GIUSEPPE BARBALINARDO

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Education

Ph.D. Candidate - Sept '16 - Current – University of California, Davis

- Computational Chemical Physics
- Coursework average GPA: 4+
- Nanoscale simulations. Lead developer and creator of kALDo, a modern Python and Tensorflow-based open-source software package for heat transport simulations, which can run on CPUs and GPUs. Development from conception to release, including unit-tests, documentation, continuous integration, and deployment using Docker and CircleCI. Implementation of Google Colab examples. Team of 5 developers. More details here: https://nanotheorygroup.github.io/kaldo.
- Amorphous and crystals. Development of a unified theoretical framework for amorphous and crystal structures, which bridges the gap between Anharmonic Lattice Dynamics and Molecular Dynamics. Theory and Simulations. In collaboration with Prof. Baroni's group at SISSA University (Trieste).
- Application of Neural Networks to model interatomic potentials.
- Recipient of the 2019-2020 Software Development Investment Fellowship by the NSF Molecular Sciences Institute.
- Recipient of the 2020 Peter A. Rock Graduate Fellowship in Chemical Physics by UC Davis.
- Thesis Advisor: Prof. Davide Donadio.
- Relevant coursework: Artificial Intelligence, Statistical Mechanics, Mathematical Methods, Quantum Chemistry, Econophysics

M.Sc. - Apr '12 – Dec '13 – University of California, San Diego

- Theoretical Physics
- Quantum Information. Theoretical study and development. Application of control theory to increase the coherence time in quantum dots qubits.
- Thesis Advisor: Prof. Lu Sham.
- Relevant coursework: Stochastic Methods, Computational Physics II: PDE and Matrices, Equilibrium Statistical Mechanics, Non-Equilibrium Statistical Mechanics, Quantum Field Theory

Work experience

Teaching Assistant - Sept '16 - Jun' 19 - University of California, Davis

- Teaching Assistant for the graduate classes of Quantum Mechanics (1 & 2) in the Chemistry Department. Helped students with Python. Collaborated with Prof. McCurdy to implement a code for students to find solutions to the Schrodinger equation using Discrete Variable Representation.

- Teaching Assistant for the graduate class of Mathematical Methods for Chemists. Helped students in implementing numerical algorithms using Python. Some examples of topics explained during the course are Fast Fourier Transform, Linear Algebra using Lanczos and Householder, Optimization using Gradient Descent and BFGS, Partial Differential Equations, and Regularization using LASSO and LARS.

Software Developer and Engineering Manager – May '14 – Aug '16 - Grio, San Francisco

Engineering Manager - Jan '16 - Aug '16

- Managed a team of 6-8 software developers across several simultaneous projects, while continuing hands-on coding.
- Designed and implemented the apprentice program and mentored junior developers.
- Organized the company's first hackathon.

Software Developer - May '14 – Aug '16

- Contributed to projects with diverse technology stacks, coding in Java, Objective C, SQL, and Python.
- Developed the new Target iPad app in an Agile-driven team of 12 people.
- Collaborated with the marketing and business team at Twitter. Developed an AngularJS dashboard to convert proprietary meta-language to Ruby and later application to over 10 marketing campaigns.
- Presented 4 Tech Talks at the company all-hands meeting.

Skills

Technologies	Mathematical Methods	Scientific Packages
Python Tensorflow JAVA C++ / C Fortran Swift AngularJS PostgreSQL Objective C MongoDB Parallel computing: MPI & CUDA	Statistics Probability Theory Linear Algebra Information Theory Stochastic Methods Markov Chain Monte Carlo Numerical Methods Algorithms	Molecular Dynamics using LAMMPS Density Functional Theory using Quantum Espresso Hartree Fock, MP2, Coupled Cluster, and Configuration Interaction using Psi4

