Dr. Jens Glaser

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Staff profile
https://www.olcf.ornl.gov/directory/staff-member/jens-glaser/
LinkedIn https://www.linkedin.com/in/jens-glaser-131b49b7/
GitHub https://github.com/jglaser

Research Profile

My research areas include drug discovery, biological self-assembly, nano-materials, and biophysics. My work has been cited 1,649 times, my h-index is 16 (April 2022, Google Scholar).

Professional History

Computational Scientist, Materials — NCCS, Oak Ridge National Laboratory, Advanced Computing for Chemistry and Materials — **2020-present**

- Develop AI models for drug discovery
- Lead a project on computational discovery of novel therapeutics against COVID-19 (DOE ASCR)
- Work with experimentalists at ORNL and LLNL to characterize predicted compounds
- Mentor a Postdoc
- Develop Monte Carlo algorithms to simulate biological self-assembly
- Implement a UCX communication layer in a GPU-accelerated database query engine on Summit
- Apply chem-informatics to large datasets from molecular docking
- Lead a workgroup on AI4Science
- Assist users for the Oak Ridge Leadership Computing Facility (OLCF)

Assistant Research Scientist — University of Michigan, Chemical Engineering — **2018-2020**

- Investigated pathways to the self-assembly to biomaterials using computer simulation
- Developed GPU-accelerated algorithms for molecular dynamics and Monte Carlo simulation
- Directly advised and mentor 2-3 students at any time in a group of 30+ students and postdocs

Postdoctoral Research Fellow — University of Michigan, Chemical Engineering, Advisor: Sharon Glotzer, *Protein Crystallization* — **2013-2018**

- Investigated protein crystallization using coarse-grained simulations for biomaterials self-assembly.
- Developed for the HOOMD-blue GPU code, used by a worldwide research community.
- Contributed to a scalable Hard Particle Monte Carlo (HPMC) code for GPUs/MPI.
- Advised graduate and undergraduate research on protein and polyhedra self-assembly.
- Contributed to research proposals and P.I. of compute-time proposals.

Postdoctoral Research Fellow — University of Minnesota, Chemical Engineering & Materials Science, Advisor: David Morse — **2011-2013**

Universality of Block Copolymer Melts

- Demonstrated universality for block copolymers using GPU simulations and well-tempered Metadynamics.
- Performed renormalized one-loop theory calculations to predict mesoscale structure of disordered melts of symmetric diblock copolymers.
- Introduced the use of GPUs into a previously CPU-based Monte Carlo simulation code.

Graduate student assistant — Leipzig University, Germany, Institute for Theoretical Physics, Advisor: Klaus Kroy — **2006-2011**
Theoretical models of reconstituted biopolymer networks

- Developed an analytical, minimal model of reconstituted cytoskeletal networks to describe light scattering experiments on F-actin solutions.
- Developed an analytical model for the experimentally observed width fluctuations of the confinement tube of semiflexible polymers.
- Simulated semidilute biopolymer solutions using Brownian dynamics on GPUs.
- Collaborated with experimental groups at the Research Center Jülich and Technical University of Munich, Germany.
- Teaching assistant for Quantum Mechanics

Educational History

Ph.D. (Dr. rer. nat., *summa cum laude)* in **Physics**, **Leipzig University, Germany** **2006-2011**
Thesis: "Semiflexible Polymer Networks"
Advisor: Klaus Kroy

Masters (Diplom-Physiker) in **Physics, Leipzig University, Germany** **1999-2006**
Thesis: "Dynamic Light Scattering of Stiff Polymers"
Advisor: Klaus Kroy

Courses at **École Normale Supérieure, Physics Department, Paris, France** **2002-2003**

Undergraduate study of **Mathematics** (Vordiplom), **Leipzig University**, **Germany** **1999-2001**

