Istituto Nazionale di Fisica Nucleare
Sezione di Milano Bicocca

Avviso di seminario

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ATOMICALLY DETAILED SIMULATION OF RARE STRUCTURAL REARRANGENTS OF MACROMOLECULES WITH QUANTUM COMPUTERS

Starting from as early as the 70s, simulating rare structural rearrangements of macromolecules with computational methods such as Molecular Dynamics (MD) has been an outstanding problem. Despite many technological and theoretical advancement, simulations still struggle to surpass the millisecond time regime when many key rare events occur. In recent years, the potential utility of Quantum Computers (QC) for a multitude of problems has attracted a lot of attention both academically and from industrial companies.Are today's admittedly suboptimal QCs -or at least the ones in the near future- good enough to help us sample the rare events in molecular systems more efficiently? To answer this question in this talk, I will introduce our newly devised hybrid path-sampling framework that combines a data-driven-based MD with QC (in the form of a quantum annealer). In contrast to the widely used Transition Path Sampling (TPS) approaches, the utilization of a Renormalization Group-based method (borrowed from nuclear physics) and QC enables us to sample transition pathways while reducing to a minimum the correlation between the paths. This allows the algorithm to search significantly different regions of the system's free energy landscape while maintaining a high acceptance rate in the Metropolis criteria. After the introduction, I will explore and demonstrate the robustness of our method by presenting three distinct cases of its application, from a prototypically simple reaction up to a considerably more complex case of protein folding.

Svolgimento Seminario
il giorno 17/03/2025 dalle **14:00** alle **15:30**, presso **U2-5017 (Auletta Seminari Teorici).**

L'invito è esteso a tutto il personale interessato, che è caldamente invitato a partecipare.