

JASON M LARKIN

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CAREER OVERVIEW AND OBJECTIVE

I have extensive experience performing experimental and numerical studies in condensed matter physics. My interests include multi-language development for applications ranging from high-performance parallel computing to smart phones, and open-source collaboration to improve the way research is performed and the way results are disseminated.

EDUCATION

Carnegie Mellon University Pittsburgh, PA • PhD Mechanical Engineering, 2013 GPA: 3.85/4.00

Thesis: Thermal Modeling of Disordered Materials. Numerically investigated thermal properties of crystal alloys, glasses, and organic materials using classical and *ab initio*-based atomistic techniques.

Coursework: molecular/electron structure · nanoscale transport phenomena · numerical methods · solid state physics · statistical mechanics

24-627 Nanophotonics: basic concepts and applications of nanophotonics, fundamental understanding of principles for manipulating light at the nanoscale. Topics: fundamentals of electromagnetics (Maxwell's equations, polarization, dipole antenna, etc.), optical properties of solids, localized and propagating surface plasmons, nanoscale thermal radiation by surface phonon polaritons, electromagnetic metamaterials with negative refraction, photonic crystals and band gap, applications in nanotechnology.

33-225 Quantum Physics and the Structure of Matter: basics of quantum mechanics, fundamentals of quantum chemistry, statistical thermodynamics, and solid state physics.

24-628 Special Topic in Energy Transport and Conversion at the Nanoscale: Energy transport and conversion processes at the nanoscale due to interactions between molecules, electrons, phonons, and photons. Understanding these processes to design heat transfer equipment, thermoelectric materials, electronics, light emitting diodes, and photovoltaics.

24-623 Molecular Simulation of Materials: theory and implementation of numerical techniques for modeling atomic-level behavior. Focus on molecular dynamics and Monte Carlo simulations. Students write their own simulation computer codes (programming in C/C++), and learn how to perform calculations in different thermodynamic ensembles. Consideration given to heat transfer, mass transfer, fluid mechanics, mechanics, and materials science applications.

CHE3920 Electronic Structure Basic Theory, Modeling and Simulations: HartreeFock calculations, Density functional theory, Pseudopotentials, Practical aspects of atomistic calculations, Quantum Monte Carlo, GW approximation. Stateoftheart atomistic simulations and modeling using ABINIT (Fortran) and VASP (Fortran, Python wrapping). Predictions of dielectric and ferroelectric properties of Phase Change Memory Materials.

University of Pittsburgh Pittsburgh, PA • MS Mechanical Engineering, 2009 GPA: 3.70/4.00

Thesis: Statistics of Particle Concentrations in Free-Surface Turbulence. Performed experiments using novel 2D and 3D flow configurations to study turbulence as a nonlinear dynamical system.

Coursework: quantum and statistical physics · turbulence · chaos and nonlinear phenomena

University of Pittsburgh Pittsburgh, PA • BS Mechanical Engineering, 2007 GPA: 3.20/4.00

Research: Used computational fluid dynamics to design a model arterial bifurcation for *in vivo* study.

EXPERIENCE

Carnegie Mellon University (2010-2012) Teaching Assistant-Heat Transfer

- Topics in conduction, convection, and radiation. Supervised recitations and substituted for lectures.

University of Pittsburgh (2008) Teaching Assistant-Advanced Fluid Mechanics

- Topics in viscous flow, boundary layer theory, and scale similarity.

University of Pittsburgh (2007-2009) Lecturer-Physics

- Lectured to students and faculty on mathematics, bio-physics, turbulence, statistical and nonlinear phenomena.

Precision Therapeutics (2006-2007) Intern-Technology Development

- Worked with team of software developers and laboratory equipment specialists.
- Used CADD to design and fabricate components of optical microscopes and laboratory automation controls.

SKILLS

- **Computing Languages:** Matlab, Fortran, Python, C/C++, Java, L^AT_EX, Shell, Perl, Markdown, HTML.
- **High-Performance Computing:** linux/unix cluster administration/computing, parallel computation (MPI, OpenMP), mixed-language development, open-source development (Git, Github, arXiv).
- **General Computing:** linux/unix, Mac OS, Windows, Microsoft Office.
- **Modeling:** atomistic simulation, quantum chemistry, nanoscale transport, statistical and nonlinear systems.
- **Hardware:** general computing, optics/lasers, DI/DO AI/AO interfaces, simple automation, machining, circuitry.

PROJECTS

- **Quantum Mechanics-Driven Prediction of Nanostructure Thermal Conductivity:** served as investigator under the AFOSR with collaborators at Carnegie Mellon and Univ. of Pitt., performing calculations on the DOD's HPCMP.

Calculations include:

- massively-parallel (100-1000 core) Molecular Dynamics simulations using LAMMPS open-source package (C/C++) together with my own ntpy package (Python, Cython) which implements the Normal Mode Decomposition algorithm.
 - parallel Lattice Dynamics calculations using GULP open-source package (Fortran), as well as my own Matlab and Python codes which implement algorithms based on eigenvalue solutions.
 - parallel ab initio (quantum-based electron structure) calculations using VASP (Fortran), ABINIT (Fortran), Quantum Espresso (Fortran) packages.
 - **disorder:** a comprehensive repository of open-source code and data from my PhD thesis, hosted on Github.
 - **ntpy:** created this open-source collaborative effort between members of NTPL and University of Toronto.
 - **GULP:** international collaboration with Julian Gale at the Nanochemistry Research Institute at Curtin University.
 - **Statistics of Free-Surface Turbulence:** international collaboration with Alain Pumir at ENS Lyon, France.
- Calculations include:
- algorithm to create virtual particle trajectories from Particle Imaging Velocimetry-derived velocity vector fields (Matlab, C/C++).
 - algorithm to temporally decorrelate velocity vector fields to study turbulence as a "white-in-time" phenomenon (Matlab).
 - algorithm to collect particle statistics in the Lagrangian frame of reference, which greatly increases statistical significance compared to the Eulerian frame of reference (Matlab).

PUBLICATIONS (SELECTED, 11 TOTAL)

- "Origin of the Exceptionally Low Thermal Conductivity of Fullerene Derivative PCBM Films", (in progress).
- "Decorrelating a Compressible Turbulent Flow: an Experiment", Phys. Rev. E 82, 016301 (2010).

PRESENTATIONS (SELECTED, 15 TOTAL)

- "Evaluation of the Virtual Crystal Approximation for Predicting Thermal Conductivity", J.M. Larkin (speaker), A.J.H. McGaughey, 2013 MRS Spring Meeting San Francisco, CA.
- "The Generalized Fractal Dimensions of a 2-D Compressible Turbulence", J. Larkin (speaker), M. Bandi, W. Goldberg, 2008 American Physical Society March Meeting New Orleans, LA.

HONORS

- 2012 ASME MHNMT International Summer Heat Transfer Conference Top 5 Technical Paper
- 2011 Bennett Conference Best Presentation
- 2011 ICES Northrop-Gruman Fellow
- 2007-2009 NSF Graduate Student Research Grant University of Pittsburgh Department of Physics.

MEMBERSHIPS

- American Physical Society · American Society of Mechanical Engineers · Materials Research Society · Society of Industrial and Applied Mathematics · DOD High Performance Computing Modernization Program