Skills

- **AI** and **Natural Language Processing** using Pytorch and HuggingFace transformers
- **Data analytics** using NVIDIA RAPIDS, BlazingSQL, dask, Apache Spark, Google BigQuery and Google Colab
- **Scientific software development** in C/C++, CUDA/HIP, MPI, Python
- **High-performance computing** on OLCF Summit, Spock, Titan, NCSA Blue Waters, XSEDE (various)
- **Developer of HOOMD-blue** molecular dynamics and Monte Carlo code
- **Analytical and numerical** methods: path integrals, field theories, statistical mechanics
- **Analysis of simulation results** using the Python software stack and Wolfram Mathematica

Awards

- Finalist paper, ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research, "Language Models for the Discovery of SARS CoV-2 Inhibitors" **2021**
- Finalist paper, ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research, "High-Throughput Virtual Laboratory for Drug Discovery Using Massive Datasets" **2020**
- Winner of the Nature Chemistry "Cover of the Year" online poll **2019**
- Research fellowship awarded by the Deutsche Forschungsgemeinschaft (German Research Foundation; DFG), "Testing Universality in Block Copolymers" **2012-2013**
- Invitation to workshop for "Young European Scientists (YES)" in Kraków, Poland, organized by the European Polymer Federation **2010**
- Member of BuildMoNa graduate school funded by German Excellence Initiative (DFG) **2008-2011**
- Second prize, BuildMoNa, for "Outstanding Scientific Results" **2009**
- Scholarship of the German National Academic Foundation (Studienstiftung) **1999-2005**

Publications

1. Glaser, J. et al. (2022) Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor, ACS Pharmacology and Translational Science, doi: 10.1021/acsptsci.2c00026
2. Glaser, J., Aramburú, F., Malpica, W., Hernández, B., Baker, Matthew, and Aramburú, R. (2022) Scaling SQL to the Supercomputer for Interactive Analysis of Simulation Data, Driving Scientific and Engineering Discoveries Through the Integration of Experiment, Big Data, and Modeling and Simulation (Springer), doi: 10.1007/978-3-030-96498-6
3. Blanchard, A.E., Shekar, M.C., Gao, S., Gounley, J., Lyngaas, I., Glaser, J., and Bhowmik, D. (2022) Automating Genetic Algorithm Mutations for Molecules Using a Masked Language Model, IEEE Transactions on Evolutionary Computation, doi: 10.1109/TEVC.2022.3144045
4. Gao, F., Glaser, J., and Glotzer, S. C. (2021) The Role of Complementary Shape in Protein Dimerization, *Soft Matter*, *doi*: 10.1039/D1SM00468A
5. Glaser, J. et al. (2021) High-Throughput Virtual Laboratory for Drug Discovery Using Massive Datasets, *International Journal of High Performance Computing Applications, doi:* 10.1177/10943420211001565
6. Acharya, A. et al. (2020) Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19, *Journal of Chemical Information and Modeling*, doi: 10.1021/acs.jcim.0c01010 (***Cover story***)
7. Vermaas, J. V., Sedova, A. Baker, M., Boehm, S., Rogers, D., Larkin, J., Glaser, J., Smith, M., Hernandez, O., Smith, J. (2020), Supercomputing Pipelines Search for Therapeutics Against COVID-19, Computing in Science & Engineering, 10.1109/mcse.2020.3036540
8. Glaser, J., Schwendeman, P., Anderson, J.A., and Glotzer S.C. (2019) Unified Memory in HOOMD-blue improves node-level strong scaling, *Computational Materials Science,* doi: 10.1016/j.commatsci.2019.109359
9. Glaser, J., Zha, X., Anderson, J. A., Glotzer, S. C. and Travesset, A. (2019) Pressure in Rigid-Body Molecular Dynamics, *Computational Materials Science,* doi: 10.1016/j.commatsci.2019.109430
10. Anderson, J.A., Glaser, J., and Glotzer, S. C. (2019) HOOMD-blue: A Python package for high-performance molecular dynamics and hard particle Monte Carlo simulations, *Computational Materials Science,* doi: 10.1016/j.commatsci.2019.109363

