Massimiliano (Max) Lupo Pasini

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🏠 https://www.ornl.gov/staff-profile/massimiliano-lupo-pasini

Citizenship	Italian
USA Legal Status	Lawful Permanent Resident (Green Card holder)

Education

2020 – present	**Master of Science - Computer Science**, *Georgia Institute of Technology*, Atlanta (USA). Major: Computer Science Minor: Machine Learning
2014 – 2018	**Doctoral studies - Applied Mathematics**, *Emory University*, Atlanta (USA), GPA − 3.976. Research areas: Numerical Linear Algebra, Scientific Computing, Parallel Computing
2011 – 2013	**Master of Science - Mathematical Engineering**, *Politecnico di Milano*, Milan (Italy). Second Level Graduation Major: Computational Science and Engineering Minor: Applied Statistics
2008 – 2011	**Bachelor of Science - Mathematical Engineering**, *Politecnico di Milano*, Milan (Italy). First Level Graduation

Languages

Italian	**Native**
English	**Fluent**
Spanish	**Fluent**
French	**Intermediate**

Interests - Scientific Topics

- Artificial Intelligence
- Machine Learning
- Scientific Computing
- Computer Science
- Numerical Analysis
- Statistics
- Matrix Analysis
- Probability
- Partial Differential Equations
- Fluid Dynamics
- Functional Analysis

Computer Skills

Advanced	Python, PyTorch, PyTorch Geometric, Keras, Scikit-learn, OpenMP, MPI, pthreads, C++, C, Matlab, R, Linux operative system, LaTeXeditor
Intermediate	CUDA, Julia, FreeFem++
Basic	FORTRAN 90, AMPL+GUSEK

Publications

2022	M. Eisenbach, M. Karabin, M. Lupo Pasini and J. Yin, *Statistical Mechanics of Materials using First Principles Calculations and Machine Learning* - Submitted to Smoky Mountains Computational Sciences and Engineering Conference 2022
2022	A. Blanchard, P. Zhang, D. Bhowmik, J. Gounley, S. T. Reeve, S. Irle, M. Lupo Pasini, *Computational workflow for accelerated molecular design using quantum chemical simulations and deep learning models* - Submitted to Smoky Mountains Computational Sciences and Engineering Conference 2022
2022	M. Lupo Pasini, S. Perotto, *Hierarchical model reduction driven by machine learning for parametric advection-diffusion-reaction problems in the presence of noisy data*, Submitted to Journal of Scientific Computing

2022   M. Lupo Pasini, L. Maleniča, K. Chong, S. Slattery, *A deep learning approach for adaptive zoning*, Submitted to Machine Learning with Applications

2022   J. Y. Choi, P. Zhang, K. Mehta, A. Blanchard, M. Lupo Pasini, *Scalable training of graph convolutional neural networks for fast and accurate predictions of HOMO-LUMO gap in molecules*, Journal of Cheminformatics, Vol 14, 70, (2022), https://jcheminf.biomedcentral.com/articles/10.1186/s13321-022-00652-1

2022   M. Lupo Pasini, J. Yin, *Stable parallel training of Wasserstein conditional generative adversarial neural networks*, Journal of Supercomputing, https://link.springer.com/article/10.1007/s11227-022-04721-y

2022   M. Lupo Pasini, P. Zhang, S. T. Reeve, J. Y. Choi, *Multi-task graph neural networks for simultaneous prediction of global and atomic properties in ferromagnetic systems*, Machine Learning: Science and Technology, Vol 3(2), 025007, (2022), https://iopscience.iop.org/article/10.1088/2632-2153/ac6a51

2022   S. Giusepponi, F. Buonocore, M. Celino, M. Lupo Pasini, A. Frattolillo, S. Migliori, *Study of solid molecular deuterium D2 growth under gas pressure*, Fusion Engineering and Design, Vol 182, 113252, https://www.sciencedirect.com/science/article/abs/pii/S0920379622002460

2022   M. Lupo Pasini, J. Yin, V. Reshniak, M. K. Stoyanov, *Anderson acceleration for distributed training of deep learning models*, The IEEE SoutheastCon 2022, IEEE Xplore Conference Proceeding, pp. 289–295 (2022) https://ieeexplore.ieee.org/document/9763953

2022   M. Lupo Pasini, S. Perotto, *Hierarchical model reduction driven by a proper orthogonal decomposition for parametrized advection-diffusion-reaction problems*, Electronic Transactions on Numerical Analysis ETNA, Vol. 55, 187-212, (2022), https://epub.oeaw.ac.at/?arp=0x003d1837

