MATHEMATICAL SCIENCES

IIT - Physics-informed Machine Learning as a powerful tool for accelerating computations: the electrostatics case

Funded By	FONDAZIONE ISTITUTO ITALIANO DI TECNOLOGIA [P.iva/CF:09198791007]
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Context of the research activity	Physics-informed machine learning (PIML) techniques frame the “learning from examples” paradigm into a set of rules deriving from the solution of differential equations or the satisfaction of physical constraints. This reduces the request for huge amounts of training data and increases the generality of the approach. Combining physical understanding of the problem at hand and adopting the most suitable ML approach for electrostatic structures is the purpose of this project.
Objectives	This project aims at specialising ML tools to electrostatic interactions in order to accelerate the computation in several applications, ranging from classical molecular dynamics (MD) to implicit solvent (IS) models. In the framework of biomolecular interaction calculation, electrostatic and desolvation contributions are of particular importance. They can be computed via explicit solvent MD or via IS models, such as the Poisson-Boltzmann equation (PBE), an elliptic partial differential equation. PBE, indeed, well describes the electrostatics in complex geometries. The behaviour of the solvent, in presence of ions, can be described with different degrees of accuracy, which unavoidably reflect on the computational cost and on the feasibility of treating large systems. Nowadays, these approaches are experiencing a significant resurgence due to the formidable amount and size of structural data that is becoming available thanks to the most modern experimental techniques such as CRYO-EM, which pose significant challenges to explicit solvent modeling. In particular, electrostatics, due to its inherent long-range effects, represents a significant computational challenge. Within this project, we aim at establishing and consolidating new theoretical and simulative approaches where electrostatic calculations are boosted by PIML techniques, also taking advantage of recent mathematical developments in the field of nonequilibrium statistical mechanics, and response theory.
Skills and competencies for the development of	Knowledge of mathematical techniques and physical theories common to bachelor and master programs in mathematics, physics, chemistry and engineering. Some familiarity with programming languages. Knowledge of statistical physics, transport theory, and machine learning techniques is

development of the activity	appreciated.