# DAIPAYAN SARKAR, PH.D.

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## SUMMARY

In my current research, I study **transport of photosynthetic metabolites across multimillion-atom bacterial microcompartments (BMCs)** using all-atom molecular dynamics (MD). Endogenous BMCs such as the carboxysome found in photosynthetic cynanobacteria, comprises of a protein shell and their biological role is towards **carbon concentration by regulating the transport of certain metabolites in the Calvin-Benson cycle, which is used in photosynthesis**. Here, MD simulations provide a mechanistic view to understand the **thermodynamics (free energy) and kinetics (mean first passage time) of small photosynthetic metabolite transport across large protein microcompartments** found in cyanobacteria. In addition to this research, which is funded by U.S. Department of Energy, Office of Basic Energy Sciences, I have experience working with biopolymers in plant secondary cell walls, namely cellulose, hemicellulose and lignin. Utilization of these biopolymers is essential towards building a **circular bio-economy** with widespread applications in **sustainable energy and engineering**. Towards this, by using the **lignin-cellulose binding free energy** derived from MD simulations, my research has provided a measure to understand the **atomistic origins of biomass recalcitrance**. Also related to plant cell walls, my work in collaboration with scientists at the National Renewable Energy Laboratory and U.S. Department of Agriculture Forest Services has shed light on the **molecular mechanisms behind the role of moisture in wood and how does the diffusion of metal cations and acetylation impact wood pretreatment**.

Another area where I have co-authored several publications is **integrative modelling**, where we combine **cryo-electron microscopy with MD to gain insight into the structure-function relationship for biomolecules**. Recent success was in determining the structure of the **AstraZeneca COVID-19 vaccine**, also known as ChAdOx1 (PDB:**7RD1**). These projects have mostly been conducted in collaboration with Dr. Abhishek Singharoy at Arizona State University and his collaborators.

Perhaps by now you may have realized that I have a diverse background in computational science and engineering and have experience **(1)** to calculate permeability for small molecule transport across protein shells and plasma membranes **(2)** integrative modelling and toolkit development **(3)** free energy calculations using enhanced sampling **(4)** free energy perturbation **(5)** computational modelling of reaction-diffusion phenomena, specifically thermodynamics and kinetics in biological and energy storage systems (mostly done as part of my doctoral thesis work in Mechanical Engineering). These diverse research areas have significant applications in energy, health and sustainable engineering applications, but have a common underlying theme called "rare events", since the biological systems are governed by the laws of thermodynamics, statistical mechanics and kinetics.

Here I have attempted to explain my journey in brief, from a postdoctoral research scientist in computational biophysics back to a graduate student in mechanical engineering, a question people often have when looking at my academic education.

Although I am not a wet lab scientist, but have nearly two years of experience working in a wet lab. Based on your interests, if you want to know about my wet lab experience, see footnote [1]

Link to all my research publications can be found here in my **Google Scholar**.

### Technical Skills:

Molecular Dynamics: NAMD, GROMACS, VMD, VMD-Python

Enhanced Sampling (REUS, ABF, Metadynamics, SMD), Free Energy perturbation (FEP)

QM- Single point energy (Gaussian16)

[1] While I worked in the lab or Dr. Zhenpeng Qin mostly doing computational modeling, I learned how to synthesize gold nanoparticle and conjugate proteins, enzymatic assay to determine enzyme-substrate kinetics using multi-well plate reader, Dynamic Light Scattering (DLS) and UV-Vis spectroscopy to characterize nanoparticles. As part of my doctoral thesis, I learned Infrared (IR) thermography.

Programming: Python, Tcl, Bash, MATLAB, Mathematica, C++ (basic level)

Bioinformatics: AlphaFold, ROSETTA, BLAST, AutoDock Vina

Structural Biology: VMD, Phenix, MolProbity, UCSF Chimera.

