

Giuseppe Barbalinardo

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Experience

Senior Data Scientist – Tonal

Jan '21 - Now

At Tonal, I design and implement smart algorithms and models applied to Fitness Science, while developing "The World's Most Intelligent Home Gym and Personal Trainer."

Ph. D. Researcher – University of California, Davis

Sept '16 - Dec '20

My contributions to the field of statistical physics and material science include theoretical modeling, software development, large-scale simulations and modern machine learning applications. Dissertation title: *Unraveling heat transport in complex materials: from glasses to nanostructures*. Advisor: Dr. D. Donadio

- Lead developer and creator of [kALDo](#), a modern 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. Integrated the code with external software, like **Quantum Espresso**, **LAMMPS**, and **ASE**. Implementation of Google Colab examples. Team of 5 developers.
- Development of a novel **theoretical model** to simulate heat transport in both amorphous and crystalline solids, while including quantum effects. Scientific collaboration supervised by Dr. D. Donadio at UC Davis and Dr. S. Baroni at SISSA.
- Theoretical and **numerical study** of the size-dependent thermal conductivity of carbon nanotubes, and one-dimensional materials by using Molecular Dynamics and Anharmonic Lattice Dynamics models, in collaboration with researchers from the College of Physical Science and Technology of Bohai University.
- Developer of [quantumGrid](#), an **educational package** for solving a 1-D time-dependent or time-independent Schrödinger equation for an arbitrary potential on any interval. This package's core is implementing a Finite Element Method with a Discrete Variable Representation (FEM-DVR) grid. Team of 3 developers. Project led by Dr. McCurdy at LBNL.
- Teaching Assistant for the graduate class of Mathematical Methods for Scientists. **Numerical algorithms** using Python, including: Optimization Methods (Gradient Descent, quasi-Newton, BFGS), Partial Differential Equations, Regularization, Dimensionality Reduction, Penalized Regressions, LASSO, Fast Fourier Transform, and Linear Algebra.
- Teaching Assistant for the graduate classes of Quantum Mechanics (1 & 2) in the Chemistry Department. Time dependent and independent. Methods: Restricted Hartree-Fock, unrestricted Hartree-Fock, Møller-Plesset perturbation theory (MP2), and configuration interaction (CI) and coupled cluster (CCSD). Python lectures to students and development of hands-on tutorials.

Software Developer and Engineering Manager – Grio, San Francisco

May '14 – Aug '16

Engineering Manager

Dec '15 - 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 – Nov '15

- Contributed to projects with diverse technology stacks, coding in **Java, Objective C, SQL, and Python**.
- Developed the Target iPad app in an Agile-driven team of 12 people.
- Developed the Texture Next Issue app, through prototyping, validation and iterations of the product.
- 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

- Python Environment and major numerical and AI libraries: Numpy, Tensorflow, Keras, Scikit Learn, Pandas, Matplotlib, PySpark, MPI4py
- Other languages: SQL, Objective C, Swift, JAVA, Fortran,
- Infrastructures and HPC: Docker, Kubernetes, MPI, Cuda, Bash, Unix, Google Cloud, AWS

Machine Learning and AI

- Optimization methods
- Dimensionality reduction
- Penalties and Regularization
- Neural Networks Architectures
- Gradient Boosting Algorithms
- Natural Language Processing
- Time Series Analysis
- Markov Chain Monte Carlo

Scientific Packages

- Molecular Dynamics, LAMMPS and OpenMM
- Density Functional Theory, Quantum Espresso
- Theoretical Chemistry methods, Psi4

Education

University of California, Davis

Ph.D. Chemical Physics, **GPA 4.0**, 2020

- Relevant coursework: Artificial Intelligence, Statistical Mechanics, Mathematical Methods, Quantum Chemistry

University of California, San Diego

M.Sc. Condensed Matter Theory, 2013

- Relevant coursework: Stochastic Methods, Computational Physics II: PDE and Matrices, Equilibrium Statistical Mechanics, Non-Equilibrium Statistical Mechanics, Quantum Field Theory

University of Milan, Italy

M.Sc. Theoretical Physics, **Summa Cum Laude**, 2011

B.Sc. Physics, 2008

- Relevant coursework: Linear Algebra, Group Theory, Probability and Statistics, Field Theory, Computational Physics

Uppsala University, Sweden

Awards

- Recipient of the **Software Development Investment Fellowship** from the National Science Foundation, Molecular Sciences Software Institute.
- Recipient of the 2020 Peter A. Rock Graduate Fellowship for the **highest academic merit** and research in Chemical Physics by UC Davis.
- Distinguished M.Sc. thesis award. Fellowship for the dissertation: "Quantum Theory of the Inverse Faraday Effect" from the Lerici Foundation in Stockholm.