Academic publications

- G Barbalinardo, Z Chen, NW Lundgren, D Donadio - Efficient anharmonic lattice dynamics calculations of thermal transport in crystalline and disordered solids - Journal of Applied Physics, 128 (13), 135104, 2020
- N. Lundgren, G. Barbalinardo, D. Donadio – Mode Localization and Suppressed Heat Transport in Amorphous Alloys - Submitted
- C Mangold, S Chen, G Barbalinardo, J Behler, P Pochet, K Termentzidis, Yang Han, Laurent Chaput, David Lacroix, Davide Donadio - Transferability of neural network potentials for varying stoichiometry: phonons and thermal conductivity of Mn - Ge compounds - Journal of Applied Physics 127 (244901). 2020
- Leyla Isaeva, Giuseppe Barbalinardo, Davide Donadio & Stefano Baroni, "Modeling heat transport in crystals and glasses from a unified

lattice-dynamical approach". Nature Communications volume 10, Article number: 3853 (2019)

- G Barbalinardo, CA Sievers, S Chen, D Donadio, "Thermal transport in finite-size van der Waals materials: Modeling and Simulations". 2018 IEEE 18th International Conference on Nanotechnology (IEEE-NANO) 18414617
- G. Barbalinardo, S. Chen, and D. Donadio, "Unraveling A New Heat Transport Regime at The Nanoscale," In preparation.
- G.. Barbalinardo, D. Donadio, and Z. Chen, "Ballistico, A Large Scale Anharmonic Lattice Dynamics Simulator." In preparation
- M Battiato, G Barbalinardo, PM Oppeneer. Quantum theory of the inverse Faraday effect. Physical Review B 89 (1), 014413, - January 2014
- M Battiato, G Barbalinardo, K Carva, PM Oppeneer. Beyond linear response theory for intensive light-matter interactions: Order formalism and ultrafast transient dynamics. Physical Review B 85 (4), 045117 - January 2012

Conferences, schools and workshops

Sept '19 – Berkeley, CA
AI for Science Town Hall at the Lawrence Berkeley National Lab. A meeting organized by the DOE.

Aug '19 - Blacksburg, VA
MolSSI Software Fellow Bootcamp on how to release an open-source scientific project at the Virginia Tech.

July '19 – Berkeley, CA
Deep Learning for Science School at the Lawrence Berkeley National Lab.

June '19 – Trieste, Italy
Conference on Nanophononics, Bridging Statistical Physics, Molecular Modeling, and Experiments and the International Centre for Theoretical Physics.
Poster presentation: Unravelling a New Heat Transport Regime at the Nanoscale

May '19 – Berkeley, CA
Northern California Theoretical Chemistry Meeting at UC Berkeley

May '19 – Davis, CA
Peter Hall Statistics and Machine Learning Conference at UC Davis

Apr '19 – Phoenix, AZ
Materials Research Science Conference.
Contributed talk: Unraveling A New Heat Transport Regime at The Nanoscale

Feb '19 – San Francisco, CA
Google AI Connect at San Francisco's Google Office

Oct '18 – Sunnyvale, CA
Design and Deployment of Deep Learning with Spark, Workshop by the Association for Computing Machinery.

Aug' 18 – Davis, CA
30th annual Conference on Computational Physics (IUPAP), University of California Davis,
Poster Presentation: "Ballistico, An Anharmonic Lattice Dynamics Simulator"

Jul' 17 – Chicago, IL
MICCoM Computational School - University of Chicago

Dec '16 – San Francisco, CA
Advanced Course on Deep Learning with Python, Keras and TensorFlow. DataWknds

Awards and extra

2020 – Now

Recipient of the 2020 Peter A. Rock Graduate Fellowship in Chemical Physics by UC Davis.

2019 – Now

Software Development Investment Fellowship from the Molecular Sciences Institute (funded by the NSF), for the project "Development of an open-source framework to model heat transport at the nanoscale."

2019 – Now

Member of the American Physical Society, Physics

2018 – Now

Referee for Physical Review B, Physical Review E

2018 – Now

Referee for The Journal of Chemical Physics

2018 – Now

Member of the Association for Computing Machinery, Bay Area

2010 – 2011

Distinguished thesis award. Scholarship for dissertation: "Quantum Theory of the Inverse Faraday Effect". Issuer: Lerici Foundation Stockholm.