Dr. Massimiliano Lupo Pasini

Data Scientist
Oak Ridge National Laboratory
Computational Sciences and Engineering

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massimiliano.lupo.pasini@gmail.com

Citisenzhip: Italian
USA Status: Green Card Holder

Interests

- Artificial Intelligence
- Machine Learning
- Deep Learning
- High-Performance Computing
- Scientific Computing
- Numerical Analysis

Profiles

- Linkedin
- Github
- ORCID
- Google Scholar
- ResearchGate
- DBLP
- OSTI.gov

Biography

Dr. Massimiliano (Max) Lupo Pasini's research focuses on the development of surrogate models and generative models for material sciences, scalable hyper parameter optimization, and numerical methods to accelerate computational physics applications. He obtained his Ph.D. in Applied Mathematics at the Computer Science and Mathematics Department at Emory University in 2018.

Working Experience

Full-Time Employment

2022 – present

R&D Associate
Data Scientist
Oak Ridge National Laboratory, Oak Ridge, TN, USA

Deep Learning | Machine Learning | Numerical Analysis | Generative AI | Materials Science | Computational Chemistry | High-Performance Computing

- (Co)-principal Investigator of multiple externally funded projects under the US Department of Energy (DoE) portfolio
- (Co)-principal Investigator of three projects (with a duration of two years each) internally funded by the ORNL Laboratory Directed Research & Development initiative
  Total budget: $1M/year
  Staffing: 6 technical staff members
  Research accomplishments: developed (1) scalable deep learning models for accelerated training on supercomputing facilities, (2) graph neural network models to accelerate materials science and computational chemistry applications, (3) flexible workflows for active learning methodologies for dynamic data collection and automated execution of experiments
- Peer-reviewer for international scientific journals
- Co-organizer of multi-institutional task forces to promote scientific engagement across the AI community
- Organizer of invited sessions at national and international conferences and workshops
- Co-mentor of 2 master students at international institutes and mentor of 1 graduate intern at ORNL

2019 – 2022

R&D Assistant
Computational Scientist
Oak Ridge National Laboratory

Deep learning | Numerical Linear Algebra | High-Performance Computing

- (Co)-principal Investigator of three projects (with a duration of two years each) internally funded by the ORNL Laboratory Directed Research & Development initiative
  Total budget: $1M/year
  Staffing: 15 technical staff members
  Research accomplishments: developed (1) scalable numerical techniques for accelerated training of deep learnign models, (2) scalable hyperparameter optimization for deep learning, and (3) surrogate models to accelerate computational fluid dynamics applications with compressible fluids
- Peer-reviewer for international scientific journals
- Organizer of invited sessions at national and international conferences and workshops
- Co-mentor of 5 master students at international institutes and mentor of 3 graduate interns at ORNL

Dr. Massimiliano Lupo Pasini

Languages

- Italian ●●●●●
- English ●●●●●
- Spanish ●●●●●
- French ●●●○○

Skills

Programming techniques

- PyTorch [5+ years] ●●●●●
- Tensorflow [5+ years] ●●●●●
- Scikit-learn [5+ years] ●●●●●
- Python [5+ years] ●●●●○
- Matlab [10+ years] ●●●●○
- MPI [10+ years] ●●●●○
- C++ [10+ years] ●●●○○
- C [10+ years] ●●●○○
- OpenMP [10+ years] ●●●○○
- CMake [10+ years] ●●●○○

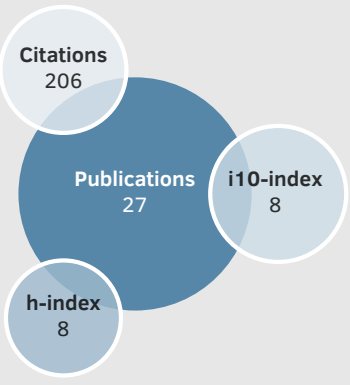
Operative Systems

- UNIX [10+ years] ●●●○○
- Windows [10+ years] ●●●○○

Version Control

- Git [10+ years] ●●●●●

Metrics



Memberships

IEEE	Institute of Electrical and Electronics Engineers
ACM	Association for Computing Machinery
SIAM	Society for Industrial and Applied Mathematics
AMS	American Mathematical Society
APS	American Physical Society
ACS	American Chemical Society
TMS	The Minerals, Metals & Materials Society

Education

Postgraduate Training

2018 – 2019 **Postdoctoral Research Associate** — Oak Ridge National Laboratory, Oak Ridge, TN, USA

Deep Learning | High-Performance Computing | Atomistic Materials Modeling

Mentor: Dr. Markus Eisenbach
Research achievements: Developed deep learning surrogate models for first-principle calculations to predict energetic and electronic structure properties of solid solution alloys using atomic information.

Graduate Training

2017 **Graduate Student Summer Internship** — Sandia National Laboratories, Livermore, CA, USA

Numerical Linear Algebra | High-Performance Computing

Mentor: Dr. Raymond S. Tuminaro
Research achievements: Developed black box multigrid (BoxMG) preconditioners for linear systems arising from the discretization of scalar PDEs on semi-structured meshes using the `MueLu` in the `Trilinos` library.

2016 **Graduate Student Summer Internship** — Sandia National Laboratories, Livermore, CA, USA

Numerical Linear Algebra | High-Performance Computing

Mentors: Dr. Raymond S. Tuminaro and Dr. Jonathan Hu
Research achievements: Developed new implementation of multiplicative two-level Schwarz preconditioners via additive variant to increase concurrency using the `MueLu` in the `Trilinos` library. Reduced computational time to appli the preconditioner by a factor of 2x with respect to standard implementation of multiplicative method using up to 3,000 cores on NERSC supercomputer Cori.