Finite Element Analysis: COMSOL, ANSYS

High performance computing (HPC): Slurm, Torque

Operating system: Unix, MacOS, Windows

Utility: Microsoft Office, LaTeX

## ACADEMIC PREPARATION

**Postdoctoral Research Associate** (PI: Prof. Josh V. Vermaas), MSU-DOE Plant Research Laboratory, East Lansing, MI May 2021 -

**Postdoctoral Research Associate** (PI: Prof. Daisuke Kihara), Department of Biological Sciences, Purdue University, West Lafayette, IN July 2019 - April 2021

**Research Associate** (PI: Prof. Zhenpeng Qin), Department of Mechanical Engineering, University of Texas at Dallas, Richardson, TX June 2017 - June 2019

**Adjunct Lecturer**, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington January 2017 - May 2017

**Enhanced Graduate Teaching Assistant**, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, TX August 2015 - May 2016

**Summer Research Fellow** (PI: Prof. Vinod Srinivasan (now at University of Minnesota, Twin Cities)), Department of Mechanical Engineering, Indian Institute of Science, Bengaluru, India May 2015 - August 2015

**Graduate Teaching Assistant**, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, TX August 2012 - May 2015

**Graduate Research Assistant**, Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, TX August 2010 - May 2012

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**Courtesy Affiliation** (PI: Prof. Abhishek Singharoy), School of Molecular Sciences, Arizona State University, Tempe, AZ August 2018 -

## EDUCATION

University of Texas at Arlington August 2012 - August 2016
**PhD**, Mechanical Engineering

University of Texas at Arlington August 2010 - May 2012
**MS**, Mechanical Engineering

University of Mumbai May 2006 - May 2010
**BE**, Mechanical Engineering

## AWARDS

ISPR-DOE travel award for 18th International Photosynthesis Congress in Dunedin, New Zealand, 2022

Doctoral Dissertation Fellowship, College of Engineering, The University of Texas at Arlington, 2016 (awarded annually by the College of Engineering to selected students)

Research Internships in Science and Engineering fellowship, Indo-US Science and Technology Forum, 2015

Enhanced Graduate Teaching Assistant, Mechanical and Aerospace Engineering Department, The University of Texas at Arlington (awarded annually by the College of Engineering to selected doctoral bound students)

## ACADEMIC MENTORSHIP

Isaiah Kaufman - Rotation PhD student, Department of Biochemistry and Molecular Biology, Michigan State University Aug - Oct, 2022

Jacob Zieba - Rotation PhD student, Department of Biochemistry and Molecular Biology, Michigan State University Jan. - April, 2022

Jessica Egelston - Senior Undergraduate, Department of Biochemistry and Molecular Biology, Michigan State University) 2021 - 22

Ian Santiago - Senior Undergraduate, Louisiana State University 2021-22

Ellen Strietweiser - Undergraduate, School of Molecular Sciences, Arizona State University (current position: PhD student at University of Washington, Seattle) 2018 - 20

Divya Chalise - Undergraduate, Mechanical and Aerospace Engineering, University of Texas at Arlington (current position: PhD student at University of California, Berkeley) 2015 - 17

## PEER-REVIEWED PUBLICATIONS

(* - equal contribution)