2022   M. Lupo Pasini, M. Burčul, S. T. Reeve, M. Eisenbach, S.Perotto, *Fast and accurate predictions of total energy for solid solution alloys with graph convolutional neural networks*, SMC 2021: Driving Scientific and Engineering Discoveries Through the Integration of Experiment, Big Data, and Modeling and Simulation pp. 79–98, (2022), https://link.springer.com/chapter/10.1007/978-3-030-96498-6_5

2021   M. Lupo Pasini, J. Yin, *Stable parallel training of Wasserstein conditional generative adversarial neural networks*, The 2021 International Conference on Computational Science and Computational Intelligence, IEEE Xplore Conference Proceeding, https://ieeexplore.ieee.org/abstract/document/9799213

2021   M. Lupo Pasini, Y. W. Li, J. Yin, M. Eisenbach, *A scalable algorithm for the optimization of neural network architectures*, Parallel Computing, Vol. 104, 102788, (2021), https://www.sciencedirect.com/science/article/abs/pii/S0167819121000430?via%3Dihub

2021   M. Lupo Pasini, V. Gabbi, J. Yin, S. Perotto, N. Laanait, *Scalable balanced training of conditional generative adversarial neural networks on image data*, Journal of Supercomputing, Vol. 77, pp. 13358-13384, (2021) https://link.springer.com/article/10.1007/s11227-021-03808-2

2020   M. Lupo Pasini, J. L. Fattebert, B. Turcksin, W. Ge, *A parallel strategy for density functional theory computations on accelerated nodes*, Parallel Computing, Vol. 100, 102703, (2020) https://authors.elsevier.com/sd/article/S0167-8191(20)30091-0

2020   M. Lupo Pasini, Y. W. Li, J. Yin, J. Zhang, K. Barros, M. Eisenbach, *Fast and stable deep-learning predictions of material properties for solid solution alloys*, Journal of Physics: Condensed Matter, (2020), https://iopscience.iop.org/article/10.1088/1361-648X/abcb10/meta

2019   M. Lupo Pasini, *Convergence analysis of Anderson-type acceleration of Richardson's iteration*, Numer Linear Algebra Appl. 2019, Vol. 26(4), e2241, (2019). https://onlinelibrary.wiley.com/doi/abs/10.1002/nla.2241

2017   M. Benzi, T. M. Evans, S. P. Hamilton, M. Lupo Pasini, S. R. Slattery, *Analysis of Monte Carlo accelerated iterative methods for sparse linear systems*, Numer Linear Algebra Appl., Vol. 24(3), e2088, (2017). https://onlinelibrary.wiley.com/doi/abs/10.1002/nla.2088

2016   M. Lupo Pasini, R. S. Tuminaro, J. Hu, *Increasing concurrency in two-level Schwarz preconditioners via additive variants*, in Center for Computing Research Summer Proceedings 2016, J.B. Carleton and M.L. Parks, eds., Technical Report SAND2017-1294R, Sandia National Laboratories, pp. 40–52, (2016).

Conference Presentations

2022   S. Reeve, M. Lupo Pasini, P. Laiu, P. Zhang, J. Y. Choi, Y. Yang, D. Shin, D. Lu, *Neural network surrogate predictions with uncertainties for materials science* - Material Science and Technology 2022 (MS&T2022), Pittsburgh, PA (USA), October 9–13

2022   A. E. Blanchard, P. Zhang, K. Mehta, D. Bhowmik, J. Gounley, S. T. Reeve, S. Irle, and M. Lupo Pasini,*Computational Workflow for Accelerated Molecular Design Using Quantum Chemical Simulations and Deep Learning Models* - Smoky Mountains Computational Sciences and Engineering Conference - Virtual Meeting - August 23-25

2022   M. Eisenbach, M. Karabin, M. Lupo Pasini, J. Yin,*Machine Learning for First Principles Calculations of Material Properties for Ferromagnetic Materials* - Smoky Mountains Computational Sciences and Engineering Conference - Virtual Meeting - August 23-25

2022   M. Lupo Pasini, P. Laiu, *Anderson acceleration with approximate least-squares calculations: applications to scientific computing* - A journey in numerical linear algebra: a workshop in honor of Michele Benzi's 60th birthday, Pisa (Italy), June 10–11

2022   M. Lupo Pasini, P. Zhang, S. T. Reeve, D. Lu, *Uncertainty-aware predictions of material properties using graph convolutional neural networks* - Artificial for Robust Engineering Systems Workshop, Oak Ridge, TN (USA), April 26–18