2015 **Graduate Student Summer Internship** — Oak Ridge National Laboratory, Oak Ridge, TN, USA

Numerical Linear Algebra | High-Performance Computing

Mentor: Dr. Steven P. Hamilton
Research achievements: 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.

Study

2014 – 2018 **Ph.D. - Applied Mathematics** — Emory University, Atlanta, GA, USA
Advisor: Prof. Michele Benzi (email: michele.benzi@sns.it)
Research areas: Numerical Linear Algebra, Scientific Computing, Parallel Computing
Dissertation title: *Deterministic and stochastic acceleration techniques for Richardson-type iterations*

2011–2013 **M.S. - Mathematical Engineering** — Polytecnique School, Milan, Italy
Advisor: Prof. Simona Perotto (email: simona.perotto@polimi.it)
Major: Computational Science and Engineering
Minor: Applied Statistics
Dissertation title: *HI-POD: hierarchical model reduction driven by a proper orthogonal decomposition for advection diffusion reaction problems*

2008 – 2011 **B.S. - Mathematical Engineering** — Polytecnique School, Milan, Italy
Advisor: Prof. Marco Fuhrman
Major: Numerical Analysis
Minor: Applied Statistics
Dissertation title: *Random variable series and their applications*

Publications

Peer-Reviewed Journals

2024 **M. Lupo Pasini, M. P. Laiu**
Anderson acceleration with approximate calculations: Applications to scientific computing
Numerical Linear Algebra with Applications, Vol XX, Article Number XXXXX
https://onlinelibrary.wiley.com/doi/full/10.1002/nla.2562

2024 **M. Lupo Pasini, M. Karabin, M. Eisenbach**
Transferring predictions of formation energy across lattices of increasing size
Machine Learning: Science and Technology, Vol 5, Art 025015
https://iopscience.iop.org/article/10.1088/2632-2153/ad3d2c/meta

2023 **P. Yoo, D. Bhowmik, K. Mehta, P. Zhang, F. Liu, M. Lupo Pasini, S. Irle**
Deep learning workflow for the inverse design of molecules with specific optoelectronic properties
Scientific Reports, Vol 13, Article Number 20031
https://www.nature.com/articles/s41598-023-45385-9

2023 **M. Lupo Pasini, K. Mehta, P. Yoo, S. Irle**
Two excited-state datasets for quantum chemical UV-vis spectra of organic molecules
Nature Scientific Data, Vol 10, 546
https://www.nature.com/articles/s41597-023-02408-4

2023 **M. Lupo Pasini, G. S. Jung, S. Irle**
Graph Neural Networks Predict Energetic and Mechanical Properties for Models of Solid Solution Metal Alloy Phases
Computational Materials Science, Vol 224, Art 112141
https://www.sciencedirect.com/science/article/pii/S0927025623001350

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
Journal of Scientific Computing, Vol 94, Art 36
https://link.springer.com/article/10.1007/s10915-022-02073-6

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, Art 70
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, Vol 79, pp. 1856–1876
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), Art 025007
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, Art 113252
https://www.sciencedirect.com/science/article/abs/pii/S0920379622002460

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, pp. 187–212
https://epub.oeaw.ac.at/?arp=0x003d1837

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, Art 102788
https://www.sciencedirect.com/science/article/abs/pii/S0167819121000430?via%3Dihub

Peer-Reviewed Journals (continued)

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
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, Art 102703
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, Vol 33, Art 084005
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
Numerical Linear Algebra with Applications, Vol 26(4), Art e2241
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
Numerical Linear Algebra with Applications, Vol 24(3), Art e2088
https://onlinelibrary.wiley.com/doi/abs/10.1002/nla.2088

Conference Proceedings

2024 **J. Bae, Jong Youl Choi, M. Lupo Pasini, K. Mehta, K. Z. Ibrahim**
MDLoader: A Hybrid Model-driven Data Loader for Distributed Deep Neural Networks Training
2024 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), 27–31 May 2024, San Francisco, CA, USA
https://ieeexplore.ieee.org/abstract/document/10596438

2024 **K. Mehta, M. Lupo Pasini, S. Irle, P. Yoo, F. Suter, D. Ganyushin, S. Klasky**
Scaling Ensembles of Data-Intensive Quantum Chemical Calculations for Millions of Molecules
2024 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), 27–31 May 2024, San Francisco, CA, USA
https://ieeexplore.ieee.org/abstract/document/10596368

2023 **J. Y. Choi, M. Lupo Pasini, P. Zhang, K. Mehta, F. Liu, J. Bae, K. Ibrahim**
DDStore: Distributed Data Store for Scalable Training of Graph Neural Networks on Large Atomistic Modeling Datasets
SC-W '23: Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis, November 2023, Vol 1690, Pages 941–950,
https://doi.org/10.1145/3624062.3624171

2023 **M. Eisenbach, M. Karabin, M. Lupo Pasini and J. Yin**
Machine Learning for First Principles Calculations of Material Properties for Ferromagnetic Materials
Smoky Mountains Computational Sciences and Engineering Conference 2022: Accelerating Science and Engineering Discoveries Through Integrated Research Infrastructure for Experiment, Big Data, Modeling and Simulation. Communications in Computer and Information Science, Vol 1690
https://link.springer.com/chapter/10.1007/978-3-031-23606-8_5