1. **D. Sarkar**, I. Santiago, J. V. Vermaas, Atomistic Origins of Biomass Recalcitrance in Organosolv Pretreatment, 2023, Chemical Engineering Science (in-revision)
2. **D. Sarkar***, M. Kulke*, J.V. Vermaas, LongBondEliminator: A Molecular Simulation Tool to Remove Ring Penetrations in Biomolecular Simulation Systems, 2023, Biomolecules, Special Issue Biomolecules In Silico: Contemporary Advances in Computational Approaches to Investigating the Molecular Dynamics of Biological Systems, doi:10.3390/biom13010107
3. C. Gupta, **D. Sarkar**, D. P. Tieleman, A. Singharoy, The ugly, bad, and good stories of large-scale biomolecular simulations, 2022, Current Opinion in Structural Biology, doi:10.1016/j.sbi.2022.102338
4. J. W. Vant, **D. Sarkar**, J. Nguyen, A. T. Baker, J. V. Vermaas, A. Singharoy, 2022, Exploring cryo-electron microscopy with molecular dynamics, Biochemical Society Transactions, doi:10.1042/BST20210485
5. A. T. Baker*, R. J. Boyd*, **D. Sarkar***, A. Teijeira-Crespo**, C. K. Chan**, E. A. Bates, K. Waraich, J.W. Vant, E.A. Wilson, C. D. Truong, M. Lipka-Lloyd, Petra Fromme, Josh V. Vermaas, D. Williams, L. Machiesky, M. Heurich, B. Nagalo, L. Coughlan, S. Umlauf, P. Chiu, P.J. Rizkallah, A.L.Parker, A. Singharoy, M. J. Borad, ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome, 2021, Science Advances, doi:10.1126/sciadv.abl8213.
6. M. Shekhar, G. Terashi, C. Gupta, **D. Sarkar**, G. Debussche, N. J. Sisco, J. Nguyen, A. Mondal, J. Vant, P. Fromme, W. D. Van Horn, E. Tajkhorshid, D. Kihara, K. Dill, A. Perez, A. Singharoy, 2021, Matter, Cell Press, doi:10.1016/j.matt.2021.09.004
7. M. Lensink, ...., C. Christoffer, G. Terashi, J. Verburgt, **D. Sarkar**, T Aderinwale, X Wang, D Kihara, ..., Shoshana J. Wodak, Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment, 2021, *Proteins: Structure, Function, and Bioinformatics*, doi:10.1002/prot.26222.
8. C.L. Lawson, A. Kryshtafovych, P.D. Adams, P. Afonine, M. L. Baker, B. A. Barad, P. Bond, T. Burnley, R. Cao, J. Cheng, G. Chojnowski, K. Cowtan, K. A. Dill, F. DiMaio, D. Farrell, J. S. Fraser, M. A. Herzik, S. W. Hoh, J. Hou, L. Hung, M. Igaev, A. P. Joseph, D. Kihara, D. Kumar, S. Mittal, B. Monastyrskyy, M. Olek, C. Palmer, A. Patwardhan, A. Perez, J. Pfab, G. D. Pintilie, J. S. Richardson, P. B. Rosenthal, **D. Sarkar**, L. U. Schaefer, M. F. Schmid, G. F. Schroeder, M. Shekhar, D. Si, A. Singharoy, G. Terashi, T. C. Terwilliger, A. Vaiana, L. Wang, Z. Wang, S. A. Wankowicz, C. J. Williams, M. Winn, T. Wu, X. Yu, K.

Zhang, H. M. Berman, W. Chiu, Outcomes of the 2019 EMDataResource model challenge: validation of cryo-EM models at near-atomic resolution, 2021, *Nature Methods*, 18, 156 - 164.