2022   D. Shin, P. Laiu, Y. Yang, S. T. Reeve, J. Y. Choi, M. Lupo Pasini, *A deep learning approach for prediction of thermodynamic properties of solid solution alloys* - Artificial Intelligence in Materials and Manufacturing (AIM) 2022, Pittsburgh, PA (USA), April 3–6

2022   K. Chong, S. Slatter, L. Maleniča, M. Lupo Pasini, *High performant portable r-adaptive particle in cell method with monotonic reconstruction remapping* - SIAM Conference on Parallel Processing for Scientific Computing 2022, Seattle, Washington (USA), February 23–26

2022   M. Lupo Pasini, P. Zhang, S. T. Reeve, J. Y. Choi, *Fast and accurate predictions of total energy for solid solution alloys with graph convolutional neural networks* - Meeting: 2022 TMS Annual Meeting & Exhibition, Symposium: ICME Case Studies: Successes and Challenges for Generation, Distribution, and Use of Public/Pre-Existing Materials Datasets, - Virtual Meeting - February 27 - March 3rd

2022   P. Zhang, S. T. Reeve, M. Lupo Pasini, J. Y. Choi, *Developing an exascale-capable graph convolutional neural network surrogate for atomic property prediction* - Meeting: 2022 TMS Annual Meeting & Exhibition, Symposium: Algorithm Development in Materials Science and Engineering, - Virtual Meeting - February 27 - March 3rd

2022   M. Lupo Pasini, P. Zhang, S. T. Reeve, J. Y. Choi, *Fast and accurate predictions of material properties from atomic information using graph convolutional neural networks* - 34th Annual CSP Workshop, Recent Developments in Computer Simulation Studies in Condensed Matter Physics February 22 - 25, 2022. Invited by David Landau (Distinguished Prof. at University of Georgia, Athens)

2022   S. Tangirala, M. Lupo Pasini, Y. W. Li, M. Eisenbach, *Neural-network predictive modeling of physical properties in binary magnetic and non-magnetic alloys* - 34th Annual CSP Workshop, Recent Developments in Computer Simulation Studies in Condensed Matter Physics February 22 - 25, 2022. Invited by David Landau (Distinguished Prof. at University of Georgia, Athens)

2021   M. Lupo Pasini, M. Burčul, S. T. Reeve, M. Eisenbach, S.Perotto, *Fast and accurate predictions of total energy for solid solution alloys with graph convolutional neural networks* - Smoky Mountains Computational Sciences and Engineering Conference - Virtual Meeting - October 19

2021   M. Lupo Pasini, M. Burčul, S. T. Reeve, M. Eisenbach, S.Perotto, *Graph convolutional neural networks for fast, accurate prediction of material properties for solid solution alloys* - Congresso Nazionale SIMAI2020 - Parma, Italy, August 30 - September 3

2020   J.-L. Fattebert, B. Turcksin, M. Lupo Pasini, *A parallel strategy for Kohn-Sham solver with GPU-accelerated nodes* - SIAM Conference on Parallel Processing for Scientific Computing 2020, Seattle, Washington (USA), February 12–15

2019   M. Lupo Pasini, J. Zhang, J. Yin, Y. W. Li, M. Eisenbach, *Machine learning assisted Monte Carlo methods for the studies of materials properties* - XXXI IUPAP Conference on Computational Physics (CCP2019) - Los Alamos, NM (USA), July 28 - August 1

2019   M. Lupo Pasini, *Convergence analysis of Anderson-type acceleration of Richardson's iteration* - International Conference On Preconditioning Techniques For Scientific and Industrial Applications 2019 - Minneapolis, Minnesota (USA), July 1-3

2018   M. Lupo Pasini, *Convergence analysis of Anderson-type acceleration of Richardson's iteration* - 15th Copper Mountain Conference on Iterative Methods - Copper Mountain, Colorado (USA), March 25-30

2016   M. Lupo Pasini, *Monte Carlo acceleration of iterative solvers for eigenvalue problems* - 14th Copper Mountain Conference on Iterative Methods - Copper Mountain, Colorado (USA), March 20-25

2016   M. Lupo Pasini, M. Benzi, T. Evans, S. Hamilton, S. Slattery, *Monte Carlo acceleration of iterative solvers for sparse linear systems* - AMS Spring Southeastern Sectional Meeting - Athens, Georgia (USA), March 5-6

2015   M. Lupo Pasini, M. Benzi, T. Evans, S. Hamilton, S. Slattery, *Monte Carlo synthetic acceleration methods for sparse linear systems* - SIAM Conference on Applied Linear Algebra (LA15) - Atlanta, Georgia (USA), October 26-30