Academic publications

- Barbalinardo, G., Chen, Z., Dong, H., Zheyong, F. and Donadio, D., *Ultrahigh but convergent thermal conductivity of carbon nanotubes from comprehensive atomistic modeling*. Submitted. 2020.
- Lundgren, N.W., Barbalinardo, G. and Donadio, D., *Mode Localization and Suppressed Heat Transport in Amorphous Alloys*. arXiv:2011.08318. Submitted. 2020.
- Barbalinardo, G., Chen, Z., Lundgren, N.W. and Donadio, D., *Efficient anharmonic lattice dynamics calculations of thermal transport in crystalline and disordered solids*. Journal of Applied Physics, 128(13), p.135104, 2020.
- Isaeva, L., Barbalinardo, G., Donadio, D. and Baroni, S., *Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach*. Nature Communications, 10, 2019.
- Mangold C, Chen S, Barbalinardo G, Behler J, Pochet P, Termentzidis K, Han Y, Chaput L, Lacroix D, Donadio D. *Transferability of neural network potentials for varying stoichiometry: phonons and thermal conductivity of $Mn_x Ge_y$ compounds*. Journal of Applied Physics 127, 244901, 2019.
- Barbalinardo, G., Sievers, C. A., Chen, S. and Donadio, D., 2018. Thermal transport in finite-size van der Waals materials: Modeling and Simulations. IEEE 18th International Conference on Nanotechnology. July, 2018.
- Battiato, M., Barbalinardo, G., Oppeneer, P.M.. Quantum theory of the inverse Faraday effect. Physical Review B 89, 014413, January, 2014.
- Battiato, M., Barbalinardo, G., Carva, K., Oppeneer, P.M.. Beyond linear response theory for intensive light-matter interactions: Order formalism and ultrafast transient dynamics. Physical Review B 85 (4), 045117, January, 2012.

Presentations, schools and workshops

- Lawrence Berkeley National Lab, CA
Workshop participant. DoE AI for Science Town Hall at the Lawrence Berkeley National Lab. Sept '19
- Virginia Tech, Blacksburg, VA
School, MolSSI Software Fellow Bootcamp. Open-source scientific projects. Aug '19
- Lawrence Berkeley National Lab, CA
School, Deep Learning for Science School at the Lawrence Berkeley National Lab. Jul '19
- International Centre for Theoretical Physics, Trieste, Italy
Poster presentation, Conference on Nanophononics, Bridging Statistical Physics, Molecular Modeling, and Experiments. Jun '19
- University of California, Berkeley, CA
Conference Attendee: Peter Hall Statistics and Machine Learning Conference May '19
- Materials Research Science Conference, Phoenix, AZ
Contributed talk: Unraveling A New Heat Transport Regime at The Nanoscale Apr '19
- University of California, Davis, CA Apr '19

- Seminar presentation: Chemistry Department Seminar
 Google, San Francisco, CA Feb '19
 Conference Attendee: Google AI Connect, San Francisco
- Association for Computing Machinery, Sunnyvale, CA Oct '18
 Workshop participant: Design and Deployment of Deep Learning with Spark
- University of California, Davis, CA Aug '18
 Poster Presentation: 30th annual Conference on Computational Physics (IUPAP)
- University of Chicago, IL Jul '17
 School: The Midwest Integrated Center for Computational Materials (MICCoM)

Projects

Co-founder of [Ergo](#) (June 2019), a dashboard powered by **Artificial Intelligence** and **Natural Language Processing**, that pulls the latest news stories across media sources and highlights relevant content to combat the spread of misinformation.

- Implementation of the main machine learning algorithms, including Sentence Transformer (SBERT), Dimensionality reduction using principal component analysis, Entity Extraction, and Clusterization, using Python, Numpy, Tensorflow and Pytorch.
- Development of the main stack, Pytorch, Flask, Postgres, Cube, VueJS, Grafana, Docker, Kubernetes, and Google Cloud.