2023 **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
Smoky Mountains Computational Sciences and Engineering Conference 2022: Accelerating Science and Engineering Discoveries Through Integrated Research Infrastructure for Experiment, Big Data, Modeling and Simulation. Communications in Computer and Information Science, Vol 1690
hhttps://link.springer.com/chapter/10.1007/978-3-031-23606-8_1

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
https://ieeexplore.ieee.org/document/9763953

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
Smoky Mountains Computational Sciences and Engineering Conference 2021: Driving Scientific and Engineering Discoveries Through the Integration of Experiment, Big Data, and Modeling and Simulation pp. 79–98
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

Magazines

2024 **M. Lupo Pasini**
A Perspective on Scalable AI on High-Performance Computing and Leadership Class Supercomputing Facilities [Industrial and Governmental Activities]
IEEE Computational Intelligence Magazine, Vol 19, Issue 3, 11 July 2024
https://ieeexplore.ieee.org/abstract/document/10595493

2024 **M. Lupo Pasini**
AI for Materials Design and Discovery Using Atomistic Scale Information [Industrial and Governmental Activities]
IEEE Computational Intelligence Magazine, Vol 19, Issue 2, 5 April 2024
https://ieeexplore.ieee.org/abstract/document/10494027

Summer Internship Proceedings

2016 **M. Lupo Pasini, R. S. Tuminaro, J. Hu**
Increasing concurrency in two-level Schwarz preconditioners via additive variants
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

Awards

2024 **Most Exciting Future Direction Award**
Office of the Laboratory Director's 2024 LDRD Poster Fair, Oak Ridge National Laboratory

2018 **Schoettle Graduate Student Research Award**
Department of Mathematics and Computer Science, Emory University

2014 **Poster Award**
30th International CAE Conference
HiMOD and HiPOD methods for solving direct and inverse problems in internal fluid dynamics
M. Aletti, A. Barone, S. Guzzetti, M. Lupo Pasini, S. Perotto and A. Veneziani

Invited Conference Presentations

2024 **M. Lupo Pasini**
Scalable Graph Neural Networks for Materials Science Applications in the US-DOE Portfolio
Machine Learning and Informatics for Chemistry and Materials, Telluride, CO, USA, October 14–18
https://meetings.telluridescience.org/meetings/workshop-details?wid=1186%20

2024 **M. Lupo Pasini, P. Balaprakash**
Overview of Oak Ridge National Laboratory's AI Initiative: Advancing Secure, Trustworthy, and Energy-Efficient AI at Scale for Scientific Discovery
Parallel Processing Applied Mathematics (PPAM2024), Keynote Speaker, Ostrava, Czech Republic, September 8–11
https://ppam.edu.pl

2024 **M. Lupo Pasini, P. Zhang, J. Y. Choi, G. Samolyuk, M. Eisenbach, Y. Yang**
Accurate extrapolations of atomization energy from binary to ternary solid solution alloys using graph neural networks
9th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS2024), Lisbon, Portugal, June 3–7
https://eccomas2024.org/event/contribution/953a9455-c10c-11ee-8aba-000c29ddfc0c

2024 **J. Y. Choi, J. Bae, M. Lupo Pasini, P. Zhang, K. Mehta, K. Ibrahim**
HydraGNN: Scalable Machine Learning and Generative AI for Accelerating Materials Design
The Platform for Advanced Scientific Computing (PASC2024), Zürich, Switzerland, June 3–5
https://pasc24.pasc-conference.org/presentation/?id=msa123&sess=sess146

2024 **K. Ibrahim, J. Y. Choi, J. Bae, M. Lupo Pasini, P. Zhang, K. Mehta**
Efficient Training of GNN-based Material Science Applications at Scale: An Orchestration of Data Movement Approach
The Platform for Advanced Scientific Computing (PASC2024), Zürich, Switzerland, June 3–5
https://pasc24.pasc-conference.org/presentation/?id=msa231&sess=sess146

2024 **J. Y. Choi, M. Lupo Pasini, P. Zhang, K. Mehta, P. Seleson**
HydraGNN: Scalable Machine Learning and Generative AI for Accelerating Materials Design
Training Program on Deep Learning Systems in Advanced GPU Cyberinfrastructure (DL-GPU 2024), Online, Texas

2023 **M. Lupo Pasini**
Artificial Intelligence for Prediction of Multi-Scale Material Properties
7th Annual Commonwealth Computational Summit, Center for Computational Sciences (CCS) and ITS/Research Computing Infrastructure (ITS/RCI), University of Kentucky, KY (USA), October 16–17

2023 **S .T. Reeve, S. Liu, P. Zhang, M. Lupo Pasini, D. Lu**
Robust graph neural network predictions of formation energy for organic and inorganic compounds using uncertainty quantification
2nd IACM Mechanistic Machine Learning and Digital Engineering for Computational Science Engineering and Technology (MMLDE-CSET 2023), El Paso, TX (USA), September 24–27

2023 **M. Lupo Pasini, G.S. Jung, S. Irle**
Graph neural network predictions of energetic and mechanical properties of solid solution alloys
10th edition of the International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED PROBLEMS 2023), Chania (Crete), June 5–7
https://coupled2023.cimne.com/event/contribution/0f6870f5-ed97-11ed-9a1c-000c29ddfc0c

