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ADVANCED COMPUTATIONAL DESCRIPTIONS OF MACROMOLECULAR MATERIALS: FROM THE ATOM TO THE FLOW

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ABSTRACT

Description of macromolecular materials involves numerous computational challenges. Accurate descriptions of such materials need for a **multiscale** description and the definition of pertinent bridges between the different scales. The finest description starts at the atomic level where **quantum mechanics** leads to **molecular dynamics simulations**. The next description scale introduces some molecular simplifications leading to a coarse grained molecular dynamics, the **DPD** being one of such approaches. Other descriptions consider molecules as interacting multi-bead-springs or multi-bead-rods. At this level **Brownian dynamics simulations** are usually employed. However, this level of description requires intensive computation resources with its significant unfavorable impact on the simulation performances (CPU time). For this reasons sometimes **kinetic theory descriptions** are preferred. In that description, the molecular conformation is described from a probability density function whose evolution is governed by the **Fokker-Planck equation**.

This approach, despite its mathematical simplicity, introduces a density function that is defined in a multidimensional space, and then the associated partial differential equations must be solved in a multidimensional domain (some times involving thousands dimensions). In this case classical discretization techniques fail because the number of required degrees of freedom could be higher than 10^{1000} (being the computational availabilities at present of about

10^9). To circumvent the **curse of dimensionality** that these **high-dimensional partial differential equations** induce, **stochastic techniques** have been applied intensively in the last decade. However, the large number of stochastic trajectories needed to reduce the statistical noise has a direct impact on its efficiency. Some improvements have been proposed, the **Brownian Configurations Fields** being one of such approaches. Recently some incipient techniques based on sparse grids or those based on **separated representations** have allowed solving models defined in highly multidimensional spaces.

The coarsest scale in the description of such material is the one related to the macroscopic flow. **Micro-macro** Lagrangian/Eulerian approaches have been intensively applied. Today **meshless approaches** are opening interesting possibilities because its natural Lagrangian character that makes possible simulate flows using the same cloud of nodes that are advected with the material velocity. In this case their coupling with microscopic descriptions becomes simple and natural. **Lattice-Boltzmann** and **particles methods** are being the more and more used.

The main aim of this mini-symposium is to cover the most relevant new and advanced numerical strategies concerning all the keywords lighted above.

Different applicative sectors are involved: medical and pharmaceutical, flows involving nanoparticles (CNT …), colloidal systems, polymer solution and melts, and more in general any nanostructured fluid as the ones usually encountered in food, cosmetic, pharmaceutical, plastic … industrial processes.