Vivin Vinod

Postdoctoral Research Associate · Computer Science

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Education

Bergische Universität Wuppertal *Wuppertal, Germany*

PhD Computer Science *2023 - 2025*

- *Final Letter Grade: Summa cum laude*
- Develop multifidelity machine learning (MFML) methods to reduce computational cost of training data resulting in high-accuracy low-cost predictions surrogates
- *Research:* Develop multi-fidelity machine learning methods with varying levels of input data precision to reduce data expense and simulation time for quantum chemistry
- *Dissertation:* Multifidelity Machine Learning Methods for Quantum Chemical Properties
- *Supervisor:* Prof. Dr. Peter Zaspel

University of Pisa *Pisa, Italy*

MS Economics *2019 - 2021*

- *Final Score:* 110/110
- *Course (brief):* Advanced statistics, Computational economics, Advanced econometric theory, Advanced microeconometric simulation, Financial Economics, Mathematical Methods for Finance, Small Area Methods for Analysis of Multidimensional Poverty Data (SAMPIEU Chair)
- *Dissertation:* Credit Risk Modeling in Application: Catastrophe Swaps and Deep Learning Approaches
- *Advisor:* Dr. Davide Radi

St. Stephen's College, Delhi University *Delhi, India*

BSc Physics(Hons) *2016 - 2019*

- *CGPA:* 8.2/10.0
- *Minors:* Philosophy, Mathematics
- *Course (brief):* Lab R&D, quantum mechanics, statistical mechanics, electrodynamics, special relativity, advanced mathematical physics, solid state physics
- *Research:* Lennard Jones mono-atomic and diatomic gas simulation, chaotic systems and basin boundaries, Ising model simulation with Metropolis Hastings algorithm and Wolf Cluster algorithm (extended to social dynamics of voter models), Non-relativistic star cluster simulation with collision, Helium atom eigen states using Genetic algorithms, time evolution of plucked string and struck sheet, chaos as secure channel for communication using Chua's circuit

Certificates

Academic Development

- IOP Trusted Reviewer - *'Outstanding review exceptionally detailed and adds valuable insight when informing decision.'* (2024)
- IBM Data Science Course - 96.4% - November 13, 2019 2:04 PM GMT
- Astrobiology capsule course - Grade A - conducted by United Nations & Indian Astrobiological Research Centre (2016)

Professional Experience

Jun 2025-present **Postdoctoral Research Associate**, Bergische Universität Wuppertal, Germany

Further research in the field of multifidelity machine learning methods for quantum chemical properties. Diversified focus on the application of multifidelity methods in fields ranging from non-adiabatic chemistry to engineering.

Jan 2026 - Mar 2026 **Visiting Researcher**, Hausdorff Research Institute for Mathematics, University of Bonn, Germany

As part of Winter School 'Bridging multiscale, limited information, and low regularity in computational mathematics'.

Apr 2026 - May 2026 **Visiting Researcher**, College of Chemistry and Chemical Engineering, Xiamen University, China

Visiting for academic exchange with Prof. Dr.Pavlo Dral's group in XMU. Work will extend multifidelity methods to neural network architecture and applications coupled with agentic AI modules.

Apr 2025 - Jul 2025 **Teaching Assistant**, Bergische Universität Wuppertal,Germany

TA for mathematical machine learning.

2023 - 2025 **Research Associate**, Bergische Universität Wuppertal, Germany
Continued work under DFG grant for machine learning simulation of large-scale molecular systems. Developed multifidelity methods for machine learning with applications in quantum chemistry. Generated multi-fidelity data for benchmarking of machine learning models. Extended methodology of multi-fidelity methods in addition to statistical analyses of the method.

2022- 2023 **Research Associate**, Constructor University Bremen gGmbH, Germany
Working under DFG grant for machine learning simulation of 150 million atoms. Implementation of multi-fidelity machine learning models for quantum chemistry under Prof. . Peter Zaspel. Developed interdisciplinary methods for machine learning in quantum chemistry.

Aug 2021 - Nov 2021 **Package Development Intern**, EMOS, INS Spain, and INE Romania

Developed packages with the national institute of statistics in Spain and Romania to analyze synthetic mobile network big-data for population statistics. Presented key findings in the uROS conference 2022.

Jan 2021- Jun 2021 **Junior Research Intern**, National Institute of Statistics, Italy (ISTAT)

Converted satellite orthophotos into a readable format as part of pre-processing metric for subsequent data manipulation. Developed U-NET DL hybrid to produce masks of orthophoto segmentation. Analyzed output in a reproducible manner. Implemented 12 channel satellite image segmentation model for integration with ISTAT policy making sector.

2021 **Graduate Teaching Assistant**, Dept. of Economics, University of Pisa
TA for mathematical methods for economics.