2023 **M. Lupo Pasini, P. Zhang, J. Y. Choi, S. Irle, Y. Cheng**
Graph neural networks prediction of spectral properties of organic molecules
Math 2 Product (M2P2023), Taormina, Sicily (Italy), May 30 – June 1
https://m2p2023.cimne.com/event/contribution/c23b38d9-ec11-11ed-9a1c-000c29ddfc0c

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, 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 **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**
Graph convolutional neural networks for fast, accurate prediction of material properties for solid solution alloys
Congresso Nazionale SIMAI2020 - Parma, Italy, August 30 - September 3

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

Contributed Conference Presentations

2024 **M. Lupo Pasini**
HydraGNN: Distributed PyTorch-based implementation of multi-tasking graph neural networks for atomistic materials modeling
MaRDA2024 Virtual Annual Meeting – Foundations to Futures: Materials Data and AI, Online, February 20–22

2023 **M. Lupo Pasini, M. Karabin, M. Eisenbach**
Transferable predictions of formation energy across lattices of increasing sizes
34th IUPAP Conference on Computational Physics (CCP2023), Kobe (Japan), August 4–8

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. 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. Slattery, 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 **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

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

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
15^{th} 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
14^{th} Copper Mountain Conference on Iterative Methods - Copper Mountain, Colorado (USA), March 20-25

Conference Posters

2024 **M. Lupo Pasini, J. Y. Choi, K. Mehta, P. Zhang, D. Rogers, J. Bae, K. Z. Ibhrahim, A. Aji, K. W. Schulz, J. Polo, P. Balaprakash**
Scalable, energy-efficient, supervised training of trustworthy graph foundation models for atomistic materials modeling
ORNL Core Universities AI Workshop at North Carolina State University (NCSU) - Raleigh, NC (USA), October 9-10

2023 **M. Lupo Pasini, P. Zhang, J. Y. Choi, K. Mehta, P. Yoo, S. Irle, Y. Cheng**
Graph neural networks prediction of spectral properties of organic molecules
Early Career Poster Session at 2023 Monterey Data Conference - Monterey, CA (USA), August 21-24

2022 **M. Lupo Pasini, P. Zhang, S. T. Reeve, J. Y. Choi**
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 **D. Calabrò, M. Lupo Pasini, S. Perotto**
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 **M. Lupo Pasini, J. Yin, Y. W. Li, M. Eisenbach**
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 **M. Lupo Pasini, J. Yin, Y. W. Li, M. Eisenbach**
A greedy constructive algorithm for the optimization of neural network architectures
7^{th} Annual Oak Ridge Postdoctoral Association Research Symposium - Oak Ridge National Laboratory, Oak Ridge, TN (USA), August 6

2019 **M. Lupo Pasini, J. Yin, Y. W. Li, M. Eisenbach**
A greedy constructive algorithm for the optimization of neural network architectures
AI Expo - Oak Ridge National Laboratory, Oak Ridge, TN (USA), July 29

2019 **M. Lupo Pasini, Y. W. Li, J. Yin, J. Zhang, M. Eisenbach**
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 **M. Lupo Pasini, Y. W. Li, J. Yin, J. Zhang, M. Eisenbach**
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 **M. Lupo Pasini, Y. W. Li, J. Yin, J. Zhang, M. Eisenbach**
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 **M. Lupo Pasini, M. Benzi, T. Evans, S. Slattery, S. Hamilton**
Deterministic and stochastic acceleration techniques for Richardson-type iterations
2018 - Salishan Conference on High Speed Computing - Gleneden Beach, Oregon (USA), April 23-26

2016 **M. Lupo Pasini, M. Benzi, T. Evans, S. Slattery, S. Hamilton**
Monte Carlo accelerated iterative methods for sparse linear systems
2016 Georgia Scientific Computing Symposium - Emory University, Atlanta, Georgia (USA), February 20

2015 **M. Lupo Pasini, S. Perotto**
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

Invited Seminars

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

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

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

2015 **Proper orthogonal decomposition for model reduction**
Invited speaker by Prof. Simona Perotto
Numerical Analysis of Partial Differential Equations II, Politecnico di Milano (ITA), May 26

Presentations

2024 **M. Lupo Pasini**
HydraGNN: a scalable graph neural network architecture for accelerated material discovery and design
Presentation given in occasion of Dr. Charlie McMillan's visit at ORNL - Oak Ridge National Laboratory, June 28

2024 **P. Balaprakash, E. Begoli, M. Lupo Pasini**
ORNL's AI Initiative: Advancing Secure, Trustworthy, and Energy-Efficient AI for Science and National Security
Presentation given in occasion of Oppenheimer Science and Energy Leadership Program (OSELP) - Oak Ridge National Laboratory, January 31

2023 **P. Balaprakash, D. Lu, J. Gounley, D. Lunga, M. Lupo Pasini**
ORNL's AI Initiative: Advancing Science, Security, and Technology Through Secure, Trustworthy, and Energy-Efficient AI
Presentation given in occasion of Dr. Henry McKoy's visit at ORNL - Director, Office of State and Community Energy Programs at US-DoE, November 13

Organized Minisymposia at International Conferences

2024 **M. Lupo Pasini**
MS140: Reduced Order Models and Artificial Intelligence for Industrial Applications
9th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS2024), June 3–7
https://eccomas2024.org/event/session/abf1a491-f81e-11ee-a60e-000c29ddfc0c
https://eccomas2024.org/event/session/fcc5fbf7-f81e-11ee-a60e-000c29ddfc0c