2015   M. Lupo Pasini, M. Benzi, T. Evans, S. Hamilton, S. Slattery, *Iterative performance of Monte Carlo linear solver methods* - SIAM Conference on Computational Science and Engineering (CSE15) - Salt Lake City, Utah (USA), March 14-18

Conference Posters

2022   *HydraGNN: Distributed PyTorch Implementation of Multi-headed Graph Convolutional Neural Networks* - ORNL Software and Data Expo - Oak Ridge National laboratory, Oak Ridge, TN (USA), May 10-11

2021   *A deep learning approach for detection and localization of leaf diseases,* - Workshop RAMSES: Reduced order models; Approximation theory; Machine learning; Surrogates, Emulators and Simulators. - SISSA, International School for Advanced Studies, Main Campus, Trieste, Italy December 14-17

2020   *A greedy constructive algorithm for the optimization of neural network architectures* - SIAM Conference on Parallel Processing for Scientific Computing (PP20) - Seattle, WA (USA), February 12-15

2019   *A greedy constructive algorithm for the optimization of neural network architectures* - 7th Annual Oak Ridge Postdoctoral Association Research Symposium - Oak Ridge National Laboratory, Oak Ridge, TN (USA), August 6

2019   *A greedy constructive algorithm for the optimization of neural network architectures* - AI Expo - Oak Ridge National Laboratory, Oak Ridge, TN (USA), July 29

2019   *Multitasking neural networks for first-principles based statistical mechanics of alloys and magnetic systems* - Deep Learning for Science School - Lawrence Berkeley National Laboratory, Berkeley, CA (USA), July 15-19

2019   *Multitasking neural networks for first-principles based statistical mechanics of alloys and magnetic systems* - 2019 OLCF User Meeting- Oak Ridge National Laboratory, Oak Ridge, TN (USA), May 21-23

2019   *Multitasking neural networks for first-principles based statistical mechanics of alloys and magnetic systems* - Computational Data Science Approaches for Materials Conference 2019 - Los Alamos, New Mexico (USA), April 8-10

2018   *Deterministic and stochastic acceleration techniques for Richardson-type iterations* - 2018 - Salishan Conference on High Speed Computing - Gleneden Beach, Oregon (USA), April 23-26

2016   *Monte Carlo accelerated iterative methods for sparse linear systems* - 2016 Georgia Scientific Computing Symposium - Emory University, Atlanta, Georgia (USA), February 20

2015   *HiMOD and HiPOD methods for solving direct and inverse problems in internal fluid dynamics* - 2015 Georgia Scientific Computing Symposium - Georgia Institute of Technology, Atlanta, Georgia (USA), February 28

2015   M. Lupo Pasini, *Implementations of Monte Carlo linear solvers in a GPU environment* - Summer Internship Workshop - Oak Ridge, TN (USA), August 10

Seminars

2023   *HydraGNN: an efficient surrogate model for predictions of material properties from atomic information.* Lawrence Berkeley National Laboratory (LBNL) Seminar Series - Invited by Bert de Jong (leader of the Applied Computing for Scientific Discovery Group)

2022   *HydraGNN: an efficient surrogate model for predictions of material properties from atomic information.* Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA) Seminar Series - Invited by Silvio Migliori (Director of ENEA ICT DIVISION)

2022   *Deep learning for prediction of material properties of solid solution alloys from multiscale information.* Computational Mechanics Seminar Series - Invited by Pablo Seleson (Research Scientist at Oak Ridge National Laboratory)

2019   *Iterative methods for neural networks* – Speaker in the *PostDoc Scientific Computing Group* seminar - Scientific Computing Group, NCCS Division, Oak Ridge National Laboratory, March 27

2017   *Operator splitting techniques for black box multigrid on semi-structured meshes* – Speaker in the *Scientific Computing Group* seminar - Department of Mathematics and Computer Science, Emory University (USA), October 27

2016   *Increasing concurrency in two level Schwarz preconditioners via additive variants* – Speaker in the *Scientific Computing Group* seminar - Department of Mathematics and Computer Science, Emory University (USA), September 23

