# NATHAN WALTER

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#### **EDUCATION**

# University of Illinois at Champaign-Urbana (UIUC)

*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) 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
Topphing Assistant	August 2012 Japuary 2014

Teaching Assistant NPRE 448: Nuclear Systems Engineering and Design

# **RESEARCH EXPERIENCE**

#### Master's Degree Research

- 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 D<sub>2</sub>O 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

August, 2013 – present

August, 2010 - January, 2014

August, 2013 – January, 2014

January 2014 – present

• Created a high dimensional molecular dynamics package to study the dimensionality of various quantities

#### 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

#### Neutron and X-ray Scattering Summer School

- 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<sub>2</sub>O performed at SEQUOIA, SNS, Oak Ridge National Laboratory (ORNL)

#### Los Alamos Computational Physics Student Summer Workshop

- 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 ratehardening 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

Undergraduate Research Assistant to Biofuel Lab Research

- 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

Student Research Assistant on Abstract Topology Project

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

#### TECHNICAL STRENGTHS

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May 2014 - May 2016

Summer 2014

Fall 2015

June 2015

ory (ORNL)

Summer 2012 Champaign, IL

Summer 2009 Chicago, IL

Computer	Programming	Languages
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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, American Conference on Neutron Scattering, "Homogeneous Nucleation and Crystal Growth in a ModelLiquid from Direct Energy Landscape Sampling SimulationsJuly, 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 ModelLiquid from Direct Energy Landscape Sampling SimulationsMarch, 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. August, 2015 – 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)