2024 **J. Gounley, M. Lupo Pasini, A. Ghosh**
MS3C: Scalable Machine Learning and Generative AI for Materials Design
The Platform for Advanced Scientific Computing Conference (PASC2024), June 3–5
https://pasc24.pasc-conference.org/presentation/?id=msa231&sess=sess146

2023 **M. Lupo Pasini**
IS05: Artificial Intelligence For Scientific Discovery
10th International Conference of Computational Methods for Coupled Problems in Science and Engineering (COUPLED2023), June 5–7
https://coupled2023.cimne.com/event/area/d3d94875-2df5-11ed-8e5b-000c29ddfc0c

2023 **M. Lupo Pasini**
IS13: Physics informed machine learning for scientific applications
1st International Conference of Math 2 Product (M2P) Emerging Technologies in Computational Science for Industry, Sustainability and Innovation, May 30th – June 1st
https://m2p2023.cimne.com/event/area/786dae44-4df0-11ed-9b3c-000c29ddfc0c

2021 **M. Lupo Pasini**
Physics informed machine learning for scientific applications
9th International Conference on Coupled Problems in Science and Engineering (COUPLED 2021) June 13 – 16
https://congress.cimne.com/coupled2021/frontal/Doc/IS/MassimilianoLupoPasini.pdf

Academic Seminars

2019 **Iterative methods for neural networks**
PostDoc Scientific Computing Group
Scientific Computing Group, NCCS Division, Oak Ridge National Laboratory, March 27

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

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

2016 **Monte Carlo acceleration of iterative solvers for eigenvalue problems**
Scientific Computing Group
Department of Mathematics and Computer Science, Emory University (USA), March 18

2015 **Implementation of Monte Carlo linear solvers for GPU architectures**
Scientific Computing Group
Department of Mathematics and Computer Science, Emory University (USA), September 11

2015 **Monte Carlo linear solvers for sparse linear systems**
Speaker in the Scientific Computing Group
Department of Mathematics and Computer Science, Emory University (USA), February 11

Software Releases

2024 **J. Y. Choi, M. Lupo Pasini, K. Mehta, P. Zhang, K. Ibrahim, J. Bae**
DDStore
February 2024, https://www.osti.gov/biblio/2305283

2024 **M. Lupo Pasini, J. Y. Choi, P. Zhang, J. Baker**
HydraGNN v3.0 - Distributed PyTorch implementation of multi-headed graph convolutional neural networks
February 2024, https://www.osti.gov/biblio/2283293

2023 **A. Cheniour, I. Greenquist, M. Lupo Pasini**
MOOSE-Python Binder
September 2023, https://www.osti.gov/biblio/2006611

2023 **M. Lupo Pasini, P. Zhang, J. Y. Choi, S. T. Reeve**
HydraGNN v2.0 - Distributed PyTorch implementation of multi-headed graph convolutional neural networks
May 2023, https://www.osti.gov/doecode/biblio/105706

2022 **M. Lupo Pasini, X. Li**
DDADL- Data driven Anderson acceleration
May 2022

2021 **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**
AADL: Anderson accelerated deep learning
September 2021, https://www.osti.gov/doecode/biblio/61115

Dataset Releases

2024 **K. Mehta, M. Lupo Pasini, S. Irle, P. Yoo, D. Ganyushin**
GDB-9-Ex_EOM-CCSD: Dataset containing Equation of Motion Coupled Cluster (EOM-CCSD) calculations for organic molecules of the GDB-9-Ex dataset
March 2024 https://www.osti.gov/biblio/2318313

2024 **K. Mehta, M. Lupo Pasini, S. Irle, P. Yoo, D. Ganyushin**
GDB-9-Ex_TD-DFT-PBE0: Dataset containing Time Dependent Density Functional Theory (TDDFT) calculations for organic molecules of the GDB-9-Ex dataset
March 2024 https://www.osti.gov/biblio/2318314

2023 **M. Lupo Pasini, G. Samolyuk, M. Eisenbach, J. Y. Choi, J. Yin, Y. Yang**
TaV_BCC_SolidSolution_128atoms_VASP6
December 2023 https://www.osti.gov/biblio/2222910

2023 **M. Lupo Pasini, G. Samolyuk, M. Eisenbach, J. Y. Choi, J. Yin, Y. Yang**
NbV_BCC_SolidSolution_128atoms_VASP6
December 2023 https://www.osti.gov/biblio/2228839

2023 **M. Lupo Pasini, G. Samolyuk, M. Eisenbach, J. Y. Choi, J. Yin, Y. Yang**
NbTa_BCC_SolidSolution_128atoms_VASP6
December 2023 https://www.osti.gov/biblio/2222906

2023 **M. Lupo Pasini, G. Samolyuk, M. Eisenbach, J. Y. Choi, Y. Yang**
NbTaV_BCC_SolidSolution_128atoms_VASP6
November 2023 https://www.osti.gov/biblio/2217644

2023 **P. Yoo, M. Lupo Pasini, K. Mehta, S. Irle**
Supplementary Material for ORNL_AISD-Ex
June 2023 https://www.osti.gov/biblio/1985737

2023 **P. Yoo, M. Lupo Pasini, K. Mehta, S. Irle**
Supplementary Material for GDB-9-Ex
June 2023 https://www.osti.gov/biblio/1985521

