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LOCAL STRESS CALCULATIONS: IMPORTANCE OF FORCE DECOMPOSITION

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We present a new methodology [1] to calculate the stress tensor from molecular dynamics (MD) simulations and investigate the non-uniqueness of local stress fields. Although we focus on biomembranes, our methodology is widely applicable.

Statistical mechanics plays a major role in the connection between Newtonian and continuum mechanics. In particular, the theoretical framework developed by Irving and Kirkwood [2] and later improved by Noll [3] and others [4-6], usually referred to as the IKN procedure, provides a definition for the fields in continuum mechanics from the statistical expectation of atomistic properties. MD simulations, due to their ability to extract statistical information from classical trajectories as simulated in a computer, have therefore become an important resource to evaluate the IKN fields.

Focusing on the stress tensor, a crucial step in the IKN procedure is the decomposition of the forces on the atoms into pairwise contributions. However, such decomposition is usually not unique and different decompositions may result in different stress tensors. This non-uniqueness is particularly acute for multibody potentials [6]. Furthermore, most force decompositions lead to non-symmetric stresses that do not satisfy the classical continuum version of conservation of angular momentum. In this case one has to resort to a micropolar theory of the continuum [7] with the introduction of a couple stress, which can also be calculated from MD simulations [5,8]. Only recently have Admal and Tadmor introduced a privileged decomposition, the central force decomposition (CFD), that results in symmetric stresses by construction [6].

A problem regarding the calculation of the stress from MD is the use of constraints, since these are usually employed in MD to accelerate the dynamics, but, up to the knowledge of the authors, they are not included in the classical theories of microscopic stress. This subject has sparkled some controversy. In a recent work [1] we have shown that, due to the invariance of Liouville's equation in the presence of constraints, constraint forces can be included in the IKN procedure as if they were normal forces.

We present a new implementation, based on the GROMACS 4.5.5 package [9] to analyze the local stress. Our implementation (1) systematically treats constraints and (2) considers two different force decompositions, CFD and the Goetz and Lipowsky decomposition (GLD) [10], which has been widely employed in biomembrane calculations.

Our results (1) highlight the lack of uniqueness of local stress measurements, (2) show the non-symmetric nature of GLD even for systems with strong symmetries, such as a lipid bilayer in equilibrium, and (3) emphasize the connection between chemistry (lipid composition) and mechanics (stress state within the membrane). This kind of chemistry-mechanics relations may become important for future engineering in biomembranes and in other fields of material science.

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