2016	*Monte Carlo acceleration of iterative solvers for eigenvalue problems* – Speaker in the *Scientific Computing Group* seminar - Department of Mathematics and Computer Science, Emory University (USA), March 18
2015	*Implementation of Monte Carlo linear solvers for GPU architectures* – Speaker in the *Scientific Computing Group* seminar - Department of Mathematics and Computer Science, Emory University (USA), September 11
2015	*Proper orthogonal decomposition for model reduction* – Invited speaker in the seminar section for the master course *Numerical Analysis of Partial Differential Equations II* (Instructor: Prof. Simona Perotto) - Politecnico di Milano (ITA), May 26
2015	*Monte Carlo linear solvers for sparse linear systems* – Speaker in the *Scientific Computing Group* seminar - Department of Mathematics and Computer Science, Emory University (USA), February 11

Software Releases

2022	M. Lupo Pasini, X. Li, *DDADL- Data driven Anderson acceleration, May 2022*
2022	M. Lupo Pasini, V. Gabbi, N. Laanait, D. Muckherjee, V. Starchenko, J. Yin, A. Prokopenko, *DistGANS- Distributed generative adversarial neural networks*, January 2022, https://www.osti.gov/doecode/biblio/68925
2021	M. Lupo Pasini, S. T. Reeve, P. Zhang, J. Y. Choi, *HydraGNN - Distributed PyTorch implementation of multi-headed graph convolutional neural networks*, October 2021 https://www.osti.gov/doecode/biblio/65891
2021	M. Lupo Pasini, V. Reshniak, M. Stoyanov, September 2021, *AADL: Anderson accelerated deep learning*, https://www.osti.gov/doecode/biblio/61115

Dataset Releases

2022	M. Lupo Pasini, P. Yoo, K. Mehta, S. Irle, *GDB-9-Ex: Quantum chemical prediction of UV/Vis absorption spectra for GDB-9 molecules*, November 2022 https://www.osti.gov/dataexplorer/biblio/dataset/1890227
2022	GS Jung, M. Lupo Pasini, S. Irle, *ORNL_AISD_NiNb*, October 2022 https://www.osti.gov/dataexplorer/biblio/dataset/1890159
2021	M. Lupo Pasini, M. Eisenbach, *CuAu binary alloy with 32 atoms - LSMS-3 data*, February 2021 https://www.osti.gov/biblio/1765349
2021	M. Lupo Pasini, M. Eisenbach, *FePt binary alloy with 32 atoms - LSMS-3 data*, February 2021 https://www.osti.gov/biblio/1762742
2021	M. Lupo Pasini, S. T. Reeve, G. Samolyuk, D. Ellis, M. Eisenbach, *FeSi binary alloy electronic structure low-Si dataset (1024 atoms)*, February 2021 https://www.osti.gov/dataexplorer/biblio/dataset/1765080

PhD Thesis

Title	**Deterministic and stochastic acceleration techniques for Richardson-type iterations**
Language	English
Advisor	Professor **Michele Benzi** (Emory University)
Year	2018

https://etd.library.emory.edu/concern/etds/rj430454t?locale=en

Master's Thesis

Title	**Hierarchical model reduction driven by a Proper Orthogonal Decomposition for advection-diffusion-reaction problems**
Language	English
Supervisor	Professor **Simona Perotto** (Politecnico di Milano)
Co-supervisor	Professor **Alessandro Veneziani** (Emory University)
Year	2013

Bachelor's Thesis

Title	**Random variable series and their applications**

Language	Italian
Supervisor	Professor **Marco Fuhrman** (Politecnico di Milano)
Year	2011

Work Experience

Full-Time Employment

November 2019 – present	**Oak Ridge National Laboratory**, *Organization: Computing and Computational Sciences Directorate - Computational Science and Engineering Division*, Scalable Algorithms and Coupled Physics group, **Computational Scientist in Artificial Intelligence**. Supervisor: Matthew T. Bement.

Post Doctorate

July 2018 – present	**Oak Ridge National Laboratory**, *Organization: Computing and Computational Sciences Directorate*, **Post Doctorate Program in Machine Learning**.
Mentor	Dr. **Markus Eisenbach**.
Description	**Machine Learning for Monte Carlo Methods**.

