Pietro Novelli

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I am a postdoctoral researcher in the Computational Statistics & Machine Learning (CSML) unit at the Italian Institue of Technology (IIT) in Genova, Italy.

My research focuses on machine learning theory and algorithms, with a particular interest on applications to the physical sciences. My main contributions involve machine learning for dynamical systems, stochastic processes, and atomistic simulations.

In a previous academic life, I got a PhD in theoretical condensed matter physics from the Scuola Normale Superiore, where I studied electronic many-body effects in 2D materials.

Alongside my academic research activities, I contribute to the machine-learning core of Zephyra, a startup developing generative design software for the manufacuring industry.

Research Output

2025

arXiv: *Self-Supervised Evolution Operator Learning for High-Dimensional Dynamical Systems* (Submitted to NeurIPS 2025)

npj Computational Materials: *Fast and Fourier Features for Transfer Learning of Interatomic Potentials*

ICML 2025: *Laplace Transform Based Low-Complexity Learning of Continuous Markov Semigroups*

2024

NeurIPS 2024: *Operator World Models for Reinforcement Learning*

NeurIPS 2024: *Neural Conditional Probability for Inference*

ICML 2024: *Consistent Long-Term Forecasting of Ergodic Dynamical Systems*

L4DC 2024: *Dynamics Harmonic Analysis of Robotic Systems: Application in Data-Driven Koopman Modelling*.

ICLR 2024: *Learning invariant representations of time-homogeneous stochastic dynamical systems*.

ArXiv: *A randomized algorithm to solve reduced rank operator regression* (Submitted to SIMODS).

2023

NeurIPS 2023 - *spotlight* paper (3.06% of all submissions): *Sharp Spectral Rates for Koopman Operator Learning*.

NeurIPS 2023: *Transfer learning for atomistic simulations using GNNs and kernel mean embeddings*.

NeurIPS 2023: *Estimating Koopman operators with sketching to provably learn large scale dynamical systems*.

2022

NeurIPS 2022: *Learning dynamical systems via koopman operator regression in reproducing kernel hilbert spaces*.

NeurIPS 2022 - workshop on ML for physical sciences: *Learning dynamical systems: an example from open quantum system dynamics*.

JCTC: *Characterizing metastable states with the help of machine learning*.

Nano Letters: *Moiré-Induced Transport in CVD-Based Small-Angle Twisted Bilayer Graphene*.

2019-2021

Nature Physics: *Observation of interband collective excitations in twisted bilayer graphene*.

Phys. Rev. B: (Editors' suggestion) *Optical and plasmonic properties of twisted bilayer graphene: Impact of interlayer tunneling asymmetry and ground-state charge inhomogeneity*.

Phys. Rev. Lett.: (Featured in "Physics" & Editors' suggestion) *Failure of conductance quantization in two-dimensional topological insulators due to nonmagnetic impurities*.

Major Collaborations

- **Massimiliano Pontil** (IIT & UCL), ML for dynamical systems and atomistic simulations.
- **Vladimir Kostic** (IIT & U. of Novi Sad), ML for dynamical systems.
- **Michele Parrinello** (IIT), ML for atomistic simulations.
- **Luigi Bonati** (IIT), ML for atomistic simulations.
- **Lorenzo Rosasco** (U. of Genova & MIT), large-scale ML.
- **Carlo Ciliberto** (UCL, UK), Reinforcement Learning & Optimization.
- **Karim Lounici** (Ecole Polytechnique), Statistical learning theory.
- **Marco Polini** (U. of Pisa), Many body theory of 2D materials.

Grants

2025: CINECA Iscra C grant (ERLO) — 80000 Compute Hours on the Leonardo Supercomputer

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2025: Lambda Labs — $1000 in Cloud Credits.

2024: Google Cloud Research Grants — $5000 in Cloud Credits to develop `kooplearn`.

2023: ELISE mobility grant (GA no 951847) — €2500.

Public outreach & awards

- January 2025: I wrote **The Operator Way**, a non-technical blog post describing operator-based methods for dynamical systems.
- December 2023: **Second place at Meta's *Open Catalyst Challenge '23***. The 2023 challenge consisted of finding the global adsorption energy of 200 given adsorbate/catalyst pairs. Invited to present our approach at the *NeurIPS AI for Science Workshop 2023*.
- May 2022: **Invited to the *Theoretical Biophysics Podcast***.
- 2022: Organizer of a **reading group on the book *High-Dimensional Probability*** by Roman Vershynin.
- Jan 2019: **My paper on 2D topological insulators was featured in *Physics Magazine***, an online magazine from the American Physical Society "focusing on results that will change the course of research, inspire a new way of thinking, or spark curiosity".

Talks

- July 2025: **Invited Talk (Novi Sad, Serbia):** Applied Linear Algebra (ALA25) conference
- July 2025: **Invited Talk (Porquerolles, France):** New Trends in Statistical Learning
- June 2025: **Talk at the Machine Learning Group (University of Padua)**
- March 2025: **Talk at DIAG (La Sapienza, Rome)**
- July 2024: **Invited talk (Field Institute, Toronto):** Fourth Symposium on Machine Learning and Dynamical Systems
- June 2024: **Invited junior talk:** International Conference on Statistics and Related Fields in honor of Vladimir Koltchinskii
- January 2024: **Talk at CMAP (École Polytechnique Paris)**
- November 2023: **Talk at Newcastle University**
- April 2023: **Talk at `ultracold` seminar on Quantum Physics and Machine Learning** (Stockholm University)
- November 2022: **Talk at Gatsby Unit (UCL)**
- May 2019: **Contributed talk at the Capri Spring School on Transport in Nanostructures**

Open Source Codes

- `franken`: A Python library to train interatomic potentials via transfer learning and random features.
- `linear-operator-learning`: A Python library for operator learning.
- `kooplearn`: A Python library to learn Koopman operators.
- `pybandstructure` (with I. Torre): A Python package to compute the band structure of periodic Hamiltonians, including tight binding or plane waves models.

Education

Scuola Normale Superiore

PhD in Nanosciences

Nov 2016 — Oct 2020 Pisa, IT

Thesis: Electron-electron interaction effects in the optical and transport properties of 2D

materials beyond graphene.
Honors: summa cum laude

University of Pisa
Master's degree in Theoretical Physics
Sep 2014 — Oct 2016 Pisa, IT

Thesis: Quantum pumping in thermoelectric systems.
Honors: summa cum laude, average grade 29.25/30.

Additional courses & schools

- **Convex optimization**
  (Jul 2020, University of Genoa)
- **RegML2020**
  (Jun 2020, MaLGa center, Genoa)
- **Numerical analysis and Optimization**
  (2019 — 2020, Scuola Normale Superiore, grade 30/30)
- **Spring School on Transport in Nanostructures** - contributed talk
  (May 2019, Capri)
- **Cargése school in 2D materials**
  (Apr 2018, Cargése (FR))
- **Quantum information I & II**
  (2016 — 2017, Scuola Normale Superiore, grade 28/30)
- **Theory of many body systems**
  (2016 — 2017, Scuola Normale Superiore, grade 30/30)

Mobility

UCL (London, Jun - Jul 2023) Research activity in collaboration with C. Ciliberto. Financed by the ELISE mobility grant (GA no 951847).

ICFO (Barcelona, Feb 2019) Research activity in collaboration with the experimental group of Prof. F.H.Koppens.

Université Paris-Saclay (Paris, Apr 2019) Invited to the "Laboratoire de physique des solides" at the University of Paris Sud for a 1-month research activity in the group of Prof. M.O. Goerbig.