2023 **P. Yoo, S. Irle, M. Lupo Pasini, K. Mehta**
ORNL_AISD_DL-HLgap
March 2023 https://www.osti.gov/dataexplorer/biblio/dataset/1996925

2023 **M. Karabin, M. Lupo Pasini, M. Eisenbach**
ORNL_AISD_NiPt_128atoms
May 2023 https://www.osti.gov/biblio/1972726

2023 **M. Karabin, M. Lupo Pasini, M. Eisenbach**
ORNL_AISD_NiPt
March 2023 https://www.osti.gov/biblio/1958172

2023 **M. Lupo Pasini, P. Yoo, K. Mehta, S. Irle**
ORNL_AISD-Ex: Quantum chemical prediction of UV/Vis absorption spectra for over 10 million organic molecules
January 2023 https://www.osti.gov/biblio/1907919

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

Leadership

2025 **Principal Investigator of LDRD project as part of the ORNL Artificial Intelligence Initiative**
Scalable generative graph foundation models for atomistic materials modeling
Team members: Jong Youl Choi, Kshitij Mehta, Pei Zhang, Zach Fox, Arindam Chowdhury, David Rogers, Junqi Yin, Prasanna Balaprakash

2024 **Principal Investigator of Research Thrust as part of the ORNL Artificial Intelligence Initiative**
Artificial Intelligence for Scientific Discovery and Design (AISD) Thrust
Team members: Stephan Irle, David Rogers, Yingqiang Cheng, German Samolyuk, Ayana Gosh, Kadir Amasyali, Pilsun Yoo, Kshitij Mehta, Paul Laiu, Pei Zhang, Jong Youl Choi, Zach Fox, John Gounley, Nolan English, Junqi Yin

2022 – 2023 **Principal Investigator of LDRD project as part of the Artificial Intelligence for Scientific Discovery and Design (AISD) Thrust within the ORNL Artificial Intelligence Initiative**
Scalable Surrogate Models for Multi-Scale Material Properties
Team members: Pei Zhang, Jong Youl Choi, Paul Laiu, Samuel T. Reeve, Dongwon Shin, Ying Yang, German Samolyuk, Junqi Yin

2021 **Principal Investigator of Research Thrust as part of the ORNL Artificial Intelligence Initiative**
Artificial Intelligence for Scientific Discovery (AISD) Thrust
Team members: Kshitij Mehta, Paul Laiu, Pei Zhang, Jong Youl Choi, Dongwon Shin, Ying Yang, Samuel T. Reeve, Junqi Yin,

2020 **Principal Investigator of LDRD project as part of the ORNL Artificial Intelligence Initiative**
Scalable stable numerical optimization for artificial intelligence applied to computed tomography
Team members: Miroslav Stoyanov, Viktor Reshniak

2019 **Principal Investigator of LDRD project as part of the ORNL Extreme Scale Computing Initiative**
Distributed agent-based modeling for sensor-limited data in materials
Team members: Vitaliy Starchenko, Debangshu Mukherjee, Junqi Yin

Training/Workshops Attended

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

2023 – 2025 **Reliable, Scalable, and Data-efficient Randomized Graph Neural Networks for Neural Combinatorial Optimization with Scientific Applications**
Amount: $ 300,000
Proposal code: DE-SC0023490
Funding agency: US Department of Energy - Advanced Scientific Computing Research (ASCR)
Principal Investigators: Thomas Strohmer (University of California Davis)
Role: Contributor to proposal and research development
Description of the program:
https://science.osti.gov/ascr
List of funded projects:
https://science.osti.gov/-/media/ascr/pdf/awards/ASCR-Randomized-Algorithms-222722-Award-List-2022.pdf

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
Proposal code: NFE-20-08282
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/Nuclear%20Energy%20Vouchers.aspx

ORNL - Laboratory Directorate Research Development Funded Grants

2025 **Scalable generative graph foundation models for atomistic materials modeling**
Proposal LDRD code: LOIS 11874
Funding agency: US Department of Energy
Role: Principal Investigator
Budget: 750,000 USD
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

2023 – 2024 **Artificial Intelligence for Scientific Discovery and Design**
Proposal LDRD code: LOIS 11122
Funding agency: US Department of Energy
Role: Principal Investigator
Budget: 1,650,000 USD
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

2023 – 2024 **Accelerating Microscopy Simulations**
Proposal LDRD code: LOIS 11522
Funding agency: US Department of Energy
Role: Contributor
Budget: 250,000 USD
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

2022 – 2023 **Neural Network Surrogate Model for Radiation Damage in Concrete**
Proposal LDRD code: LOIS 11223
Funding agency: US Department of Energy
Role: Contributor
Budget: 250,000 USD
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

2021 – 2023 **Surrogate models for prediction of material properties from multi-scale information**
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
Budget: 850,000 USD
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
Budget: 250,000 USD
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
Budget: 400,000 USD
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
Budget: 600,000 USD
Description of the program:
https://www.ornl.gov/content/laboratory-directed-research-development/

Node Computational Hours Grants for Supercomputing Facilities

2024 – 2025 **National Energy Research Scientific Computing (NERSC) Center - ERCAP (Energy Research Computing Allocations Process)**
Title: Generative graph-based AI for scalable, accurate, and transferable exploration of large chemical spaces for accelerated alloy design
Amount: 20,000 node hours
Proposal code: ERCAP0030519
Funding agency: Advanced Scientific Computing Research (ASCR) - US Department of Energy
Granted Early Access to NERSC-Perlmutter
Role: Principal Investigator

