Joshua A. Anderson, Ph.D.

Lead Research Area Specialist

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https://github.com/joaander/
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Experience

Software Development

HOOMD-blue
- http://glotzerlab.engin.umich.edu/hoomd-blue
- 174,000 lines of **CUDA**, **C++**, and **Python**.
- I am the lead developer of **HOOMD-blue**, a general purpose Molecular Dynamics and hard particle Monte Carlo software written from the ground up for GPUs and highly tuned for performance.
- I wrote initial implementation myself, including the GPU algorithms (cell list, neighbor list, pair force, bond force, integration), data structures, and the python scripting interface.
- Over 10 years, I have worked with 67 group members and outside contributors to add additional features to **HOOMD-blue**, including Brownian dynamics, DPD, non-equilibrium methods, rigid body dynamics, multi-GPU execution with MPI, DEM simulations of polyhedral particles, hard particle Monte Carlo, BVH accelerated neighbor lists, and many more.

Freud
- https://github.com/glotzerlab/freud
- 36,000 lines of **C++**, **Cython** and **Python**.
- **Freud** is a high performance library for analyzing simulation results. It implements distribution functions, clustering, order parameters, correlation functions, structure factor, and other computations. All methods are threaded for fast performance on CPUs. I wrote the underlying design and initial implementation and have supervised further development of the project.

fresnel
- https://github.com/glotzerlab/fresnel
- 15,000 lines of **CUDA**, **C++**, and **Python**.
- I implemented **fresnel**, a rendering engine that path-traces publication quality images interactively.

GSD
- https://github.com/glotzerlab/gsd
- 3500 lines of **C** and **Python**.
- **GSD** is a lightweight binary container file format that can efficiently access sequences of dense arrays sequentially and randomly. I designed the file format to meet the needs of **HOOMD-blue**.

Research

2014 –
- **Lead Research Area Specialist**, Dept. of Chemical Engineering, University of Michigan
- Mentored a team of developers that built numerous open-source software packages for computational soft matter research: https://github.com/glotzerlab/.
- Led the continued development of **HOOMD-blue**, a general purpose and high performance Molecular Dynamics and hard particle Monte Carlo software.
- Implemented a lightweight binary container file format for molecular simulation trajectories.
- Implemented a rendering engine that path-traces publication quality images in real time.
- Studied the fluid to hexatic to solid transition using Monte Carlo simulations of millions of polygons.
- Coauthored many successful **INCITE** and **XSEDE** proposals for compute resources.
- Administered a University of Michigan Visualization Hub with high-end visualization workstations, 4k displays and a 10ft tiled display.
- Served on the Advanced Research Computing Future Infrastructure committee which determined possible directions for improving cyberinfrastructure at the University of Michigan.
- Administered computation and storage resources for a research group with more than thirty members.
- Deployed software builds with **Docker** container images and on **conda-forge**.
- Employed continuous integration to validate scientific software using **Jenkins** and **CircleCI**.

2009 – 2014
- **Senior Research Area Specialist**, Dept. of Chemical Engineering, University of Michigan
- Led the continued development of **HOOMD-blue**. Designed and implemented the **Freud**.
- Mentored and worked with many graduate students on research projects, including: polymer nanoparticle telechelics, phase separation in binary systems, self-assembly of complimentary particles, formation of complex crystals from potentials, and self-assembly of driven rotating particles.

Experience (continued)

- Co-PI on the University of Michigan NVIDIA CUDA Research Center award
- Worked with HPC system administrators to specify, purchase, configure and troubleshoot GPU and CPU clusters (1200 CPU cores, 256 GPUs).
- Co-PI on the Blue Waters GLCPC: *Many-GPU Simulations of Soft Matter Design*

2005 – 2009
- **Ph.D. graduate student**, Dept of Physics and Astronomy Iowa State University, Ames IA
- Developed algorithms for performing Molecular Dynamics on Graphics Processing Units
- Characterized phase diagrams of polymer and polymer-nanoparticle composite systems using Molecular Dynamics
- Studied dynamics of phase transitions in polymer systems

2001 - 2005
- **Undergraduate Research**, Dept of Physics Michigan Technological University, Houghton, MI

Teaching

2009 – 2011
- Local instructor at the University of Michigan site for yearly summer school events on GPU and MPI programming. http://www.vscse.org

2010
- Introduction to CUDA as a summer school course

Extracurricular

2001 - 2005
- Hybrid vehicle design and construction, Michigan Technological University
- Designed and constructed high voltage electrical systems on the vehicle as well as low voltage control electronics
- Designed and implemented real-time controls software to control the hybrid power train and other electrical systems using Matlab and Simulink