9. S. Ramadesikan, L. Skiba, J. Lee, K. Madhivanan, **D. Sarkar**, A. De La Fuente, C. B. Hanna, T. Hazbun, D. Kihara, R. C. Aguilar, Specific OCRL1 patient mutations differentially impact Lowe Syndrome cellular phenotypes, 2021, *Human Molecular Genetics*, ddab025
10. T. Aderinwale, C. W. Christoffer, **D. Sarkar**, E. Alnabati, D. Kihara, Computational structure modeling for diverse categories of macromolecular interactions, 2020, *Current Opinion in Structural Biology*, 64, 1-8.
11. J. W. Vant, **D. Sarkar**, E. Strietweiser, G. Fiorin, R. D. Skeel, J. V. Vermaas, A. Singharoy, Data-guided Multi-Map variables for ensemble refinement of molecular movies, 2020, *Journal of Chemical Physics*, 153, 214102.
12. J.W. Vant, SL J. Lahey, K. Jana, M. Shekhar, **D. Sarkar**, B. H. Munk, U. Kleinekathofer, S. Mittal, C. Rowley, A. Singharoy, Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials, 2020, *Journal of Chemical Information and Modeling*, 60, 5, 2591–2604.
13. **D. Sarkar***, P. Kang*, S.O. Nielsen, Z. Qin, Non-Arrhenius Reaction-Diffusion Kinetics for Protein Unfolding over a Large Temperature Range, 2019, *ACS Nano*, 13, 8, 8669-8679.
14. S. Luhar, **D. Sarkar**, A. Jain, Steady state and transient analytical modelling of non-uniform convective cooling of a microprocessor chip due to jet impingement, 2017, *International Journal of Heat and Mass Transfer*, 110, 768-777 2017.
15. D. Anthony, **D. Sarkar**, A. Jain, Non-invasive, transient measurement of the core temperature of a solid body, 2016, *Scientific Reports*, 6, 35886:1-1.
16. D. Anthony, **D. Sarkar**, A. Jain, Contactless, non-intrusive core temperature measurement of a solid body in steady-state, 2016, *International Journal of Heat and Mass Transfer*, 101, 779-788.
17. **D. Sarkar**, A. Jain, R. J. Goldstein, V. Srinivasan, Corrections for lateral conduction error in steady-state heat transfer measurements, 2016, *International Journal of Thermal Sciences*, 109, 413-423.
18. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Thermal conduction in an orthotropic sphere with spatial variation in convective heat transfer coefficient, 2016, *International Journal of Heat and Mass Transfer*, 96, 406-412.
19. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Steady-state temperature distribution in tissue due to heat generating tumor, 2015, *International Journal of Heat and Mass Transfer*, 96, 406-412.
20. **D. Sarkar**, K. Shah, A. Haji-Sheikh, A. Jain, Analytical modelling of temperature distribution in an anisotropic cylinder with circumferentially-varying convective heat transfer, 2014, *International Journal of Heat and Mass Transfer*, 39, 1027-1033.
21. **D. Sarkar**, A. Haji-Sheikh, A view of thermal wave in thin plates, 2012, *International Communications in Heat and Mass Transfer*, 39, 8, 1009-1017.

## Book Chapters

1. J. W. Vant*, **D. Sarkar***, C. Gupta*, M. Shekhar, S. Mittal and A. Singharoy, Molecular Dynamics Flexible Fitting: All you want to know about flexible fitting, Methods in Molecular Biology, Protein Structure Prediction, 4t̂h Ed - in press, 2019 (role: equal contribution)
2. E. Wilson, J. W. Vant, J. Layton, R. Boyd, H. Lee, M. Turilli, B. Hernandez, S. Wilkinson, S. Jha, C. Gupta, **D. Sarkar** and A. Singharoy, All You Want to Know About Large System Simulations, Methods in Molecular Biology -submitted, 2019 (role: corresponding author)

## Pre-print Manuscripts

1. **D. Sarkar**, I. Santiago, J. V. Vermaas, Atomistic Origins of Biomass Recalcitrance in Organosolv Pretreatment, 2022, ChemRxiv, doi:110.26434/chemrxiv-2022-9j7zv

2. **D. Sarkar***, H. Lee*, J. W. Vant, M. Turilli, S. Jha, A. Singharoy, (2021). Scalable Adaptive Protein Ensemble Refinement Integrating Flexible Fitting, bioRxiv, doi:10.1101/2021.12.07.471672 (role: corresponding author)

## INVITED ABSTRACTS, TALK, PRESENTATION AND POSTERS

(* - equal contribution)