Publications

Preprints

V. Vinod, P. Zaspel. LFaB: Low fidelity as Bias for Active Learning in the chemical configuration space. *arXiv*, 10.48550/arXiv.2508.15577, **(2025)**.

Published

V. Vinod. Multifidelity Machine Learning Methods for Quantum Chemical Properties. *Ph.D. Dissertation*, Bergische Universität Wuppertal, 10.25926/BUW/0-851 , **(2025)**.

V. Vinod, P. Zaspel. Investigating Benchmarking data efficiency in Δ-ML and multifidelity models for quantum chemistry. *J. Chem. Phys. 163 (2): 024134*, 10.1063/5.0272457, **(2025)**. [IF - 3.8]

D. Lyu, V. Vinod, M. Holzenkamp, Y. M. Holtkamp, S. Maity, C. R. Salazar, U. Kleinekathöfer, P. Zaspel. Excitation Energy Transfer between Porphyrin Dyes on a Clay Surface: A study employing Multifidelity Machine Learning. *Adv. Theory Simul., e00271*, 10.1002/adts.202500271, **(2025)**. [IF - 2.9]

V. Vinod, P. Zaspel. Investigating Data Hierarchies in Multifidelity Machine Learning for Excitation Energies. *J. Chem. Theory Comput., 21(6), 3077–3091*, 10.1021/acs.jctc.4c01491, **(2025)**. [IF - 6.4]

V. Vinod, D. Lyu, M. Ruth, U. Kleinekathöfer, P. R. Schreiner, P. Zaspel. Predicting Molecular Energies of Small Organic Molecules with Multifidelity Methods. *J. Comput. Chem., 46, e70056.*, 10.1002/jcc.70056, **(2025)**. [IF - 4.8]

V. Vinod, P. Zaspel. QeMFi: A Multifidelity Dataset of Quantum Chemical Properties of Diverse Molecules. *Sci. Data, 12, 202*, 10.1038/s41597-024-04247-3 **(2025)**. [IF - 8.7]

V. Vinod, P. Zaspel. Assessing non-nested configurations of multifidelity machine learning for quantum-chemical properties. *Mach. Learn.: Sci. Technol., 5 045005*, 10.1088/2632-2153/ad7f25 **(2024)**. [IF - 6.4]

V. Vinod, P. Zaspel. [Zenodo dataset]. QeMFi: A Multifidelity Dataset of Quantum Chemical Properties of Diverse Molecules (1.1.0) [Data set]. *Zenodo* 10.5281/zenodo.13925688 **(2024)**.

V. Vinod, U. Kleinekathöfer, P. Zaspel. Optimized Multi-Fidelity Machine Learning for Quantum Chemistry. *Mach. Learn.: Sci. Technol, 5 015054*, 10.1088/2632-2153/ad2cef **(2024)**. [IF - 4.6]

V. Vinod, S. Maity, P. Zaspel, U. Kleinekathöfer. Multi-Fidelity Machine Learning for Excited State Energies of Molecules. *J. Chem. Theory Comput., 19 (21), 7658-7670*. 10.1021/acs.jctc.3c00882 **(2023)**. [IF - 6.4]

V. Vinod. Credit Risk Modeling in Application: Catastrophe Swaps and Deep Learning Approaches. *UNIPI Biblio* **(2021)**.

Awards, Fellowships, & Grants

Jul 2021	**SAMPIEU Award**, Jean Monnet Chair
Dec 2019	**International Student Award**, University of Pisa
Feb 2018	**Meera Memorial Award**, St. Stephen's College, DU
Jul 2017	**College Bursary Grant**, St. Stephen's College, DU

Presentations

** presenting author; + collaborative*

Talks and Posters

Mar 2025. *Optimal Combination and Data Hierarchies in Multifidelity Machine Learning for Quantum Chemistry*. MESIGA25: Numerical Methods in Applied Mathematics, Potsdam, DE.

Jul 2024. *Optimized Multi-Fidelity Machine Learning for Quantum Chemical Properties*. CECAM: Machine Learning of First Principles Observables, Berlin, DE.

Mar 2024. *Optimized Multi-Fidelity Machine Learning for Quantum Chemistry*. Leopoldina Symposium, Halle (Saale), DE.

Feb 2024. *Optimized Multi-Fidelity Machine Learning for Quantum Chemistry*. Young Chemists Summit 2024, Salzburg, AT.

May 2023. *Multi-Fidelity Machine Learning for Excited State Energies*. SIMPLAIX Workshop on "Machine Learning for Multi-scale Molecular Modeling", Heidelberg, DE.

Sep 2022. *Multi-Fidelity Machine Learning for Quantum Chemistry*. Poster: CECAM Flagship School, Paris, FR.

