

# Giuseppe Barbalinardo

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I am interested in the overlapping areas between software development and scientific modeling, and passionate about AI and Natural Language Processing.

## Research Highlights

My Ph.D research focuses on modeling heat transfer at the atomistic level. I contributed to this field with a novel theory development (Nature Communications 2019), numerical solutions (Journal of Applied Physics 2020) and by using modern machine learning techniques (Journal of Applied Physics 2020).

I am the main developer of kALDo, a modern open-source Python-Tensorflow package for Anharmonic Lattice Dynamics calculations: [github.com/nanotheorygroup/kaldo](https://github.com/nanotheorygroup/kaldo)

## Experience

**Graduate Student Researcher** Jul' 19 - Dec '20  
Nanotheory Research Group led by Dr. D. Donadio,  
University of California Davis

- Awarded the Software Development Investment Fellowship from the National Science Foundation - Molecular Sciences Software Institute.
- 2020 recipient of the Peter A. Rock Graduate Fellowship in Chemical Physics by UC Davis.

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

- Teaching Assistant for the graduate class of Mathematical Methods for Chemists. Helped students in learning numerical algorithms using Python: Fast Fourier Transform, Eigenvalues using Lanczos and Householder, Optimization using Gradient Descent and BFGS, Partial Differential Equations, and Regularization and dimensionality reduction using LASSO and LARS.
- Teaching Assistant for the graduate classes of Quantum Mechanics (1 & 2) in the Chemistry Department. Taught Educational Python lectures and tutorials. Implemented a code for students to numerically solve Schrodinger equation using Discrete Variable Representation.

**iOS Engineering Manager** Jan '16 - Aug '16  
Bitalign Inc. dba Grio San Francisco

- Managed and led the iOS team of 8 software developers across several simultaneous projects.
- Collaborated with several companies in the Bay Area and delivered high-quality software. Examples include Texture by Next Issue Media (now acquired by Apple).
- Designed and implemented the apprentice program and mentored junior developers.
- Organized the company's first hackathon and presented Tech Talks.

**Software Engineer** May '14 - Dec '15  
Bitalign Inc. dba Grio San Francisco

- Developed software using Swift, Objective C, Java (Android) and Ruby on Rails in an Agile-methodology driven environment.
- Partnered with clients in the Bay Area including the development of the Target iPad app.

- Designed high-level software architecture for new projects, including a collaboration with Twitter where I developed a dashboard to convert proprietary meta-language to Ruby and later applied to over 10 marketing campaigns.

## Education

**Ph.D.** Computational Chemical Physics. Sept '16 - Dec '20  
University of California Davis

- Coursework average GPA: 4.0.
- Relevant coursework: Mathematical Methods, AI and NLP, Statistical Mechanics.

**M.Sc.** Condensed Matter Theory. Apr '12 - Dec '13  
University of California San Diego

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

**M.Sc.** Theoretical Physics Dec '08 - Jul '11  
University of Milan, Bicocca Milan, Italy  
Uppsala University (Master Thesis) Uppsala, Sweden

- Distinguished thesis award fellowship for the dissertation: "Quantum Theory of the Inverse Faraday Effect", issued by the: Leric Foundation in Stockholm.
- Graduated with academic honor, magna cum laude.
- Relevant coursework: Linear Algebra, Group Theory, Probability and Statistics, Field Theory, Computational Physics.

## Other Activities

I am the co-founder of ERGO, an AI powered platform that pulls the latest news stories across media sources and highlights relevant content to combat the spread of misinformation: [www.searchergo.com](http://www.searchergo.com)  
Technologies: Python, Postgres, VueJS, NLP algorithms, in particular the Transformer (sentence).

## Skills

### Mathematical Methods

Statistics / Probability Theory / Linear Algebra / Information Theory / Stochastic Methods / Differential Equations / Markov Chain Monte Carlo / Numerical Methods / Algorithms

### Machine Learning

Regressions and penalized regressions / Bayesian optimization / Dimensionality reduction using LASSO, Single Value Decomposition and Principal Component Analysis / Optimization methods / Deep Neural Networks / Time series analysis using LSTM and Wavenet / NLP algorithms / BERT and Sentence Transformer.

### Technologies

Python / Objective C / Swift / Tensorflow / Pytorch / PostgreSQL / MySQL / JAVA SE / Android / Javascript / VueJS / Ruby on Rails / Docker / Kubernetes / Fortran / BLAS / Lapack / MPI / CUDA



## Links

[1] Ballistico, open-source project. Release in mid-2020. While the repo is currently private, I am providing access to it with the following credentials: <https://github.com/gbarbalinardo/ballistico> / ballistico-ald / Physics&AI0

[2] This project has been published in Nature Communications and several other press agencies covered it, including PhysicsWorld, Ceramics, SpaceDaily, AskaNews (italian), and N+1 (russian)

[3] A few projects I participated as a software developer and engineering manager at Grio, dba Bitalign, San Francisco.  
Target iPad app. iOS Developer. Participated in a two scrum team sized project that developed the new iPad application for Target. As an iOS developer, I developed many features in the new application. Among others, store pickers and major components on the home screen. Dev team size ~ 15 people.

Texture / Next Issue Media. iOS Developer. Implemented a functional prototype to perform user-testing. Developed several features in the legacy app: Facebook free magazine, analytics, and rebranding. Dev team size ~ 12 people.

iPracticeBuilder. iOS Developer. Developed the iPhone version of the app. Multi-device synchronization with Core-Data and new UI/UX. Dev team size ~ 5 people

Twitter Cards: Built new cards using Twitter's native language. Designed the algorithm and produced several variants of it. Dev team size ~ 3 people

[4] A few tech talks I gave at Grio, as a part of an introductory course on minimization problems

Monte-Carlo simulation of the NCAA March Madness using GPU and CUDA and NumbaPro as I discuss in this blog post

World Cup simulator, used to explain importance sampling algorithms to software developers as discussed in this post.

An introduction to probabilistic programming. Video here.

Mathematical Methods	Technologies
	Python Objective C / Swift Tensorflow / Pytorch PostgreSQL / MySQL JAVA SE / Android Javascript / VueJS Ruby on Rails Docker / Kubernetes Fortran / BLAS / Lapack MPI / CUDA

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## Academic publications

- 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  
MoSSI Software Fellow Bootcamp on how to release an open-source scientific project at 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. DataWeekends

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