11. Simon, A. J., Zhou, Yi, Ramasubramani, V., Glaser, J., Pothukuchy, A., Gerberich, J., Leggere, J., Golihar, J., Jung, C., Glotzer, S. C., Taylor, D. W. & Ellington, A. D., (2019) Supercharging enables organized assembly of synthetic biomolecules, *Nature Chemistry 11:204–212, doi:* 10.1038/s41557-018-0196-3 (***Cover story***)
12. Karas, A. S., Glaser, J. & Glotzer, S.C. (2016) Using Depletion to Control Colloidal Crystal Assemblies of Hard Cuboctahedra, *Soft Matter*, 12:5199, doi: 10.1039/C6SM00620E
13. Hsiao, L. C., Schultz, B. A., Glaser, J., Engel, M., Szakasits, M. E., Glotzer, S. C. & Solomon, M. J. (2015) Metastable orientational order of colloidal discoids, *Nature Communications* 6:8507, doi: 10.1038/ncomms9507
14. Glaser, J., Karas, A.S., & Glotzer, S.C. (2015) A parallel algorithm for implicit depletant simulations, *The Journal of Chemical Physics* 143:184110, doi: 10.1063/1.4935175
15. Glaser, J., Nguyen, T., Anderson, J., Lui, P., Spiga, F., Millan, J., Morse, D. & Glotzer, S. C. (2015) Strong scaling of general-purpose molecular dynamics simulations on GPUs, *Computer Physics Communications*, 192, 97-107, doi: 10.1016/j.cpc.2015.02.028 (***highly cited paper***)
16. Medapuram, P., Glaser, J. & Morse, D. (2015) Universal Phenomenology of Symmetric Diblock Copolymers Near the Order-Disorder Transition, *Macromolecules*, 48, 819-839, doi: 10.1021/ma5017264
17. Glaser, J., Medapuram, P., Beardsley, T., Matsen, M. & Morse, D. (2014). Universality of Block Copolymers, *Physical Review Letters*, 113, 068302, doi: 10.1103/PhysRevLett.113.068302
18. Glaser, J., Qin, J., Medapuram, P. & Morse, D. (2014). Collective and single-chain correlations in disordered melts of symmetric diblock copolymers: Quantitative comparison of simulations and theory. *Macromolecules*, 47(2), 851-869, doi: 10.1021/ma401694u
19. Glaser, J., Qin, J., Medapuram, P., Mueller, M., & Morse, D. (2012). Test of a Scaling Hypothesis for the Structure Factor of Disordered Diblock Copolymer Melts. *Soft Matter*, 8(44), 11310–11317, doi: 10.1039/c2sm26536b
20. Chakraborty, D., Gnann, M. V., Rings, D., Glaser, J., Otto, F., Cichos, F., & Kroy, K. (2011). Generalised Einstein Relation for Hot Brownian Motion. *EPL*, 96(6), 60009, doi: 10.1209/0295-5075/96/60009
21. Glaser, J., & Kroy, K. (2011). Tube-Width Fluctuations of Entangled Stiff Polymers. *Physical Review E*, 84(5), 051801, doi: 10.1103/PhysRevE.84.051801
22. Glaser, J., Chakraborty, D., Kroy, K., Lauter, I., Degawa, M., Kirchgeßner, N., Hoffmann, B., Merkel, R. & Giesen, M. (2010). Tube Width Fluctuations in F-Actin Solutions. *Physical Review Letters*, 105(3), 037801, doi: 10.1103/PhysRevLett.105.037801
23. Glaser, J., Hallatschek, O., & Kroy, K. (2008). Dynamic Structure Factor of a Stiff Polymer in a Glassy Solution. *The European Physical Journal. E, Soft Matter,* 26(1-2), 123–36, doi: 10.1140/epje/i2007-10321-2
24. Semmrich, C., Storz, T., Glaser, J., Merkel, R., Bausch, A. R., & Kroy, K. (2007). Glass Transition and Rheological Redundancy in F-actin Solutions. *Proceedings of the National Academy of Sciences of the United States of America*, 104(51), 20199–203, doi: 10.1073/pnas.0705513104 (***Cover article***)
25. Kroy, K., & Glaser, J. (2007). The Glassy Wormlike Chain. *New Journal of Physics, 9(11), 416,* doi: 10.1088/1367-2630/9/11/416

Proceedings and Book-Chapters

26. Glaser, J., & Kroy, K. (2010). Fluctuations of Stiff Polymers and Cell Mechanics. In M. Elnashar (Ed.), Biopolymers (pp. 509–534). Sciyo Publishers.
27. Kroy, K., & Glaser, J. (2009). Rheological redundancy - from Polymers to Living Cells. AIP Conference Proceedings, 1151, 52–55.

