. joined the Biophysics faculty at Johns Hopkins University in 2013. She received her BS in Applied Math from Columbia University and her PhD in BioEngineering from UC Berkeley. She completed postdoctoral training in the Laboratory of Chemical Physics at the National Institutes of Health in Bethesda, Maryland. Her research focuses on understanding how the individual interactions between thousands of diverse components in the cell generate order and collective function at the right time and the right place. She develops theoretical and computational approaches to study the evolution and mechanics of dynamic systems of interacting and assembling proteins.

Vivek Narsimhan

Member

Vivek Narsimhan, Ph.D. is an Assistant Professor of Chemical Engineering at Purdue University. Dr. Narsimhan received his bachelors in Chemical Engineering from the California Institute of Technology, his Master in Advanced Study in Mathematics from the University of Cambridge, his Ph.D. in Chemical Engineering from Stanford University, and completed his Post-doctoral research at MIT. His research uses a mixture of theory, simulations, and experiments to examine problems in the areas of suspensions, complex interfaces, fluid mechanics, and polymers. He has developed mathematical models, performed simulations, and conducted experiments to describe the mechanics of droplets, red blood cells, and vesicles under various flow types and microfluidic geometries. These investigations provide insight into how complex membranes alter the mechanical stability and motion of fluid-filled particles, both individually and as a suspension.

Carol B. Post

Member

Carol B. Post, Ph.D. is Distinguished Professor of Medicinal Chemistry and Molecular Pharmacology at Purdue University. She specializes in Computational Chemistry and Biological NMR and is also an NIH principal investigator. Since 1990, she has directed a research program toward understanding protein structure and molecular mechanisms that regulate molecular interactions and enzymatic activity. Her research program utilizes primarily computer simulation methods and NMR spectroscopy to study the structure and function of proteins and protein complexes associated with signaling, with current efforts being focused on Src and Syk tyrosine kinase. Molecular dynamics simulation methods and NMR spectroscopy are the approaches taken to study proteins and protein complexes associated with cancer and human viruses. Post is an internationally recognized leader in the regulation and function of protein-protein interactions associated with cell signaling and viruses. She has an exceptional record of scientific research and impact in such critical areas as cancer biology, therapeutics, and infectious and immune diseases. Post was recognized in 2009 with the Lions Club Award for Outstanding Achievements in Cancer Research, the Chaney Faculty Scholar Award from the College of Pharmacy in 2013, the Provost’s Award for Outstanding Graduate Mentor in 2016, and appointment as Fellow of the AAAS in 2020 and Fellow of the Biophysical Society in 2021. Dr. Post has served on previous molecular dynamics review committees convened by the National Academies.

Pengyu Ren

Member

Pengyu Ren, Ph.D. is E.C.H. Bantel Professorship for Professional Practice at The University of Texas at Austin. studies the structure and function of biomolecules, with pharmaceutical and biomedical applications. Dr. Ren's research team uses a range of computational tools to study the structure, dynamics and interactions of proteins, nucleic acids and other macromolecules, and to search for compounds mimicing and interfering with biomolecues for diagnostic and therapeutic purposes. His lab is developing a multi-scale modeling technique that allows scientists to efficiently study bimolecular assemblies. Dr. Ren is an elected Fellow of American Institute for Medical and Biological Engineering. He has published about 80 journal articles and 5 book chapters. He received a Ph.D. in Chemical Engineering from the University of Cincinnati.

Steven W. Rick

Member

Steven W. Rick, Ph.D., is a Professor in the Chemistry Department at the University of New Orleans. Dr. Rick received his Bachelors from the University of California, Los Angeles, his Ph.D. from the University of California, Berkeley in 1989, and completed his postdoctoral research at Columbia University. His research applies theoretical and computational approaches to a variety of chemically interesting systems. His work involves the development of more efficient computer simulation methods and better models for molecular interactions. Dr. Rick's group is applying these methods to the study of liquid water, interfaces, aqueous solutions, proteins, and ion transport through various materials. Dr. Rick has served on a previous molecular dynamics review committee convened by the National Academies.