Internships

May–August 2017	**Sandia National Laboratories**, *Organization: Quantitative Modeling & Analysis (8754)*, Student Intern Programs.
Mentor	Dr. **Raymond S. Tuminaro**. **Task description** Development of C++ libraries for linear algebra operations using MPI distributed memory parallelization. Code available at https://github.com/trilinos/Trilinos/tree/develop/packages/muelu/research/max/XpetraSplitting
May–August 2016	**Sandia National Laboratories**, *Organization: Quantitative Modeling & Analysis (8954)*, Student Intern Programs.
Mentors	Drs. **Raymond S. Tuminaro and Jonathan Hu**. **Task description:** Development of C++ libraries for linear algebra operations using MPI distributed memory parallelization. Increased concurrency by reducing computational time up to 50%. Numerical experiments run on NERSC supercomputers Edison and Cori using up to 8,000 MPI processes. Code available at https://github.com/trilinos/Trilinos/tree/develop/packages/muelu/research/max/AdditiveMG **Increasing concurrency in Two-Level Schwarz preconditioners via additive variants**, *Summer Proceedings - Center for Computing Research (CCR)*, August, 2016.
June–August 2015	**Oak Ridge National Laboratory**, *Reactor and Nuclear System Division (RNSD)*. Nuclear Engineering Science Laboratory Synthesis (NESLS) program.
Mentor	Dr. **Steven P. Hamilton**. **Task description** Development of C++ linear algebra libraries with CUDA kernels for GPU acceleration of Monte Carlo applications. Reduced computational time up to 70% with respect to CPU version of the code. Code available at https://github.com/ORNL-CEES/Profugus/commits/adaptive_mc/packages **Implementation of Monte Carlo Linear Solvers in GPU environment**, *Poster session*, August 5, 2015.

Training/Workshops

March – April 2022	**Systems at Scale**, *Organization: Meta (previously known as Facebook AI)*, Invited and organized by Francois Richard (Meta).
July 15 –July 19 2019	**Deep Learning for Science School**, *Organization: Lawrence Berkeley National Laboratory, Berkeley, CA*, Scientific Organizing Committee: Wahid Bhimji (LBL), Ben Brown (LBL), Steve Farrell (LBL), Mustafa Mustafa (LBL), Michela Paganini (FAIR).
July 29 –August 10 2018	**Argonne Training Program on Extreme-Scale Computing**, *Organization: Argonne National Laboratory, Lemont, IL*, Coordinator: Marta Garcia Martinez.

Programmatic Funded Grants

2022 – 2023 **High Performance Computing For Energy Innovation (HPC4EI)**,
Amount: $ 300,000
Proposal code: FP-E-20.2-23777,
Funding agency: US Department of Energy,
Principal Investigators: John Khalil and John Gangloff (Raytheon Technologies Research Center (RTRC)).
Role: Contributor to proposal and research development
Description of the program:
https://hpc4energyinnovation.llnl.gov/
List of funded projects:
https://www.energy.gov/eere/amo/articles/14-projects-receive-42m-high-performance-computing-based-research

2021 **Gateway for Accelerated Innovation in Nuclear (GAIN) Voucher**,
Amount: $ 150,000,
Funding agency: US Department of Energy,
Principal Investigator: Danielle Castley (CEO of BecQ).
Role: Contributor to research development
Description of the program:
https://gain.inl.gov/SitePages/Home.aspx

ORNL - Laboratory Directorate Research Development Funded Grants

2021 – 2023 **Surrogate models for prediction of material properties from multi-scale information - Part of the Artificial Intelligence for Science and Discovery Thrust of the ORNL Artificial Intelligence Initiative**,
Proposal LDRD code: LOIS 10585,
Funding agency: US Department of Energy.
Role: Principal Investigator
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

2020 – 2021 **Scalable stable numerical optimization for artificial intelligence applied to computed tomography**,
Proposal LDRD code: LOIS 10261,
Funding agency: US Department of Energy.
Role: Principal Investigator
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

2020 **Distributed agent-based modeling for sensor-limited data in materials**,
Proposal LDRD code: LOIS 9350,
Funding agency: US Department of Energy.
Role: Principal Investigator
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

2019 **Exascale GPUs based particle in cell solver**,
Proposal LDRD code: LOIS 9791,
Funding agency: US Department of Energy.
Role: Co-PI
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

Node Computational Hours Grants to access Supercomputing Facilities

2023 – 2024 **Oak Ridge Leadership Computing Facility (OLCF) Directorate Discretionary Allocation**,
Amount: 20,000 node hours
Proposal code: LRN026,
Funding agency: US Department of Energy, Granted Access to Summit.
Role: Principal Investigator
Description of the program:
https://www.olcf.ornl.gov/for-users/documents-forms/olcf-directors-discretion-project-application/

2023 – 2024	**National Energy Research Scientific Computing (NERSC) Center - ERCAP (Energy Research Computing Allocations Process)**,

2023 – 2024 **National Energy Research Scientific Computing (NERSC) Center - ERCAP (Energy Research Computing Allocations Process)**,
Amount: unlimited node hours
Proposal code: ERCAP0025216,
Funding agency: Advanced Scientific Computing Research (ASCR) - US Department of Energy, Granted Early Access to Perlmutter.
Role: Principal Investigator
Description of the program:
https://www.nersc.gov/users/accounts/allocations/first-allocation/