Invited Talks

Apr 2019
- *Best practices for engineering molecular science simulation, analysis, and visualization codes* – ACS national meeting

Oct 2018
- *Managing Data Spaces, Performing MD, and Analyzing Trajectories with Signac, HOOMD-Blue, and Freud* – AiChE annual meeting

Mar 2018
- *Research computing on massively parallel systems with open source software* – Research computing days keynote, Boise State University

Mar 2018
- *Attaining maximum GPU execution performance in the HOOMD-blue particle simulation toolkit* – Computing PhD Colloquium, Boise State University

Nov 2017
- *Recent Developments in the HOOMD Simulation Ecosystem* – Software Engineering in and for the Molecular Sciences, AiChE annual meeting

Nov 2017
- *Managing Data Spaces, Performing MD, and Analyzing Trajectories with Signac, HOOMD-Blue, and Freud* – Workshop: Hands On With Molecular Simulation, AiChE annual meeting

Jun 2017
- *HOOMD-blue software design and development model* – 2017 Current trends in molecular dynamics software design Workshop at Temple University.

May 2017
- *Simulations of complex soft matter crystals enabled by GPUs* – 2017 OLCF user meeting.

Aug 2016
- *Computer simulations on today's massively parallel architectures* – 2016 Machine-Ground Interaction Consortium (MaGIC) Workshop

Apr 2016
- *Examining the fluid to solid transition of hard polygons with large scale Monte Carlo simulations* – Chemical Engineering dept. seminar at the University of Rochester.

Nov 2015
- *Computer Simulations in the Massively Parallel Era and Beyond* – CoMSEF Young Investigator Award for Modeling and Simulation, AiChE annual meeting

Sep 2013
- *Powering Soft Matter Self-assembly Simulations with GPUs* – Michigan Technological University Physics Dept. Colloquium

May 2013
- *Efficient techniques for massively parallel many-particle simulations on GPUs* – Computer Simulations on GPU International Symposium

Dec 2011
- *Intro to GPUs* – Cyberinfrastructure Days at the University of Michigan.

Jun 2011
- *HOOMD-Blue, General-Purpose Many-Body Dynamics On the GPU* – Computer Simulations on GPU International Symposium

Jan 2011
- *Utilizing GPUs for fast and flexible many-particle dynamics simulations* – Applied Interdisciplinary Mathematics seminar at the University of Michigan.

Invited Talks (continued)

Sep 2010	• *Simulating nano-materials, polymers, and complex fluids on GPUs with HOOMD-blue* – Bio-molecular Simulations Workshop at ORNL.
Jul 2009	• *FOMMS 2009 GPU Programming Tutorial* – FOMMS 2009.
Mar 2008	• *Molecular dynamics on graphics processing units* – ORNL.
Nov 2007	• *Molecular dynamics on graphics processing units* – Beckman Institute, UIUC.

List of Publications

[24] Wenbo Shen, James Antonaglia, **Joshua A. Anderson**, Michael Engel, Greg van Anders, and Sharon C. Glotzer. Symmetries in hard polygon systems determine plastic colloidal crystal mesophases in two dimensions. *Soft Matter*, 2019.

[23] Carl S. Adorf, Vyas Ramasubramani, **Joshua A. Anderson**, and Sharon C. Glotzer. How to professionally develop reusable scientific software — and when not to. *Computing in Science & Engineering*, pages 1–1, 2018.

[22] **Joshua A. Anderson**, James Antonaglia, Jaime A. Millan, Michael Engel, and Sharon C. Glotzer. Shape and symmetry determine two-dimensional melting transitions of hard regular polygons. *Physical Review X*, 7(2):021001, 2017.

[21] Matthew Spellings, Ryan L. Marson, **Joshua A. Anderson**, and Sharon C. Glotzer. GPU accelerated Discrete Element Method (DEM) molecular dynamics for conservative, faceted particle simulations. *Journal of Computational Physics*, 334:460–467, 2017.

[20] **Joshua A. Anderson**, M. Eric Irrgang, and Sharon C. Glotzer. Scalable Metropolis Monte Carlo for simulation of hard shapes. *Computer Physics Communications*, 204:21–30, 2016.

[19] Michael P. Howard, **Joshua A. Anderson**, Arash Nikoubashman, Sharon C. Glotzer, and Athanassios Z. Panagiotopoulos. Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. *Computer Physics Communications*, 203:45–52, 2016.

[18] Jens Glaser, Trung Dac Nguyen, **Joshua A. Anderson**, Pak Lui, Filippo Spiga, Jaime A. Millan, David C. Morse, and Sharon C. Glotzer. Strong scaling of general-purpose molecular dynamics simulations on GPUs. *Computer Physics Communications*, 192:97–107, 2015.

