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Hybrid Particle-Field Coarse-grained models for biological simulations

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Molecular Dynamics (MD) is a powerful computational technique used to understand the physical basis of the structure and function of biological systems.[1] In this context, coarse-grained (CG) models have been successfully applied to a broad range of bio-molecular systems, including the self-assembly of lipids in aqueous solutions. However, many biologically relevant processes occur on timescales that far exceed the timescales of typical MD simulations using CG models. Thanks to an innovative simulation technique, name hybrid particle-field (hPF),[2,3] is possible to study large scale systems beyond what is feasible with traditional MD and CG models.[4] A special class of CG models, developed for the hPF technique, have been successfully used to investigate several problems in biophysics.5–8 The first application of CG hPF models, with parameters for phospholipids only, was published by the Milano group in 2011.[5] Thanks to the speed up of dynamics, due to the hPF approach, the self-diffusion acceleration lead to a fast self-assembly process. The net effect is that the developed CG models can reproduce, via self-assembly, the lamellar and non-lamellar structure phases of many lipids and surfactants.[5–8] Our aim is to highlight recent applications and provide a comprehensive overview of hPF CG models for biological applications.

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Department

Scuola Superiore Meridionale

Primary author(s) : Dr. DE NICOLA, Antonio (Scuola Superiore Meridionale, Universita' di Napoli Federico II)

Presenter(s) : Dr. DE NICOLA, Antonio (Scuola Superiore Meridionale, Universita' di Napoli Federico II)