UNIMORE Dipartimento di Scienze Fisiche, Informatiche e Matematiche

UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

CNR NANO MODENA S3

FIM-S3 SEMINAR

Machine learning unleashed: breaking symmetries and conservation laws in foundation models for atomistic simulations

Friday June 27th, 2025 – 10.00 (sharp)

S3 Seminar Room, 3rd Floor, Physics building
Remote link: Teams

Speaker

Filippo BIGI – EPFL, Switzerland

Abstract

Symmetry-conserving machine learning models, while physically principled, often suffer from limited computational efficiency. Here, we investigate symmetry-free approaches from different axes, showing that non-equivariant and non-energy-conserving machine-learned force fields can be used to provide remarkable acceleration of atomistic simulations, while producing correct physical observables. Furthermore, we present both symmetric and symmetry-free approaches for the long-time-step prediction of molecular dynamics simulations. This emerging paradigm, which aims to directly predict future positions and momenta in a simulation, affords an acceleration factor of up to two orders of magnitude compared to machine-learned interatomic potentials, with the potential to dramatically extend the time scales accessible to atomic-scale modeling.

Host: Federico Grasselli

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