28. Glaser, J., Hubert, C., & Kroy, K. (2008). Dynamics of Sticky Polymer Solutions. In W. Janke & A. Pelster (Eds.), Path Integrals - New Trends and Perspectives. Proceedings of the 9th International Conference Dresden, Germany, 23 – 28 September 2007 (pp. 537–542). Singapore: World Scientific.

Open-Source Developer Activities

HOOMD-blue (general-purpose many-particle dynamics, http://glotzerlab.engin.umich.edu/hoomd-blue)

- Designed multi-GPU molecular dynamics capability using MPI domain decomposition
- Implemented time-reversible and measure-preserving integrators for constant-pressure in a shape-varying cell and constant-temperature ensembles.
- Implemented the multi-GPU enabled rigid body framework and P3M electrostatics.
- Designed and implemented support multi-GPU nodes (e.g. OLCF Summit) using NVLINK
- Port the GPU kernels to AMD GPUs using HIP

HPMC (Parallel Hard Particle Monte Carlo component of HOOMD-blue, doi: 10.1016/j.cpc.2016.02.024)

- Implemented and accelerated geometric overlap checks for various shapes including faceted spheres, triangle meshes and sphere unions.
- Designed capability to perform simulations with implicit depletants.

Simpatico (C++ framework for simulation of polymeric liquids, http://github.com/dmorse/simpatico)

- Integration with HOOMD-blue for GPU execution
- Constant-pressure integrators

Plug-ins and libraries

- Developed *dfftlib*, a multi-GPU Fast Fourier transform library based on CUFFT with MPI support.
- Developed *metadynamics-plugin* to HOMD-blue to perform free energy calculations for order-disorder transitions in block copolymers.

Other contributions:

- Triangle mesh geometry in *fresnel*, a GPU-accelerated raytracing library (http://github.com/glotzerlab/fresnel)
- Support for OLCF Summit in *signac-flow* workflow management tool

Industry Collaboration

- NVIDIA Corp., Santa Clara, CA — performance testing of HOOMD-blue on new GPUs, collaborate on chem-informatics and data-analytics with RAPIDS
- Roivant Sciences, Boston, MA — drug discovery
- BlazingDB, Inc., San Francisco, CA — port of BlazingSQL software to Power9 and UCX communications
- Google Cloud, Mountain View, CA — analytics on large datasets
- AMD, Santa Clara, CA — porting HOOMD-blue to AMD GPUs
- Mellanox Technologies, Sunnyvale, CA (now NVIDIA) — benchmarking of GPUDirect RDMA technology

Invited Presentations at Conferences and Workshops

1. OLCF User Meeting 2021, User-led talks in modeling and simulation, “Structure-Based Virtual Screening and Data Analytics on Summit for COVID-19”
2. Dask Distributed Summit, 2021, Dask in HPC Workshop, “Towards Scalable Data Analytics for Drug Discovery”
3. Supercomputing Conference, 2020, COVID-19 Gordon Bell Session: “High-Throughput Virtual Laboratory for Drug Discovery Using Massive Datasets”
4. Supercomputing Conference, 2020, Workshop: Interactive HPC, Keynote and panelist, “Rapid-Response Data Analytics for COVID-19 Using GPUs"
5. NVIDIA GPU Technology Conference Digital Fall 2020, “The Summit Supercomputer as Virtual Drug Discovery Laboratory for COVID-19”
6. Summit on Summit, Sierra and Perlmutter VI, 2020, “Molecular docking and massively parallel data analytics for COVID-19 on Summit”
7. 31th annual workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, University of Georgia, Athens, 2019, “Using computer simulation to study the assembly of protein crystals and complexes”
8. 4th annual MVAPICH User Group meeting, Ohio State University, Columbus, 2016, “Distributed algorithms for GPU-enabled Molecular Dynamics”
9. 29th annual workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, University of Georgia, Athens, 2016 “Using GPUs for the computational design of soft and biological materials”
10. 3rd annual MVAPICH User Group meeting, Ohio State University, Columbus, 2015, “How parallelism helps computational physics discovery”
11. CECAM Workshop, The Physics of Protein Self-Assembly, Lausanne, Switzerland 2015, Poster, “Self-assembly of anisotropic shapes through entropy”
12. 2nd annual MVAPICH User Group meeting, Ohio State University, Columbus, 2014, “HOOMD-blue: Scalable Molecular Dynamics on Thousands of GPUs”