2021 – 2022 **National Energy Research Scientific Computing (NERSC) Center - ERCAP (Energy Research Computing Allocations Process)**,
Amount: unlimited node hours
Proposal code: ERCAP0022058,
Funding agency: Advanced Scientific Computing Research (ASCR) - US Department of Energy, Granted Early Access to Perlmutter.
Role: Principal Investigator
Description of the program:
https://www.nersc.gov/users/accounts/allocations/first-allocation/

2021 – 2022 **Oak Ridge Leadership Computing Facility (OLCF) Directorate Discretionary Allocation**,
Amount: 20,000 node hours
Proposal code: MAT250,
Funding agency: US Department of Energy, Granted Access to Summit.
Role: Principal Investigator
Description of the program:
https://www.olcf.ornl.gov/for-users/documents-forms/olcf-directors-discretion-project-application/

2020 – 2021 **Oak Ridge Leadership Computing Facility (OLCF) Directorate Discretionary Allocation**,
Amount: 20,000 node hours
Proposal code: CSC457,
Funding agency: US Department of Energy, Granted Access to Summit.
Role: Principal Investigator
Description of the program:
https://www.olcf.ornl.gov/for-users/documents-forms/olcf-directors-discretion-project-application/

Student Mentoring

Summer 2022 **National Science Foundation (NSF) Mathematical Sciences Graduate Internship (MSGI)**.
Doctorate student: Mashu Gupta, Department of Mathematics,University of Texas at Arlington, Arlington, TX, USA.
Project title: Scalable hyperparameter optimization for neural network architectures
https://public.orau.org/SAWD/NSF-msgi/SitePages/NSFCatalogView.aspx

Spring 2022 – present **Master thesis research**.
Master student: Andrea Consonni, Department of Electronics and Informatics, Politecnico di Milano, Milan, MI, Italy
Master thesis title: Deep learning models for prediction of consumers' satisfaction

Spring – Summer 2022 **National Science Foundation (NSF)**.
Doctorate student: Yuanyuan Zhao, Department of Mathematics, University of Alaska Fairbanks, Fairbanks, AK, USA.
Project title: Solving partial differential equations on graphs by convolutional neural networks
https://public.orau.org/SAWD/NSF-msgi/SitePages/NSFCatalogView.aspx

Fall 2021 – Spring 2022 **Master thesis research**.
Master student: Giuseppe Paolini, Department of Electronics and Informatics, Politecnico di Milano, Milan, MI, Italy
Master thesis title: Artificial intelligence for biomedical high resolution 3D images

Fall 2021 – Spring 2022 **Master thesis research**.
Master student: Davide Calabro', Department of Electronics and Informatics, Politecnico di Milano, Milan, MI, Italy
Master thesis title: A deep learning approach for detection and localization of leaf diseases

Spring 2021 – Fall 2021 **Master thesis research**.
Master student: Evandro Maddes, Department of Electronics and Informatics, Politecnico di Milano, Milan, MI, Italy
Master thesis title: Reinforcement learning for mesh adaptivity

Spring 2021 – Fall 2021	**Project course research.** **Master students: Simona Caputi, Francesco Mantegazza**, Department of mathematics, Politecnico di Milano, Milan, MI, Italy **Project title**: Machine learning driven techniques for hierarchical model reduction
Summer 2021	**National Science Foundation (NSF) Mathematical Sciences Graduate Internship (MSGI).** **Doctorate student: Xingjian Li**, Department of Mathamtics, Emory University, Atlanta, GA, USA. **Project title**: Scalable and communication-avoiding strategies for artificial intelligence and deep learning models https://public.orau.org/SAWD/NSF-msgi/SitePages/NSFCatalogView.aspx
Fall 2020 – Spring 2021	**Master thesis research.** **Master student: Marko Burčul**, Department of Electronics and Informatics, Politecnico di Milano, Milan, MI, Italy **Master thesis title**: A deep learning approach for fast, accurate predictions of material properties for solid solution alloys
Spring-Fall 2020	**Master thesis research.** **Master student: Vittorio Gabbi**, Department of Electronics and Informatics, Politecnico di Milano, Milan, MI, Italy **Master thesis title**: Scalable numerical optimization for distributed multi-agent deep learning
Summer 2020	**Department of Energy Science Undergraduate Laboratory Internships (SULI).** **Undergraduate student: Emmit Benitez**, Department of Physics, Iowa University, Iowa City, IA, USA **Project title**: Accelerated statistical mechanics for the study of material properties via deep learning

