

NATHAN P. WALTER

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EDUCATION

University of Illinois at Champaign-Urbana (UIUC) 08.2013 – present
PhD Candidate in Nuclear, Plasma, and Radiological Engineering (NPRE) Expected: 08.2018
Master of Science in Nuclear, Plasma, and Radiological Engineering (NPRE) 08.2018
Graduate Minor in Computational Science and Engineering
Advisor: Yang Zhang

- Master's Thesis Topic: Direct Energy Landscape Sampling of the Homogeneous Nucleation and Crystal Growth of a Model Liquid

University of Illinois at Champaign-Urbana (UIUC) 08.2010 – 12.2014
Bachelor of Science in Nuclear, Plasma, and Radiological Engineering (NPRE)
Minor in Mathematics Overall GPA: 3.84/4.00

RESEARCH INTERESTS

Understanding slow material processes from a atomistic scale; Rare event sampling methods such as metadynamics; Neutron and X-ray scattering; Classical and Ab Initio molecular dynamics for modeling and simulation; Materials undergoing irradiation; Large deformation constitutive material equations. Machine Learning algorithms

AWARDS, HONORS, CLUBS, AND CERTIFICATES

American Physical Society, GSOF Travel Award 03.2017
Graduate Specialization in Computational Science and Engineering 08.2016
U.S. Department of Energy, Naval Reactors (NR), *Rickover Fellowship Program* Honorable Mention 00.2014
Nuclear Regulatory Commission Undergraduate Scholarship 12.2011 – 06.2013
University of Illinois at Champaign-Urbana Dean's List Recipient 06.2011 – 0.62013
The Hacker Within, An organization for computational scientists to share and practice computational skills.
Member: 08.2015 – present
Treasure: 08.2016 – present

TECHNICAL STRENGTHS

Computer Programming Languages	C, C++, Matlab, Python, Fortran, Java, L ^A T _E X, Swift (novice), AJAX, R, OpenMP, MPI, HTML, CSS, Julia (novice)
Software	GROMACS, LAMMPS, VASP, SRIM/TRIM, FLAG, VMD, IGOR Pro, Dave, gnuplot, Adobe Photoshop, Illustrator, Flash, SPSS

RESEARCH EXPERIENCE

PhD Research 08.2016 – present

- Implemented a method of directly sampling the energy landscape into the molecular dynamics package GROMACS in order to study the activation barrier statistics of various protein systems
- Used energy landscape sampling to provide insight to protein folding and unfolding dynamics
- Developed a new method of directly sampling the energy landscape with higher computational efficiency than the one implemented in my master's work.
- Sampled and studied the energy landscapes of vary potentials to determine the affect of potential softness on the landscape

Master's Degree Research

01.2014 – 08.2016

- Implemented a method of directly sampling the energy landscape into the molecular dynamics package GROMACS in order to study the activation barrier statistics of glass forming and crystal forming systems
- Developed reduction codes to extract quantities from classical and *ab initio* molecular dynamics simulations relevant for comparing simulations to scattering experiments (i.e. intermediate scattering function, density of states, etc.).
- Developed an open-source package, *LiquidLib*, to analyze molecular dynamics trajectories to study the structure and dynamics of liquids and compare the results to neutron scattering experiments
- Performed *ab initio* molecular dynamic simulations to study the vibrational modes in D₂O and compare to neutron scattering experiments conducted at SEQUOIA, SNS, ORNL.
- Performed *ab initio* molecular dynamic simulations to study the effects of hydrogen impurities on liquid lithium transport properties
- Created a high dimensional molecular dynamics package to study the dimensionality of various quantities

Neutron and X-ray Scattering Summer School

06.2015

- Studied x-ray scattering methods at the Advanced Photon Source, APS, Argonne National Laboratory (ANL)
- Studied neutron scattering methods at SNS and HFIR, Oak Ridge National Laboratory (ORNL)

Scattering Experiments

- Participated in pair distribution experiments on glass forming metallic liquids using a neutron electrostatic levitator performed at NOMAD, SNS, Oak Ridge National Laboratory (ORNL)
- Participated on Inelastic Neutron Scattering experiments on liquid metals performed at CNCS, SNS, Oak Ridge National Laboratory (ORNL)
- Analyzed scattering data on D₂O performed at SEQUOIA, SNS, Oak Ridge National Laboratory (ORNL)

Los Alamos Computational Physics Student Summer Workshop

Summer 2014

- Implemented a strain-based constituent equation for large material deformation under high strain-rates into a production hydrocode
- Developed concepts for extending the strain-based formulation from perfectly plastic materials to rate-hardening materials.
- Studied the advantages of the strain-based with pertaining to advection in Lagrangian mode, finite material rotations, and artificial viscosity.