Invited Talks at Research Institutions and Industry

13. Oak Ridge National Laboratory, Oak Ridge, Tennessee, NCCS Seminar, “Computational Tools for the Pandemic”, 2021
14. Oak Ridge National Laboratory, Oak Ridge, Tennessee, Scientific Computing group, Invited seminar, “Too complex to model? Why the next biomaterial will be discovered on a supercomputer”, 2019
15. Rensselear Polytechnic Institute, Troy, New York, Department of Chemical Engineering, Invited seminar, “Self-assembly of Soft And Biological Matter”, 2017
16. Johannes-Gutenberg University of Mainz, Theory of Condensed Matter group, invited seminar, “Self-Assembly of Colloids and Proteins: Depletion Interactions and Implicit Solvent”, 2016
17. Yale University, Department of Chemical Engineering, invited seminar, “Computational Design of Soft and Biological Materials”, 2016
18. University of Texas at Austin, Center for Systems & Synthetic Biology (Ellington group), “Insights from simulations of colloidal self-assembly for the assembly of proteins”, 2016
19. FU Berlin, Faculty of Mathematics and Computer Science, invited seminar, “High Performance Computing in Molecular Dynamics”, 2014
20. University of Göttingen, Institute of Theoretical Physics, “Computational design of novel materials by self-assembly: from block copolymers to protein crystals”, 2014

21. Technical Summit for Chemistry and Life Sciences Developers, NVIDIA headquarters Santa Clara, California, 2014, presentation on scaling bottlenecks encountered during development of HOOMD-blue and discussion with NVIDIA engineers
22. Group seminar, Laboratory for Computational Nanoscience and Soft Matter Simulation, BioInterfaces Institute, University of Michigan, 2013, "Universal phase behavior of diblock copolymers and massively parallel simulations on multiple GPUs"
23. Computation Institute Seminar, University of Chicago, 2013, "Identifying the Order-Disorder Transition of Diblock Copolymers Using Metadynamics and Massively Parallel Many-Particle Simulations on Multiple GPUs"
24. Technical Summit for Chemistry and Life Sciences Developers, NVIDIA headquarters Santa Clara, California, 2014, discussion with NVIDIA engineers
25. Group seminar, Statistical and Biological Physics, University of Munich, Germany, 2012, "Diblock Copolymers: How Universal are Coarse-grained Simulations?"
26. Physics Department seminar, North Dakota State University, 2011, "From Stiff Polymers to Cell Mechanics"
27. YES, 4th workshop of Young European Scientists, Cracow, Poland 2010 "From Stiff Polymers to Cell Mechanics"
28. Research seminar, Department of Physics, Technical University of Chemnitz, Germany, 2010, "GPU-accelerated Brownian Dynamics of Effective Stiff Polymer Solutions"
29. Simulations on GPU symposium, Leipzig University, Germany, 2009, "Brownian Dynamics of Stiff Polymers"
30. Group seminar, Laboratory for Molecular and Integrative Cellular Dynamics (Fredberg group), Harvard University, 2008, "The glassy wormlike chain"
31. Group seminar Biophysics, Experimental Soft Condensed Matter (Weitz group), Harvard University, 2008, "The glassy wormlike chain"