Teaching

2019	**Iterative Methods for linear systems (Online lectures)**, *Lecturer.* Lecture 1: https://www.youtube.com/watch?v=UoYrAZ8FVsg Lecture 2: https://www.youtube.com/watch?v=fY3m16QXkMU Complex Systems Spectral Methods, Online Winter School on Spectral Methods for Complex Systems Organizer: Francesco Caravelli (Los Alamos National Laboratory, Los Alamos, NM, USA)
2018	**Math 111 - Calculus 1**, *Instructor.* Mentor: Prof. Bree Ettinger Department of Mathematics and Computer Science, Emory University
2017	**Math 116 - Life Sciences Calculus**, *Teaching assistant.* Instructor: Prof. Dwight Duffus Department of Mathematics and Computer Science, Emory University

Awards

2018	**Schoettle Graduate Student Research Award.** Department of Mathematics and Computer Science, Emory University
2014	**Poster Award**, *Title: "HiMOD and HiPOD methods for solving direct and inverse problems in internal fluid dynamics"*, Authors: M. Aletti, A. Barone, S. Guzzetti, M. Lupo Pasini, S. Perotto and A. Veneziani, 30th International CAE Conference. Pacengo del Garda, Italy, October 27-28

Conferences Attended (without presentations/posters)

2017	SIAM Conference on Computational Science and Engineering - Atlanta, Georgia (USA), February 27-March 3
2016	Georgia Scientific Computing Symposium - Emory University - Atlanta, Georgia (USA), February 20
2015	Georgia Scientific Computing Symposium - Georgia Institute of Technology - Atlanta, Georgia (USA), February 28
2014	SIAM Annual Meeting (AN14) - Chicago, Illinois (USA), July 7-11
2014	13th Copper Mountain Conference on Iterative Methods - Copper Mountain, Colorado (USA), April 6-11
2014	SIAM Conference on Parallel Processing for Scientific Computing (PP2014) - Portland, Oregon (USA), February 18-21

Scientific Affiliations

January 2020 – present	**Institute of Electrical and Electronics Engineers (IEEE).** Position: Member
January 2020 – present	**American Mathematical Society (AMS).** Position: Member

January 2014 – present	**Society for Industrial and Applied Mathematics (SIAM)**. Position: Member
January 2022 – present	**The Minerals, Metals & Materials Society: TMS**. Position: Member
August 2016 – July 2018	**Emory SIAM Student Chapter**. Position: President
August 2015 – August 2016	**Emory SIAM Student Chapter**. Position: Treasurer

Service to Scientific Community

Reviewer for peer-reviewed scientific journals and conferences

2019 – present	**IMA Journal of Numerical Analysis**, *Oxford Academic*, Role: Reviewer.
2019 – present	**Computers and Mathematics with Applications**, *Elsevier*, Role: Reviewer.
2020	**MSML2020 - Mathematical and Scientific Machine Learning Conferences**, *July 15 - July 17, 2020*, Princeton University, Princeton, NJ USA, Role: Reviewer.
2021	**MSML2021 - Mathematical and Scientific Machine Learning Conferences**, *August 16 - 19, 2021*, Virtual Event, Role: Reviewer.
2022	**MSML2022 - Mathematical and Scientific Machine Learning Conferences**, *August 16 - 19, 2021*, Virtual Event, Role: Reviewer.
2021 – present	**Journal of Supercomputing**, *Springer*, Role: Reviewer.
2021 – present	**Linear Algebra and its Applications**, *Elsevier*, Role: Reviewer.
2022 – present	**Parallel Computing**, *Elsevier*, Role: Reviewer.
2022 – present	**Mathematics of Computations**, *American Mathematical Society*, Role: Reviewer.
2022 – present	**Nature Communications**, *Springer*, Role: Reviewer.
2022 – present	**Numerical Algorithms**, *Springer*, Role: Reviewer.
2022 – present	**International Journal of Human-Computer Interaction**, *Taylor & Francis Online*, Role: Reviewer.

Miscellaneous

July 2018 – present	**United Nations**. Volunteered Spanish/English translator
2010 – 2012	**Examiner Assistant**, ***Wall Street Institute***, English School for foreigners. Task: Supervising and giving instructions concerning the exam procedures to the candidates applying for certificate in English communication skills.
2006 – 2013	**Science Study Support**. Task: Volunteer to help middle school, high school and college students in Mathematics and Physics.