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

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 (2023). 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, 112141, Vol 224, (2023). https://www.sciencedirect.com/science/article/pii/S0927025623001350

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, (2023). 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, (2023). hhttps://link.springer.com/chapter/10.1007/978-3-031-23606-8_1

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, 36, (2022). https://link.springer.com/article/10.1007/s10915-022-02073-6

2022   M. Lupo Pasini, L. Malenica, K. Chong, S. Slattery, *A deep learning approach for adaptive zoning*, ArXiv preprint, arXiv:2301.13162, https://arxiv.org/abs/2301.13162, (2022)

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*, 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, (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, Vol 33, 084005, (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

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, 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

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

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

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. 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   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

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* - 7th 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

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

2023   M. Lupo Pasini, P. Zhang, J. Y. Choi, S. T. Reeve, *HydraGNN v2.0 - Distributed Py-Torch implementation of multi-headed graph convolutional neural networks*, October 2021
https://www.osti.gov/doecode/biblio/65891

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

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

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

December 2022 – November 2023
Oak Ridge National Laboratory, *Organization: Computing and Computational Sciences Directorate - Computational Science and Engineering Division*, Computational Coupled Physics group, **Data Scientist**.
Supervisor: Matthew T. Bement.

November 2019 – November 2023
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)**, *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 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

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

July 2023 – present	**Government Task Force (GTF)**, *Industrial and Government Activities (IGA)*, IEEE Computational Intelligence Society (CIS). Position: Member
March 2023 – present	**American Chemical Society (ACS)**. Position: Member

March 2023 – present	**American Physical Society (APS)**. Position: Member
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.
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.

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.