Contributed Talks and Posters at Conferences

1. Smoky Mountains Conference, virtual, 2021, "Scaling SQL to the Supercomputer for Interactive Analysis of Simulation Data" (poster)
2. AIChE Annual Meeting, Orlando, 2019, "Using Unified Memory and Nvlink for Node-Level Strong Scaling of Molecular Dynamics Simulations" (talk)
3. AIChE Annual Meeting, Orlando, 2019, "Controlling Protein Crystallization through Wetting Near a Critical Point" (talk)
4. Gordon Research Conference on Chemistry and Physics of Liquids, Holderness School, NH, 2019, "Shape Driven Phase Separation and Crystallization of Proteins" (poster)
5. OLCF User Meeting, 2019, Oak Ridge, TN, "Unified memory in HOOMD-blue improves node-level strong scaling" (poster)
6. APS March Meeting, 2019, Boston, "Large-Scale Simulations of Protein Self-Assembly" (talk)
7. AICHE Annual Meeting, Pittsburgh, 2018, "Modeling the Self-Assembly of Super-Charged Green Fluorescent Proteins" (talk)
8. FOMMS, Delavan, 2018, "Large-Scale Self-Assembly of Janus ellipsoids" (poster)
9. ACS Colloids, State College, 2018, "Necessity of non-specific interactions for protein self-assembly" (talk)
10. OLCF User Meeting, Oak Ridge, 2018, "Nucleation of Protein Crystals and Strong Scaling on Summit" (poster)

11. APS March Meeting, Los Angeles, 2018, “Metadynamics study of protein crystal nucleation and growth”, (talk)
12. AIChE Annual Meeting, Minneapolis, 2017, “Self-Assembly of Open Structures Using Depletion” (talk)
13. AIChE Annual Meeting, Minneapolis, 2017, “Self-Assembly of Proteins: The Role of Shape and Specific Interaction” (talk)
14. APS March Meeting, New Orleans, 2017, “The role of shape vs. patches in protein crystallization” (talk)
15. AIChE Annual Meeting, San Fransisco, 2016, “Towards Biomolecular Simulations with HOOMD-blue 2.x” (talk)
16. AIChE Annual Meeting, San Francisco, 2016, “Patches or Shape? Towards Minimal Models for Protein Crystallization” (talk)
17. APS March Meeting, Baltimore, 2016, “Implicit depletion of anisotropic particles” (talk)
18. AICHE Annual Meeting, Salt Lake City, 2015, “Entropic Depletion Interactions Between Anisotropic Particles Studied Using a Rigorous, Efficient and Parallelizable Monte Carlo Method” (talk)
19. ACS Colloid and Surface Science Symposium, Carnegie Mellon, Pittsburgh, 2015, “Attraction from entropy: Implicit simulation of depletion for anisotropic particles” (talk)
20. Blue Waters symposium, Sun River (Oregon), 2015, “Scalable Molecular Dynamics and Monte Carlo simulations of millions of particles on thousands of GPUs” (talk)
21. Meeting of the American Institute of Chemical Engineers, Atlanta, 2014, “HOOMD-Blue — Development of a Highly Scalable General Purpose Molecular Dynamics code” (talk)
22. CCP International Conference on Computational Physics, Boston, 2014, “Strong Scaling of a Molecular Dynamics code on 1000’s of GPUs” (talk)
23. GPU Technology Conference, San Jose, 2014, “Strong Scaling Multi-GPU Simulations with HOOMD-blue” (poster)
24. APS March Meeting, Denver, 2014, “HOOMD-blue — scaling up from one desktop GPU to Titan” (talk)
25. 2nd International Symposium Computer Simulations on GPU, Freudenstadt, Germany, 2013, ”HOOMD-blue: Massively Parallel Many-Particle Simulations on Multiple GPUs” (poster)
26. APS March meeting, Baltimore, 2013, “Identifying the ODT in Simulations of Diblock Copolymers using Metadynamics” (talk)
27. APS March meeting, Baltimore, 2013, “Highly Scalable many-GPU Simulations with HOOMD-blue” (poster)
28. Statistical mechanics: Interplay of Theory and Computer Simulations, Mainz, Germany 2012, “Using Metadynamics to Investigate the Order-Disorder Transition of Symmetric Diblock Copolymer Melts” (poster)
29. Gordon Research Conference and Seminar, Polymer Physics, South Hadley, 2012, “How Universal are Coarse-grained Simulations of Block Copolymers?” (poster)
30. APS March meeting, Boston, 2012, “Universality in Block Copolymers: a Corresponding States Hypothesis” (talk)
31. International Soft Matter Conference, Granada, Spain, 2010 “Tube-Width Fluctuations in F-Actin solutions” (poster)
32. Spring Meeting of the German Physical Society (DPG), Regensburg, Germany, 2010, “Tube-Width Fluctuations in F-actin solutions” (talk)
33. Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 2009, “A Liquid State Theory for Biopolymers” (talk)
34. Spring Meeting of the German Physical Society (DPG), Berlin, Germany, 2008, “Nonlinear rheology of a glassy solution of semiflexible polymers” (talk)

