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Title: Dinámica Molecular y Browniana: Realidad y perspectivas en paralelización

Abstract:

The biological activy of biological macromolecules is straight forward related with its conformation in solution. So far, di erent experimental techniques have been used to link their conformation and function, such as X-Ray, neutron scattering or NMR technique, among others.

Parallely, during the last decades, with the arising of the computer power, di erent simulation techniques have been developed to study these complicated systems. Thus, two of the most widely used techniques are, the Molecular Dynamics Simulations and Brownian Dynamics Simulation. The first one presents the advantage that provides an insight of the system with atomic detail, but on the other hand, the scale of time simulated is far away from the scale of time required to study properties with biological relevance. Concerning Brownian Dynamics Simulation, this simulation technique is capable to reach longer simulation time, even closer to the scale of time with biological relevance, but on the other hand, the information provide by this technique corresponds to the mesoescale level, loosing in part information at atomic level.

In both cases, Brownian Dynamics Simulation and Molecular Dynamics Simulation, the tra jectory length is the limiting step for studying bigger and more complex systems.

A strategy for avoiding this limiting step is to develop optimized parallel algorithm that permits the study these complex systems.

Here, we shall introduce the actual state of the art of these two techniques, and what are the most relevant challenges that remain to be solved.

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