1. **D. Sarkar**, M. Sutter, C. A. Kerfeld, J. V. Vermaas, Tracking photosynthetic metabolites across bacterial microcompartments using computational microscopy , DOE Physical Biosciences PI meeting, 2022, (poster presentation - PI: Christoph Benning).
2. **D. Sarkar**, J. V. Vermaas, Large scale molecular dynamics simulation of photosynthetic metabolites across bacterial micro-compartments, American Chemical Society, Fall 2022 meeting (platform talk).
3. **D. Sarkar**, L. Bu, J. Jakes, J. Zeiba, V. Bharadwaj, M. Crowley, M. Crowley, P. Ciesielski, J. V. Vermaas, Diffusion in plant cell wall models at different relative humidity using molecular dynamics simulations, American Chemical Society, Fall 2022 meeting (platform talk).
4. M. Kulke*, **D. Sarkar***, J. V. Vermaas, Quantifying temperature dependent mesophyll conductance within leaf plasma membranes, American Chemical Society, Fall 2022 meeting (platform talk).
5. J. L. Egleston*, **D. Sarkar***, J. V. Vermaas, Structural principles governing substrate selectivity in small multidrug resistance proteins, American Chemical Society, Fall 2022 meeting (poster presentation)
6. **D. Sarkar***, J. L. Egleston*, J. V. Vermaas, Correlating the transport cycle of small multidrug resistance transporters, Annual Biophysical Society Meeting 2022, doi:10.1016/j.bpj.2021.11.800
7. F. T. Doole, C. K. Chan, E. Streitwieser, **D. Sarkar**, A. V. Struts, A. Singharoy, M. F. Brown, Rivalry of cholesterol and antimicrobial peptides as seen by molecular simulations and NMR spectroscopy., Annual Biophysical Society Meeting 2022, doi:10.1016/j.bpj.2021.11.1922
8. I. Santiago, **D. Sarkar**, J. V. Vermaas, Quantifying solvent impacts on lignin-cellulose interactions in diverse solvents, American Chemical Society, Fall 2021 meeting (virtual presentation).
9. **D. Sarkar**, M. Shekhar, A. Singharoy, 2021 EM Challenge Committee Meeting, Stanford University (invited talk, presented virtually).
10. G Terashi, C Christoffer, **D Sarkar**, D Kihara, Modeling SARS-CoV2 proteins in the CASP-commons experiment, CASP14-COVID 19 paper (invited abstract, manuscript in preparation), 2021.
11. C Christoffer, G Terashi, J Verburgt, **D Sarkar**, T Aderinwale, X Wang, D Kihara, Kihara human team and LZerD server in CAPRI 50 / CASP 14, (invited abstract, manuscript in preparation), *CAPRI50/CASP14 extended abstract*, 2021.
12. C Christoffer, G Terashi, J Verburgt, **D Sarkar**, T Aderinwale, X Wang, D Kihara, Kihara human team and LZerD server in CAPRI 50 / CASP 14, *CAPRI50/CASP14 extended abstract*, 2021.
13. **D. Sarkar**, J. Verburgt, C. Christoffer, Y. Kagaya, G. Terashi, K. Lundquist, X. Zhu, L. Gorenstein, D. Kihara, Integrative modeling for protein structure refinement using Molecular Dynamics with flat- bottom harmonic restraints, enhanced sampling and ROSETTA iterative hybridize, Critical Assessment of Structure Prediction (CASP 14), 2020 - virtual conference. (Team leader invited to chair protein structure refinement session and to give oral presentation for protein cryoEM and NMR data guided modeling session).
14. G. Terashi, C. Christoffer, J. Verburgt, S. R. M. V. Subramanya, A. Jain, Y. Kagaya, **D. Sarkar**, T. Aderinwale, X. Wang, D. Kihara, Distance Prediction, Structure Prediction, Refinement, Quality Assessment, and Protein Docking in KiharaLab, Critical Assessment of Structure Prediction (CASP 14), 2020 - virtual conference.
15. F. Doole, C. K. Chan, E. Streitwieser, **D. Sarkar**, M. Kim, A. Singharoy, M. F. Brown, Antimicrobial peptide-Membrane interactions: Insights from Molecular Simulations, Annual Biophysical Society Meeting, 2021 - virtual Poster Presentation.

