NATHAN WALTER

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EDUCATION

University of Illinois at Champaign-Urbana (UIUC) August, 2013 – present
PhD Candidate in Nuclear, Plasma, and Radiological Engineering (NPRE)
Master of Science in Nuclear, Plasma, and Radiological Engineering (NPRE)
Graduate Minor in Computational Science and Engineering
Expected PhD Completion: August, 2018
Master's Degree Completion: August, 2016
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) August, 2010 – January, 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

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

TECHNICAL STRENGTHS

Computer Programming Languages	C, C++, Matlab, Python, Fortran, Java, LaTeX, 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 D_2O 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

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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 levatator 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 Labratory (ORNL)
- Analyzed scattering data on D_2O 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

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Institute for Genomic Biology Summer 2012
Undergraduate Research Assistant to Biofuel Lab Research Champaign, IL

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

University of Northeastern Illinois Summer 2009
Student Research Assistant on Abstract Topology Project Chicago, IL

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

PRESENTATIONS

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

Contributed Talk, Los Alamos Student Summer Symposium, *"A New Strain-Based Method for Plastic Flow Simulations"* 08.2014

PUBLICATIONS

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"*, LA-UR-14-26946, Los Alamos Unlimited Release (2014).

AWARDS, HONORS, CLUBS, AND CERTIFICATES

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