Nov 2021. *Delauney Triangulation for Voronoi Partition for implementation in Simulated Mobile Network Data*. Invited talk: International Conference Use of R in Official Statistics (uRosConf 2021), Bucharest, Romania (Virtual).

Jul 2021. *Living conditions and Poverty in Italy - 2017. Small Area estimation and machine learning methods*. competitive participant (Winner), Erasmus+ & Centro Camilo Dagum & Jean Monnet Chair EU, Pisa, Italy.

Feb 2018. *Chua diode circuit as a secure communication device using chaos theory*. Invited talk: Meera Memorial Paper Presentation, Delhi, India.

Contributed Presentations

L. Dongyu *[+], M. Holzenkamp*[+], and V. Vinod[+]. 2023. *Multifidelity Machine Learning and Active Learning Strategies for Quantum Chemistry*. SPP Annual Meeting, 2023, Halle (Saale), DE.

D. Salgado *[+], M. Necula[+] and B. Oancea[+], S. Barragan[+], and V. Vinod[+]. 2021. *simviz: a package to visualize simulated telecommunication mobile network event data*. uROS Conference 2021, Bucharest, Romania (Virtual).

V. Vinod*[+] and Y. Funk[+]. 2021. *Small area estimation methods for NUTS3 level poverty estimation in Italy*. University of Pisa and Scuola S'ant Anna, Pisa, Italy.

Teaching Experience

Summer 2025	**Mathematical Machine Learning**, Teaching Assistant	*Bergische Universität Wuppertal, Germany*
Winter 2021	**Mathematical methods for economics**, Teaching Assistant	*University of Pisa, Italy*

Research Experience

Institutional Research

Bergische Universität Wuppertal - School of Mathematics and Natural Science *Wuppertal, Germany*

Supervisor: Prof. Dr. P. Zaspel *2023 - 2025*

- Carried forward from Constructor University Bremen due to relocation of supervisor
- Generating multifidelity quantum chemistry datasets on high performance computing clusters.

Constructor University Bremen - Dept of Computer Science *Bremen, Germany*

Supervisor: Prof. Dr. P. Zaspel *2022 - 2023*

- Interdisciplinary field of machine learning for quantum chemistry and molecular biophysics.
- Replace computationally expensive quantum chemistry calculations with generalised and scalable Multi-Fidelity machine learning (MFML) models.
- Simulate 150 million atom Bacterio-Chlorophyll (BChl) Light Harvesting complex (LHC) by focusing on excitonic energy and coupling in the organelle.
- Employ cheap classical molecular dynamics to provide detailed quantum mechanical description of LHCs.
- Reduce amount of expensive data required to train model for excitonic energy prediction.
- Develop MFML models with consistent average accuracy at least equivalent to DFT methods.
- Train MFML model with augmentation to accommodate environments of large complex in a flat membrane and subsequently a full scale chromatophore complex.

INE Spain - Dept of methodology for OS & INS Romania - Dept Innovative tools in OS *Romania*

Supervisors: Dr. D. Salgado & Dr. M. Necula & Dr. B. Oancea & Dr. S. Barragan *Sep 2021 - Jan 2022*

- Voronoi partition analysis for simulated network big data analysis for use in official statistics (OS).
- Develop visualisation packages for `simviz` package in R to be integrated into big data analysis of ground truth network data.
- Voronoi neighbourhood assessment to study nearest antenna connection fallacy in mobile network data analysis. Results show benefit of `simviz` over conventional methods of analysis.

University of Pisa & Scuola S'ant Anna Pisa - Dept of Economics & Management *Pisa, Italy*

Advisor: Dr. D. Radi *Jan 2021 - Jul 2021*

- Thesis: "Credit Risk Modeling in Application: Catastrophe Swaps and Deep Learning Approaches".
- Self organizing maps applied to hands-on approach for study of credit risk defaulting to banks.
- Compound Poisson process modeling of Catastrophe swaps with both ex-ante and loss re-estimation pricing.
- Using U-NET CNN and hybrid deep learning to estimate catastrophe swap prices during loss re-estimation.

National Institute of Statistics - Department of Statistical Production *Rome, Italy*

Supervisors: Dr. C. Guisti, Dr. A. Ferruzza, Dr. L. Constanzo & Dr. S. Mugnoli *Jan 2021 - Jun 2021*

- Projects: Satellite image segmentation to study urbanisation and generate higher level metrics of poverty for policy making.
- Deployed deep U-NET convolutional neural network (CNN) model in interest of 5-fold image segmentation of 12-channel satellite image input.
- Data cleaning and analysis from noisy satellite channels by incorporating multi-channel inputs.
- Test ANN models to predict urbanization as a function of different input variables including foliage cover, buildings, roads, and crop cover change.
- Proposed work on converting .ecw files to python readable formats to assist future development of this branch of work.