16. F. Doole, C. K. Chan, **D. Sarkar**, M. Kim, A. Singharoy, M. F. Brown, Antimicrobial Peptide Functionalized Biomaterials Investigated by Molecular Dynamics Simulations, Annual Biophysical Society Meeting 2020, San Diego, CA, USA - Poster Presentation.

17. **D. Sarkar**, R.D. Skeel and A. Singharoy, String like simulations outside the friction dominated regime, $4^{th}$ NAMD Developers Meeting, Beckman Institute, University of Illinois Urbana-Champaign, Champaign, IL.

18. J.W. Vant, **D. Sarkar**, R.D. Skeel and A. Singharoy MDFF Error Analysis, $4^{th}$ NAMD Developers Meeting, Beckman Institute, University of Illinois Urbana-Champaign, Champaign, IL, USA.

19. **D. Sarkar**, P. Kang, Z. Qin, Examining Arrhenius Kinetics over a Large Temperature Range, Summer Biomechanics, Bioengineering, and Biotransport (SB3C) Conference, June 2019, Seven Springs, Pennsylvania, USA - Invited talk for John Pearce $70^{th}$ Birthday.

20. P. Kang, **D. Sarkar**, Z. Qin, Laser Fragmentation of Plasmonic Gold Nanoparticles: Coulomb Explosion versus Photothermal Evaporation, Summer Biomechanics, Bioengineering, and Biotransport (SB3C) Conference, June 2019, Seven Springs, Pennsylvania, USA - Poster Presentation.

21. **D. Sarkar**, J. W. Vant, M. Shekhar, J. S. Richardson, R. Skeel, A. Singharoy, MDFF Error Analysis: A Tool for Determining Stereochemical and Thermodynamic Correct Structures, Biophysical Journal, 116, 3, supp. 1, 140A-141A (694-Pos) – Annual Biophysical Society Meeting 2019, Baltimore, MD.

22. **D. Sarkar**, P. Kang, S. O. Nielsen, Z. Qin, Reaction-Diffusion Kinetics During Selective Photo-Inactivation of Proteins by Molecular Hyperthermia, NEMB2018-6203, ASME 2018 NanoEngineering for Medicine and Biology Conference (NEMB), August 21 -24, 2018, Los Angeles, CA.

23. **D. Sarkar**, P. Kang*, Z. Qin, Molecular Hyperthermia to Manipulate Individual Proteins: Feasibility and Non-Arrhenius Kinetics, 8th World Congress of Biomechanics, 8-12 July 2018, Dublin, Ireland - Oral presentation.

24. P. Kang, **D. Sarkar**, T. Price, Z. Qin, Molecular Hyperthermia: the final frontier of bio-thermal science, Photo thermal effects in plasmonics (PEP18), Summer School, Special focus on biology, June 24-29, 2018, Porquerolles island, France.

25. **D. Sarkar**, P. Kang*, S.O. Nielsen, Z. Qin, Non-Arrhenius Reaction-Diffusion Kinetics for Protein Unfolding, Inactivation and Inhibition Over a Large Temperature Range, The Bluebonnet Symposium on Thermal-Fluid Sciences, 27 April 2018, The University of Texas at Dallas, Richardson, TX, USA – Invited talk.

26. R. Raj, **D. Sarkar**, A. Jain, Thermal modelling of memory access operations in microprocessors, Proc. ASME 2016 International Mechanical Engineering Congress and Exposition, IMECE2016-67697, November 11-17, Phoenix, AZ, USA 2016.

27. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Thermal transport in perfused biological tissue due to gold/magnetic nanoparticle heating, ASME NEMB 2016 Nano-Engineering for Medicine and Biology Conference, NEMB2016-6118, February 21-24, Houston, TX, USA 2016.

28. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Theoretical analysis of transient bio-heat transfer in multi-layer tissue, Proc. ASME 2015 International Mechanical Engineering Congress and Exposition, IMECE2015-53392, November 13-19, Houston, TX, USA 2015.