Machine Learning Experience

- Enrolled in several high level statistics courses, including the course on machine learning
- Participated in the Kaggle competition for Springleaf as a team.
- For the competition, used various machine learning methods to reduce the data space, and build predictive models
- Used several machine learning regression and clustering methods to create a model to predict the value of a hand written input number

Institute for Genomic Biology

Undergraduate Research Assistant to Biofuel Lab Research

Summer 2012
Champaign, IL

- Worked on British Petroleum (BP) Biofuel Project
- Analyzed soil samples for carbon/nitrogen make-up
- Studied different plants' potential as a biofuel

- Implemented Java code to simulate contact points
- Developed mathematical and programming algorithms for the project

PRESENTATIONS

- Talk, American Physical Society March Meeting, “*Protein Folding and Unfolding Dynamics from Direct Energy Landscape Sampling Simulations*” 03.2017
- Talk, University of Illinois Urbana-Champaign Nuclear Engineering Graduate Seminar, “*Direct Energy Landscape Sampling of the Homogeneous Nucleation and Crystal Growth of a Model Liquid*” 12.2016
- Discussion, The Hacker Within: University of Illinois Urbana-Champaign, “*An Overview of Techniques and Methods in Machine Learning with Application to Sci-Kit (sklearn) in Python*” 11.2016
- Talk, University of Illinois Urbana-Champaign Soft Materials Seminar, “*Direct Energy Landscape Sampling of the Homogeneous Nucleation and Crystal Growth of a Model Liquid*” 09.2016
- Talk, American Conference on Neutron Scattering, “*Homogeneous Nucleation and Crystal Growth in a Model Liquid from Direct Energy Landscape Sampling Simulations*” 07.2016
- Discussion, The Hacker Within: University of Illinois Urbana-Champaign, “*Understanding Classification of Hand-Written Numbers with Machine Learning Techniques*” 05.2016
- Talk, University of Illinois Urbana-Champaign Nuclear Engineering Undergraduate Seminar, “*Homogeneous Nucleation and Crystal Growth in a Model Liquid from Direct Energy Landscape Sampling Simulations*” 04.2016
- Talk, American Physical Society March Meeting, “*Homogeneous Nucleation and Crystal Growth in a Model Liquid from Direct Energy Landscape Sampling Simulations*” 03.2016
- Poster, American Physical Society March Meeting, “*Energy Landscape Statistics of Kob-Andersen Liquid From Direct Energy Barrier Sampling*” 03.2015
- Talk, Los Alamos Student Summer Symposium, “*A New Strain-Based Method for Plastic Flow Simulations*” 08.2014

PUBLICATIONS

- T. P. Money Penny, **N. P. Walter**, Z. Cai, Y. Miao, D. L. Gray, J. J. Hinman, S. Lee, Y. Zhang, J. S. Moore, “*Impact of Shape Persistence on the Porosity of Molecular Cages*” JACS (2017)
- Nathan Walter**, Zhikun Cai, Abhishek Jaiswal, Yang Zhang, “*LiquidLib: A comprehensive tool for post processing of classical and ab initio molecular dynamics simulations of liquids with application to neutron scattering experiments*”, to be submitted
- Zhikun Cai, Abhishek Jaiswal, **Nathan Walter**, Yang Zhang, “*Validity boundary of the Stokes-Einstein relation in water*” to be submitted
- Nathan Walter**, Yang Zhang, “*Direct Energy Landscape Sampling of the Homogeneous Nucleation and Crystal Growth of a Model Liquid*”, to be submitted
- Zhikun Cai, **Nathan Walter**, Yang Zhang, “*Energy Landscape Statistics And Coarsening In Liquids: A Relaxation Excitation Mode Analysis: Part I*”, to be submitted.
- Zhikun Cai, **Nathan Walter**, Yang Zhang, “*Energy Landscape Statistics And Coarsening In Liquids: A Relaxation Excitation Mode Analysis: Part II*”, to be submitted.
- Nathan Walter**, Zhikun Cai, Yang Zhang, “*Energy Landscape Statistics And Coarsening In Liquids: A Relaxation Excitation Mode Analysis: Part III*”, to be submitted.
- Nathan Walter**, Paul Friedrichsen, Scott Runnels, “*Extending a Strain Space Formulation for Plasticity to Rate-Hardening Materials and Finite Rotations*”, submitted to Mathematics and Computers in Simulation .
- Nathan Walter**, Paul Friedrichsen, Scott Runnels, “*Extending a Strain Space Formulation for Plasticity to Rate-Hardening Materials and Finite Rotations*”, LA-UR-15-23329, Los Alamos Unlimited Release (2015).
- Nathan Walter**, Paul Friedrichsen, “*Improving Plasticity Modeling in Hydrocodes with Hypoelastic Frameworks*”,

APPOINTMENTS

Research Assistant Yang Zhang's Research Group	January, 2014 – present
Nuclear Regulatory Commission Graduate Fellowship	January 2014 – present
Teaching Assistant , NPRE 448: Nuclear Systems Engineering and Design	August, 2013 – January, 2014