35. Diffusion Fundamentals III, Athens, Greece, 2010, “Tube Geometry and Brownian Dynamics in Semiflexible Polymer Networks” (poster)
36. 34th conference of the Middle European Cooperation in Statistical Physics, Leipzig, Germany, 2009, “A Liquid-state Approach to Biopolymers” (poster)
37. Jülich Soft Matter Days, Bonn, Germany, 2008, “Packing Structure and Dynamics of Stiff Polymers” (poster)
38. International Soft Matter Conference, Aachen, Germany, 2007, “Glass Transition and Rheological Redundancy in F-Actin solutions” (poster)
39. Spring Meeting of the German Physical Society (DPG), Regensburg, Germany, 2007, “Dynamic Light Scattering of F-Actin solutions” (poster)
40. Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 2006, “Dynamic Light Scattering of Stiff Polymers” (talk)
41. Jülich Soft Matter Days, Bonn, Germany, 2005, “Hydrodynamic Interactions for Stiff Polymers” (poster)

Teaching Competencies and Outreach

- Mentor at NVIDIA GPU Hackathons: Princeton University (2021), and NERSC (2021)
- Organized Invite-only Workshop on GPU-accelerated Data Analytics Virtual Lab on Summit: From Drug discovery to Radiation Physics, OLCF, 2020
- Invited webinar, “HOOMD-blue 1.0: Easy-to-use and Highly Scalable Molecular Dynamics on GPUs”, NVIDIA GTC Express series, 2014
- Co-organizer and presentation “Multi-GPU Molecular Dynamics with HOOMD-blue”, NVIDIA CUDA days at University of Michigan, 2014
- Advanced webinar “Using HOOMD-blue for Polymer Simulations and Big Systems”, Virtual School for Computational Science and Engineering, University of Michigan, 2014
- Teaching assistant for Quantum Mechanics I/II, Leipzig University for three semesters
- Mentoring a high school student

Students and postdocs

Darren Hsu (postdoc), AI models for drug discovery
Fengyi Gao (graduate student), Self-assembly of protein complexes
Vyas Ramasubramani (graduate student), Depletion interactions and implicit solvent models
Rose Cersonsky (graduate student), Protein modeling
Andrew Karas (graduate student), Depletion interactions between hard shapes
Carissa Skye (undergraduate summer student), Self-assembly of particles on the 3-sphere using Monte Carlo
Joalix Bajandas (SROP undergraduate exchange student), Dimerization of GFP molecules

Conference sessions

- Panelist, Benchmarking in the Data Center: Expanding to the Cloud, ACM SIGPLAN workshop, April 2022
- OLCF User Meeting, Oak Ridge, TN, 2021, Session Organizer: “**User-led talks in traditional modeling and simulation**”
- AIChE Annual Meeting, Orlando, 2019, Session Chair, “**Thermophysical Properties of Biological Systems**”

