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Long-time atomistic simulations with the Parallel Replica Dynamics method[1]

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Molecular Dynamics (MD) — the numerical integration of atomistic equations of motion — is a workhorse of computational materials science. Indeed, MD can in principle be used to obtain any thermodynamic or kinetic quantity, without introducing any approximation or assumptions beyond the adequacy of the interaction potential. It is therefore an extremely powerful and flexible tool to study materials with atomistic spatio-temporal resolution. These enviable qualities however come at a steep computational price, hence limiting the system sizes and simulation times that can be achieved in practice. While the size limitation can be efficiently addressed with massively parallel implementations of MD based on spatial decomposition strategies, allowing for the simulation of trillions of atoms, the same approach usually cannot extend the timescales much beyond microseconds. In this article, we discuss an alternative parallel-in-time approach, the Parallel Replica Dynamics (ParRep) method, that aims at addressing the timescale limitation of MD for systems that evolve through rare state-to-state transitions. We review the formal underpinnings of the method and demonstrate that it can provide arbitrarily accurate results for any definition of the states. When an adequate definition of the states is available, ParRep can simulate trajectories with a parallel speedup approaching the number of replicas used. We demonstrate the usefulness of ParRep by presenting different examples of materials simulations where access to long timescales was essential to access the physical regime of interest and discuss practical considerations that must be addressed to carry out these simulations.

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