2024 – 2025 **National Energy Research Scientific Computing (NERSC) Center - ERCAP (Energy Research Computing Allocations Process)**
Title: Accelerated scalable training of physics informed deep learning models for materials science
Amount: 45,000 node hours
Proposal code: ERCAP0027259
Funding agency: Advanced Scientific Computing Research (ASCR) - US Department of Energy
Granted Early Access to NERSC-Perlmutter
Role: Principal Investigator

2024 **Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Allocation**
Title: Scalable Deep Learning for Phonon Contribution in Non-Zero Temperature Alloys
Amount: 500,000 node hours
Proposal code: CPH161
Funding agency: US Department of Energy
Granted Access to OLCF-Frontier
Role: Principal Investigator

2023 – 2024 **Oak Ridge Leadership Computing Facility (OLCF) Directorate Discretionary Allocation**
Title: Scalable accelerated training of physics informed graph convolutional neural networks for material science and chemistry
Amount: 20,000 node hours
Proposal code: LRN026
Funding agency: US Department of Energy
Granted Access to OLCF-Summit
Role: Principal Investigator

2023 – 2024 **National Energy Research Scientific Computing (NERSC) Center - ERCAP (Energy Research Computing Allocations Process)**
Title: Scalable accelerated training of physics informed deep learning models for material science
Amount: 45,000 node hours
Proposal code: ERCAP0025216
Funding agency: Advanced Scientific Computing Research (ASCR) - US Department of Energy
Granted Early Access to NERSC-Perlmutter
Role: Principal Investigator

2022 – 2023 **National Energy Research Scientific Computing (NERSC) Center - ERCAP (Title: Scalable accelerated training of physics informed deep learning models for material science**
Energy Research Computing Allocations Process)
Amount: 10,000 node hours
Proposal code: ERCAP0022058
Funding agency: Advanced Scientific Computing Research (ASCR) - US Department of Energy
Granted Early Access to NESC-Perlmutter
Role: Principal Investigator

2021 – 2022 **Oak Ridge Leadership Computing Facility (OLCF) Directorate Discretionary Allocation**
Title: Scalable accelerated training of physics informed deep learning models for material science
Amount: 20,000 node hours
Proposal code: MAT250
Funding agency: US Department of Energy
Granted Access to OLCF-Summit
Role: Principal Investigator

2020 – 2021 **Oak Ridge Leadership Computing Facility (OLCF) Directorate Discretionary Allocation**
Title: Scalable stable numerical optimization for artificial intelligence
Amount: 20,000 node hours
Proposal code: CSC457
Funding agency: US Department of Energy
Granted Access to OLCF-Summit
Role: Principal Investigator

Research Scientists Mentoring

Fall 2024 – Present **Postdoctoral Research Associate**
Arindam Chowdhury
Computational Sciences and Engineering Division, TN, USA.
Project title: Robust and Scalable Graph Neural Networks for Scientific Computing

Summer 2024 – Spring 2025 **SIAM Postdoctoral Research Fellow**
Nicolas Barnafi
Assistant Professor at Pontificia Universidad Católica de Chile, Santiago, Chile.
Project title: Robust and Scalable Graph Neural Networks for Scientific Computing

Student Mentoring

Summer 2024 – Fall 2024	**ORNL Research Student Internships (RSI)** ***Doctorate student: Rylie Weaver*** *Department of Mathematics, Claremont Graduate University, Claremont, CA, USA.* **Project title**: Invariant and Equivariant Graph Neural Networks for Materials Science
Summer 2024 – Fall 2024	**Graduate Research at ORNL (GRO)** ***Doctorate student: Adithya Raman*** *University of Buffalo, Buffalo, NY, USA.* **Project title**: Energy Profilers for Large-Scale Training of Graph Neural Networks
Summer 2024 – Fall 2024	**Graduate Research at ORNL (GRO)** ***Doctorate student: Chaojian Li*** *Georgia Institute of Technology (GeorgiaTech), Atlanta, GA, USA.* **Project title**: Enabling Large-Scale Foundation Graph Neural Network Training
Summer 2024 – Fall 2024	**Graduate Research at ORNL (GRO)** ***Doctorate student: Julian Barra Otondo*** *University of Massachusetts Lowell (UMass Lowell), Lowell, MA, USA.* **Project title**: Machine Learning Assisted Design of Molten Salts
Summer 2024	**Graduate Research at ORNL (GRO)** ***Doctorate student: Zhifan Ye*** *Georgia Institute of Technology (GeorgiaTech), Atlanta, GA, USA.* **Project title**: Enabling Large-Scale Foundation Graph Neural Network Training
Summer 2024	**Graduate Research at ORNL (GRO)** ***Doctorate student: Erdem Caliskan*** *University of Tennessee-Knoxville, Knoxville, TN, USA.* **Project title**: Fiber composite homogenization using Graph Neural Networks
Summer 2024	**Educational Collaboration at ORNL (ECO)** ***Undegraduate student: Ridhima Singh*** *Massachusetts Institute of Technology (MIT), Cambridge, MA, USA.* **Project title**: Reinforcement Learning for Residential Smart Buildings
Summer 2024	**ORNL Research Student Internships (RSI)** ***Undegraduate student: Pranav Murthy*** *Georgia Institute of Technology (GeorgiaTech), Atlanta, GA, USA.* **Project title**: Physics-Informed Graph Neural Networks for Atomistic Materials Modeling Applications
Summer 2024 – Fall 2024	**Graduate Research at ORNL (GRO)** ***Doctorate student: Arindam Chowdhury*** *Rice University, Austin, TX, USA.* **Project title**: Global Attention Graph Neural Networks for Materials Science
Fall 2023 – Fall 2024	**Master thesis research** ***Master student: Lorenzo Nebolosi***, *Department of Electronics and Informatics, Politecnico di Milano, Milan, MI, Italy* **Master thesis title**:
Summer 2023	**ORNL Graduate Research Student Internships (GRSI)** ***Doctorate student: Justin Baker*** *Department of Mathematics, University of Utah, Salt Lake City, UT, USA.* **Project title**: Equivariant Graph Neural Networks for Materials Science
Spring 2022 – Spring 2023	**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
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 – 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 Mathematics, 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

