Vincenzo Di Florio, PhD

Curriculum vitae

Genova, Italy vincenzo.diflorio@polimi.it / vincenzo.diflorio97@gmail.com

CURRENT POSITION

Post-doctoral Research Fellow at MOX - Modeling and Scientific Computing Jan 2025 – Present
Dipartimento di Matematica, Politecnico di Milano, Italy

ABOUT ME

Physicist and mathematician specializing in numerical methods for molecular simulation and non-equilibrium statistical mechanics. Author of NextGenPB, a parallel finite element PDE solver for the linearized Poisson-Boltzmann equation, built from scratch, with applications to biomolecular free energy calculations and drug discovery workflows. Research combines rigorous mathematical modeling, from first-principles statistical mechanics to data-driven approaches such as PINNs and PGNNs, to develop scalable and accurate tools for biophysics. Further research interests include non-equilibrium molecular dynamics and response theory, with focus on transport phenomena in low-dimensional systems.

EDUCATION

Ph.D, in Pure and Applied Mathematics [EQF 8] 2021-2025
Politecnico di Torino, Turin, Italy
Istituto Italiano di Tecnologia, Genoa, Italy

Research topics: Biomolecular modeling, continuum electrostatics, and the development and customization of protocols and software tools for biological systems
Thesis: Mathematical, Algorithmic and Numerical Solutions to enhance Electrostatic Calculations for Biomolecules in Electrolytic Solutions
Supervisors: Dr. Walter Rocchia, Prof. Lamberto Rondoni

Masters in Physics of Complex Systems [EQF 7] 2019-2021
Università degli studi di Torino, Turin, Italy

GPA: 110/110 cum Laude and Distinction (received from the examination board)
Related coursework: Statistical Physics and Mathematical modelling
Thesis: State equations and order fluctuations in 1D and 3D
Advisor: Prof. Lamberto Rondoni

Bachelor Studies in Physics [EQF 6] 2016-2019
Università degli studi di Trieste, Trieste, Italy

GPA: 110/110 cum Laude
Related coursework: Major in Physics with minor courses in Numerical Analysis and Dynamical Systems
Thesis: Quantum dots for quantum computation
Advisor: Prof. Angelo Bassi

RESEARCH EXPERIENCE

Post-doctoral Research Fellow at Politecnico di Milano Jan 2025 – Present

Milan, Italy

- Developing advanced numerical methods and adaptive mesh refinement strategies for the Poisson-Boltzmann equation, targeting super-resolution accuracy in molecular electrostatics.
- Designing hybrid physics-guided machine learning models (PINNs/PGNNs) to accelerate biomolecular electrostatic potential calculations.
- Contributed talk at SIAM PP26, Berlin (Mar 2026): *NextGenPB – A Modern Parallel Finite Element Solver for the Poisson-Boltzmann Equation*.

Collaboration with IIT Concept Lab Nov 2024 – Dec 2024
Genoa, Italy

- Evaluated and selected the theoretical numerical model for a nonlinear Poisson-Boltzmann solver; conducted mathematical feasibility analysis and benchmarking of candidate discretization strategies.

Internship at City College of New York (CUNY) May 2024 – Aug 2024
New York, USA

- Integrated NextGenPB as the electrostatic solver within the MCCE multi-conformation continuum electrostatics workflow for biomolecular free energy calculations.
- Developed and validated a benchmark pipeline for pK_a prediction, comparing physics-based electrostatic results against experimental reference data for a set of proteins.

Internship at SISSA Sep 2018 – Dec 2018
Trieste, Italy

- Applied sparse regression methods (SINDy framework) to identify governing equations of dynamical systems from time-series data.

PUBLICATIONS

Journal Articles

- Carbone, D., **Di Florio, V.**, Lepri, S., & Rondoni, L. (2026). *Computing nonequilibrium transport from short-time transients: From Lorentz gas to heat conduction in one-dimensional chains*. The Journal of Chemical Physics, 164(10), 104108. DOI: 10.1063/5.0320325.
- Mazzeo, M. D., **Di Florio, V.**, Rocchia, W., & Decherchi, S. (2026). *Patch-Based Ray Tracing in NanoShaper Boosts Molecular Surface Computation*. Journal of Chemical Information and Modeling, 66(1), 461–471. DOI: 10.1021/acs.jcim.5c02287.
- **Di Florio, V.**, Ansalone, P., Siryk, S. V., Decherchi, S., De Falco, C., & Rocchia, W. (2025). *NextGenPB: An analytically-enabled super resolution tool for solving the Poisson-Boltzmann equation featuring local (de)refinement*. Computer Physics Communications, 317, 109816. DOI: 10.1016/j.cpc.2025.109816.
- **Di Florio, V.**, Giberti, C., Rondoni, L., & Zhao, H. (2024). *Microscopic state equation for oscillator chains*. The European Physical Journal Plus, 139(7), 622. DOI: 10.1140/epjp/s13360-024-05419-1.
- Rondoni, L., & **Di Florio, V.** (2024). *Probability Turns Material: The Boltzmann Equation*. Entropy, 26(2), 171. DOI: 10.3390/e26020171.

PRESENTATIONS

Contributed talk

- *"NextGenPB: A Modern Parallel Finite Element Solver for the Poisson-Boltzmann Equation"*, SIAM Conference on Parallel Processing for Scientific Computing (PP26), Berlin, Germany (Mar 2026)
- *"State equation for oscillator chain"*, ICIAM 2023, Tokyo, Japan (Aug 2023)

Poster Presentation

- *"Biomolecular Electrostatics applications of the NextGenPB solver"*, Protein Electrostatics 2025, Lisbon, Portugal (June 2025)
- *"NextGenPB: a novel Poisson-Boltzmann Solver leveraging super-resolution and local refinement"*, ACS Fall 2024, Denver, USA (Aug 2024)
- *"Efficient and Scalable implementation of a Linearized Poisson-Boltzmann Solver on Hierarchically refined Cartesian Meshes"*, Protein Electrostatic 2023, Genoa, Italy (June 2023)

SCHOOLS & CONFERENCES

- 50th Summer School on Mathematical Physics, Ravello, Italy (Aug 2025)
- Boltzmann Equation and Irreversibility: after 150 years an evergreen problem, Pisa, Italy (Nov 2022)
- XLVII Summer School on Mathematical Physics, Ravello, Italy (Aug 2022)
- Machine Learning Crash Course 2022, Genova, Italy (June 2022)

TEACHING

Tutor – Methods for environmental engineering Feb 2024 – Apr 2024
Politecnico di Torino, Turin, Italy
Teaching assistant – Calculus 1 Sep 2022 – Jan 2023
Politecnico di Torino, Turin, Italy
Teaching assistant – Physics 1 Mar 2021 – May 2021
Università degli studi di Torino, Turin, Italy

SKILLS

Computational

- **C++**: *Daily user*, focused on numerical methods and scientific code development.
- **Python**: *Daily user*, applied to data analysis, scientific computing, development of interfaces for C++/C codes, and ML model development (PyTorch).
- **MPI / OpenMP**: *Working knowledge*, used for parallelization of scientific computing codes (NextGenPB).
- **OCTAVE/MATLAB**: *Daily user*, applied to numerical methods and code development.
- **BASH**: *Basic knowledge*, used for scripting.

Operating Systems

- **Linux**: *Daily user*.
- **MacOS**: *Daily user*.

Document Creation

- **LaTeX**: *Daily user*.
- **Microsoft Office Suite**: *Intermediate proficiency*.

Languages

- **Italian**: Native speaker.
- **English**: Fluent.