Leonor Saiz

Member

Leonor Saiz, Ph.D. is a Professor in the Biomedical Engineering Department at the University of California, Davis. Dr. Saiz received her Ph.D. in Physics from the University of Barcelona. Her research involves the study of the dynamics of biological networks at the cellular and molecular level. Her lab combines computational and theoretical approaches together with experimental data to (1) understand how cellular behavior arises from the physical properties and interactions of the cellular components; and to (2) infer detailed molecular properties, such as the in vivo DNA mechanics, from the cellular physiology. By developing novel methodologies that consider multiple spatial and temporal scales and multiple levels of biological organization, including atomic, molecular, and cellular, their work has provided new avenues to integrate the molecular properties of cellular components directly into the dynamics of cellular networks. The ultimate goal of her work is to understand and follow the impact of molecular perturbations in the cellular components, such as a mutation in a protein or interventions with small molecules or drugs, through the different cellular processes up to the cellular behavior; one of the major challenges of modern biomedical sciences.

Janani Sampath

Member

Janani Sampath, Ph.D. is an Assistant Professor of Chemical Engineering at the University of Florida. She joined the department in January 2021. Her expertise lies in using molecular dynamics simulations to understand the behavior of polymers, proteins and their hybrids. Her group uses a combination of coarse grained and atomistic models to study systems ranging from synthetic polymer membranes, polymer-protein bioconjugate self-assembly, and polymers for therapeutic applications. Prior to this, she was a postdoctoral researcher at the University of Washington and Pacific Northwest National Lab. She obtained her Ph.D. in chemical engineering from the Ohio State University in 2018.

Jeffrey Skolnick

Member

Jeffrey Skolnick, Ph.D. is Professor and Mary and Maisie Gibson Chair and GRA Eminent Scholar in Computational Systems Biology at Georgia Institute of Technology. He received his BA in Chemistry, from Washington University, St. Louis in 1975, his M. Phil. in Chemistry from Yale University in 1977, and his PhD in Chemistry from Yale University in 1978. His research interests include using systems and computational biology approaches to solve health problems. He uses these tools to better understand important areas of study such as cancer metabolomics, drug design, and protein evolution. An additional area of research includes the prediction of protein structure from DNA sequences to better characterize human genes.

Kayla G. Sprenger

Member

Kayla G. Sprenger, Ph.D, is an assistant professor in the Department of Chemical and Biological Engineering at the University of Colorado, Boulder. At the Massachusetts Institute of Technology, Dr. Sprenger was a postdoctoral associate at the Institute for Medical Engineering and Science in the Chakraborty Laboratory for Computational Immunology. Her research interests include using molecular dynamics simulations, mathematical modeling, and machine learning to investigate host immune responses to infectious disease pathogens and neurological disease pathways. She has a BS and an MS in chemical engineering and earned her PhD from the University of Washington in 2017. Dr. Sprenger has served on a previous molecular dynamics review committee convened by the National Academies.

Juan Vanegas

Member

Juan M. Vanegas, Ph.D. is currently an Assistant Professor at the University of Vermont in the Department of Physics with appointments in the Materials Science and Cellular, Molecular, and Biomedical Sciences Graduate Programs. Dr. Vanegas received his master's in Biochemistry and Biophysics from Oregon State University, and his PhD in Biophysics from the University of California, Davis. His research uses coarse-grained, atomistic, and ab initio molecular simulation methods to understand how chemical structure determines mechanical properties of biomolecules and their response to mechanical stimuli. Some applications of this research include understanding elastic properties of lipid biomembranes and force transduction mechanisms in mechanosensitive channels. His lab leads the development of computational tools for local stress calculations from molecular dynamics simulations.

Josh Vermaas

Member

Josh Vermaas, Ph.D. is a computational biophysicist within the scientific computing group. During his PhD training at the University of Illinois, Josh performed and analyzed molecular dynamics simulations at all scales. This time included graduate research opportunities throughout the national lab system at the National Renewable Energy Laboratory, Oak Ridge National Laboratory, and Sandia National Lab. This membrane-focused research was expanded during his postdoctoral tenure at the National Renewable Energy Laboratory to encompass biomass materials, with a particular focus on lignin. Josh is now applying this experience towards adapting molecular dynamics codes to trends in HPC architecture and enable advances at the bleeding edge of computational science.