[17] Eric S. Harper, Ryan L. Marson, **Joshua A. Anderson**, Greg van Anders, and Sharon C. Glotzer. Shape allophiles improve entropic assembly. *Soft Matter*, 11(37):7250–7256, 2015.

[16] Ryan L. Marson, Carolyn L. Phillips, **Joshua A. Anderson**, and Sharon C. Glotzer. Phase behavior and complex crystal structures of self-assembled tethered nanoparticle telechelics. *Nano Letters*, 14(4):2071–2078, 2014.

[15] **Joshua A. Anderson**, Eric Jankowski, Thomas L. Grubb, Michael Engel, and Sharon C. Glotzer. Massively parallel Monte Carlo for many-particle simulations on GPUs. *Journal of Computational Physics*, 254(1):27–38, 2013.

[14] Michael Engel, **Joshua A. Anderson**, Sharon C. Glotzer, Masaharu Isobe, Etienne P. Bernard, and Werner Krauth. Hard-disk equation of state: First-order liquid-hexatic transition in two dimensions with three simulation methods. *Physical Review E*, 87(4):042134, 2013.

[13] Carolyn L. Phillips, **Joshua A. Anderson**, Greg Huber, and Sharon C. Glotzer. Optimal Filling of Shapes. *Physical Review Letters*, 108(19):1–5, 2012.

[12] Trung Dac Nguyen, Carolyn L. Phillips, **Joshua A. Anderson**, and Sharon C. Glotzer. Rigid body constraints realized in massively-parallel molecular dynamics on graphics processing units. *Computer Physics Communications*, 182(11):2307–2313, 2011.

[11] Carolyn L. Phillips, **Joshua A. Anderson**, and Sharon C. Glotzer. Pseudo-random number generation for Brownian dynamics and dissipative particle dynamics simulations on GPU devices. *Journal of Computational Physics*, 230(19):7191–7201, 2011.

[10] Sharon C. Glotzer and **Joshua A. Anderson**. Nanoparticle assembly: Made to order. *Nature Materials*, 9(11):885–887, 2010.

[9] **Joshua A. Anderson**, Rastko Sknepnek, and Alex Travesset. Design of polymer nanocomposites in solution by polymer functionalization. *Physical Review E*, 82(2):021803, 2010.

[8] **Joshua A. Anderson**. *Phases of polymer systems in solution studied via molecular dynamics*. PhD thesis, Iowa State University, 2009.

[7] Christian D. Lorenz, Paul S. Crozier, **Joshua A. Anderson**, and Alex Travesset. Molecular Dynamics of Ionic Transport and Electrokinetic Effects in Realistic Silica Channels. *Journal of Physical Chemistry C*, 112(27):10222–10232, 2008.

[6] Rastko Sknepnek, **Joshua A. Anderson**, Monica H. Lamm, Jörg Schmalian, and Alex Travesset. Nanoparticle ordering via functionalized block copolymers in solution. *ACS nano*, 2(6):1259–65, 2008.

List of Publications (continued)

[5] **Joshua A. Anderson**, Christian D. Lorenz, and Alex Travesset. General purpose molecular dynamics simulations fully implemented on graphics processing units. *Journal of Computational Physics*, 227(10):5342–5359, 2008.

[4] **Joshua A. Anderson**, Christian D. Lorenz, and Alex Travesset. Micellar crystals in solution from molecular dynamics simulations. *The Journal of chemical physics*, 128(18):184906, 2008.

[3] Chris D. Knorowski, **Joshua A. Anderson**, and Alex Travesset. Self-assembled ordered polymer nanocomposites directed by attractive particles. *The Journal of chemical physics*, 128(16):164903, 2008.

[2] Michael Garland, Scott Le Grand, John Nickolls, **Joshua A. Anderson**, Jim Hardwick, Scott Morton, Everett Phillips, Yao Zhang, and Vasily Volkov. Parallel computing experiences with CUDA. *Ieee Micro*, 28(4):13–27, 2008.

[1] **Joshua A. Anderson** and Alex Travesset. Coarse-Grained Simulations of Gels of Nonionic Multiblock Copolymers with Hydrophobic Groups. *Macromolecules*, 39(15):5143–5151, 2006.

Honors

Nov 2015 • CoMSEF Young Investigator Award – AIChE
May 2009 • Research Excellence Award – Iowa State University Physics Department
May 2005 • Ian W. Shepard Award – Michigan Technological University Physics Department

Education

2005-2009 • Doctorate of Philosophy in Condensed Matter Physics from Iowa State University
2001-2005 • Bachelor of Science in Physics and Computer Science from Michigan Technological University