NATHAN WALTER

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Current Address: 120 Talbot Laboratory, 104 S. Wright St. ⋄ Urbana, Illinois 61801

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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: May, 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; 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

RESEARCH EXPERIENCE

Master's Degree Research

January 2014 – 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 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

Machine Learning Experience

Fall 2015

- 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

Neutron and X-ray Scattering Summer School

June 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

May 2014 - May 2016

- 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 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.

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

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

PUBLICATIONS

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).

Zhikun Cai, **Nathan Walter**, Yang Zhang, "Energy Landscape Statistics And Coarsening In Liquids: A Relaxation Mode Analysis", to be submitted.

Nathan Walter, Paul Friedrichsen, "Improving Plasticity Modeling in Hydrocodes with Hypoelastic Frameworks", LA-UR-14-26946, Los Alamos Unlimited Release (2014).

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" November, 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" November, 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" September, 2016

Talk, American Conference on Neutron Scattering, "Homogeneous Nucleation and Crystal Growth in a Model Liquid from Direct Energy Landscape Sampling Simulations"

July, 2016

Discussion, The Hacker Within: University of Illinois Urbana-Champaign, "Understanding Classification of Hand-Written Numbers with Machine Learning Techniques" May, 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" April, 2016

Talk, American Physical Society March Meeting, "Homogeneous Nucleation and Crystal Growth in a Model Liquid from Direct Energy Landscape Sampling Simulations" March, 2016

Poster, American Physical Society March Meeting, "Energy Landscape Statistics of Kob-Andersen Liquid From Direct Energy Barrier Sampling" March, 2015

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

August, 2014

AWARDS, HONORS, CLUBS, AND CERTIFICATES

U.S. Department of Energy, Naval Reactors (NR), Rickover Fellowship Program in Nuclear Engineering Honorable Mention

April, 2014

Nuclear Regulatory Commission Undergraduate Scholarship

 $Fall,\ 2011-Spring,\ 2013$

University of Illinois at Champaign-Urbana Dean's List Recipient

Spring, 2011 – Spring, 2013

The Hacker Within: University of Illinois Urbana-Champaign, An organization for computational scientists to share and practice computational skills.

Member: August, 2015 – present Treasure: August, 2016 – present

Successfully completed the following Coursera and Udemy online courses:

- Become a Certified Web Developer (Udemy)
- The Data Scienties's ToolBox (Coursera)
- Statistical Inference (Coursera)
- Machine Learning by Standford University (Coursera)