- AIChE Annual Meeting, Pittsburgh, 2018, Session Chair, "**Thermophysical Properties of Biological Systems**"
- APS March Meeting, New Orleans, 2017, Invited Session "**Biological Materials Self-Assembly**" (organizer)
- APS March Meeting, New Orleans, 2017, GSOFT Short Course "**Fundamental Tools and Concepts in Computational Soft Matter Physics**" (co-organizer)
- APS March Meeting, Baltimore, 2016, Focus Session "**Phase Transitions and Self-Assembly in Biological Systems**" (chair)
- **Abstract Sorter,** GSOFT, APS March Meeting 2016
- APS March Meeting, Baltimore, 2013, "**Elastomers and Gels"** (chair)

Funding and Compute Time Awards

1. "Scalable Transformer language models for drug discovery", INCITE 2022, Co-Investigator, P.I. Andrew Blanchard
2. "Data Centric Approach to Drug Discovery for COVID-19", OLCF Director's discretionary allocation on Summit, P.I.
3. OLCF-NVBL Collaboration "Data-Centric Approach to the Design of Novel Therapeutics against COVID-19", Project Lead ($560k funding for 6 months)
4. Computing credits ($2M) on Google Cloud "Covid Computational Drug Discovery Initiative", GCP Subgroup 2020, P.I. Jeremy Smith, Co-Investigator
5. "Scalable Computational Biodefense for COVID-19 and beyond" (investigator), P.I. Ada Sedova, LDRD SEED proposal 2020
6. "Colloidal crystallization pathways", INCITE Award 2020 (co-investigator), P.I. Glotzer
7. "Nucleation and Growth of Colloidal Crystals", INCITE Award 2019 (contributor), P.I. Glotzer
8. "Large-Scale Simulation of Biological Crystallization", Early Science Project on the DOE Summit supercomputer, 2019, P.I. Glotzer
9. Design of protein biomaterials through tailored shape and packing strategies of patchy particles", Army Research Office, 2018-2021, with P.I.s Glotzer and Ellington (renewal)
10. "GPU-enabled Simulations of the Hydrophobic Effect in Biological Self-Assembly", XSEDE grant on Stanford xStream Supercomputer, 2016-2017, P.I.
11. "Design of protein biomaterials through tailored shape and packing strategies of patchy particles", Army Research Office, 2015-2018, with P.I.s S.C. Glotzer and A. Ellington
12. "Many-GPU Simulations of Soft Matter Design", Great Lakes Consortium for Petascale Computation, allocation on NCSA Blue Waters supercomputer, 2014-2015, Co-P.I., P.I.: S.C. Glotzer
13. Proposal for NVIDIA Research Center at the University of Michigan, 2014-2016, Co-P.I., P.I.: S.C. Glotzer
14. "Mapping the Universal Phase Diagram of Finite Block Co-Polymers", XSEDE grant on Keeneland GPU Supercomputer, 2013-2014, Co-P.I., P.I.: David Morse
15. "Testing Universality in Diblock Copolymers Using Graphics Processing Units", XSEDE grant on Keeneland GPU Supercomputer, 2012-2013, Co-P.I., P.I.: David Morse
16. "Optimization of a General-Purpose Molecular Dynamics Code Running on Multiple GPUs", Oak Ridge National Laboratory, Director's discretionary allocation on the Titan supercomputer 2013
17. "Testing universality in block copolymers", DFG Research Fellowship 2012-2013

Reviewer Activities

- **Scientific Journals**: Physical Review Letters, ACS Nano, ACS Macro Letters, Physical Review E, Langmuir, Soft Matter, New Journal of Physics, The Journal of Chemical Physics, Biophysical Journal, Journal of Computational Physics, Computer Physics Communications, Computational Materials Science, Proceedings of the National Academy of Sciences of the USA, ACS Central Science, Wiley Advanced Science
- **Funding Organizations**: ACS Petroleum Fund, Netherlands Organisation for Scientific Research, Office of Science - Department of Energy

Professional Societies

American Institute of Chemical Engineers
American Physical Society
Deutsche Physikalische Gesellschaft (German Physical Society)
Association for Computing Machinery

Language Proficiency

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