29. **D. Sarkar**, A. Haji-Sheikh, A. Jain, Analytical temperature distribution in a multilayer tissue structure in the presence of a tumor, Proc. ASME 2013 International Mechanical Engineering Congress and Exposition, IMECE2013-63275, November 15- 21, San Diego, CA, USA 2013.

## PROFESSIONAL DUTIES

Review editor for Frontiers in Molecular Biosciences - see reviewer profile

Peer-review for Biophysical Journal, Scientific Reports, IEEE Transactions on Components, Packaging and Manufacturing Technology, Microelectronics Reliability, Microorganisms, ASME Journal of Electrochemical Energy Conversion and Storage.

Judge for Biophysical Society (BPS2023) image competition

Judge for University of Texas at Arlington, College of Engineering's Innovation Day, 2021.

## COMPUTATIONAL GRANT EXPERIENCE

DOE NERSC ERCAP 2023, ERCAP0024719, Large Scale Molecular Simulations for Diffusive Carbon Dioxide and Bicarbonate Transport across Bacterial Microcompartments - Awarded 17,316 GPU-node hours ($\sim$ $ 36,550) - PI: Dr. Josh Vermaas

DOE NERSC ERCAP 2023, ERCAP0024719, Permeation across bacterial microcompartments for designer catalysis - Awarded 14,679 GPU-node hours ($\sim$ $ 30,984) - PI: Dr. Josh Vermaas

NSF ACCESS 2023, BIO210061, Molecular Simulations for Smarter Plant Systems and Materials - Awarded 91,707.0 GPU Hours ($\sim$ $ 48,394.13) - PI: Dr. Josh Vermaas

DOE NERSC ERCAP 2022, ERCAP0021030, Large Scale Molecular Simulations for Diffusive Carbon Dioxide and Bicarbonate Transport across Bacterial Micro Compartments - Awarded 2,680 GPU node-hours ($\sim$ $ 5656) - PI: Josh Vermaas

NSF XSEDE Anvil HPC, 2022 - Awarded early user period - PI: Dr. Josh Vermaas

## THESIS & DISSERTATION

General solutions to temperature distribution in orthotropic systems subject to variable heat transfer and biological systems during bioheat transfer, ProQuest/UMI, Ph.D. Dissertation, The University of Texas at Arlington, 2016.

Thermal behavior of dielectric materials during rapid heating, ProQuest/UMI, M.S. Thesis, The University of Texas at Arlington, 2012.

## RELATED ACADEMIC COURSEWORK

**Graduate**

Mechanical Engineering: Advanced Thermodynamics, Microscale Thermal Phenomena, Thermal Conduction (Diffusion), Fluid Dynamics, Convection Heat Transfer, Radiation Heat Transfer, Finite Element Methods, Non-Linear Systems & Control, Engineering Analysis, Advanced Engineering Mathematics

Mathematics (sub-track Applied Mathematics): Applied Mathematics-I, Applied Mathematics-II, Applied Differential Equations, Numerical Solution to Differential Equations.

Other courses: Advanced Physical Chemistry (UT-Dallas), Physical Biochemistry (UT-Dallas), Cell Physiology (UT-Southwestern and UT-Arlington)

**Undergraduate**

Mechanical Engineering: Thermodynamics, Heat and Mass Transfer, Fluid Mechanics, Computational Mathematics, Computer Programming.

## WORKSHOPS

NAMD Developers meeting - September 2021

NAMD Developers meeting - August 2019

Free Energy and Enhanced Sampling with NAMD – September 2017

Molecular Dynamics with LAMMPS – August 2016

## AFFILIATIONS

Current member of MSU-DOE Plant Research Laboratory Community Building and Outreach Committee (PRL-CBOC) where we work closely with the Diversity, Equity and Inclusion (DEI) committee of College of Natural Sciences and Michigan State University.