Tutorials Delivered

2024	**M. Lupo Pasini, J. Y. Choi, P. Zhang, K. Mehta, P. Seleson** *HydraGNN: a scalable graph neural network architecture for material property predictions* ORNL Artificial Intelligence - AI for Science Tutorial Series, Online, 28 March https://ornl.github.io/events/ai-tutorials-series-2024/
2023	**M. Lupo Pasini, J. Y. Choi, P. Zhang** *Scalable Graph Neural Network training using HPC and supercomputing facilities* Learning on Graphs Conference 2023 (LoG2023), Online, 28 November http://log2023.logconference.org

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

Service to Scientific Community

Engagement in scientific associations

January 2024 – present **IEEE Government Task Force**
Position: Vice-President, CIM Columns coordinator and Newsletters coordinator
Government Activities Committee (GAC) - IEEE Computational Intelligence Society (CIS)

July 2023 – January 2024 **IEEE Government Task Force**
Position: CIM Columns coordinator and Newsletters coordinator
Industrial and Government Activities (IGA) - IEEE Computational Intelligence Society (CIS)

August 2016 – July 2018 **Emory SIAM Student Chapter**
Position: President

August 2015 – August 2016 **Emory SIAM Student Chapter**
Position: Treasurer

Reviewer for peer-reviewed scientific journals

2019 – present **IMA Journal of Numerical Analysis**
Oxford Academic
Role: Reviewer

2019 – present **Computers and Mathematics with Applications**
Elsevier
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

2023 – present **Journal of Scientific Computing**
Springer
Role: Reviewer

2023 – present **Scientific Reports**
Springer
Role: Reviewer

2023 – present **Applied Sciences**
MDPI
Role: Reviewer

2023 – present **Mathematical Reviews**
American Mathematical Society
Role: Reviewer

2023 – present **Sustainability**
MDPI
Role: Reviewer

2023 – present **Electronics**
MDPI
Role: Reviewer

2024 – present **Digital Discovery**
Royal Society of Chemistry
Role: Reviewer

2024 – present **International Journal of Mechanical Sciences**
Elsevier
Role: Reviewer

2024 – present **Neural Networks**
Elsevier
Role: Reviewer

2024 – present **Journal of Computational and Applied Mathematics (ELSCAM)**
Elsevier
Role: Reviewer

2024 – present **ournal for Numerical Methods in Engineering (INME)**
Wiley
Role: Reviewer

2024 – present **SIAM Journal of Multiscale Modeling and Simulation (MMS)**
SIAM
Role: Reviewer

2024 – present **SIAM Journal of Scientific Computing (SISC)**
SIAM
Role: Reviewer

2024 – present **SIAM Journal on Matrix Analysis and Applications (SIMAX)**
SIAM
Role: Reviewer

Reviewer for peer-reviewed conferences

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 15 - 17, 2022
Virtual Event
Role: Reviewer

2024 **IEEE SoutheastCon 2024**
March 15 - 17, 2024
IEEE
Role: Reviewer

2024 **ICLR 2024 - Twelfth International Conference on Learning Representations**
May 7 - 11, 2024
AI4DiffEqtnsInSci workshop
Role: Reviewer

Media Exposure

October 2022 **Discover Frontier - YouTube video**
https://www.youtube.com/watch?v=cWnDU8FauqE

October 2022 **Groq Customer Spotlight :: GroqDay - YouTube video**
https://www.youtube.com/watch?v=qBT7Y2wLsqc

November 2023 **Scalable Graph Neural Network training using HPC and supercomputing facilities**
Tutorial delivered at the conference Learning on Graphs 2023 (LoG2023)
YouTube video (tutorial starts at 1:01:00)
https://www.youtube.com/watch?v=U5oHXGcHBdk

December 2023 **Data Curation for the Exascale Era - Quotation cited in OLCF article**
https://www.olcf.ornl.gov/2023/12/11/data-curation-for-the-exascale-era/

December 2023 **ORNL Scientists Generate Molecular Datasets at Extreme Scale - Author of OLCF article**
https://olcf.ornl.gov/2023/12/12/ornl-scientists-generate-molecular-datasets-at-extreme-scale/

Miscellaneous

July 2018 – present **United Nations**
Volunteered Spanish/English translator

2010 – 2012 **Wall Street Institute - English School for foreigners**
Role: Examiner Assistant
Task: Supervising and giving instructions concerning the exam procedures to the candidates applying for certificate in English communication skills.

2006 – 2013 **Private Tutoring**
Task: Volunteer to help middle school, high school, and college students in Mathematics and Physics.

Extra-Curricular Activities

Education Taking virtual private French classes with teacher at Alliance Francaise of Atlanta