Hybrid Molecular Dynamics - hydrodynamics modelling of liquid solutions: whole virus at atomistic resolution

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Our novel methodology for modelling liquid molecular systems at very different space and time scales simultaneously with consistent transition between the scales is described. Regions of atomistic representation of the liquid of arbitrary shape and time evolution coexist with fluctuating hydrodynamics environment which in turn is coupled to macroscopic hydrodynamics at larger scales. In the model, the hydrodynamics description is used as an effective boundary condition to close the molecular dynamics solution without resorting to standard periodic boundary conditions. A nominally two-phase liquid model is considered as a representation of the same chemical substance. The 'phases' are immersed into each other as 'fine grains', the surface tension effects are irrelevant, and both 'phases' simultaneously occupy the same control volume. The partial concentrations of the MD 'phase' and the hydrodynamics 'phase' are equal to s and 1-s, respectively, where s is a parameter of the model $0 \le s \le 1$. s is a user-defined function of space and time which controls how much atomistic information is required in a particular region of the simulation domain. The approach is implemented in a popular Molecular Dynamics package GROMACS.

As an example, a virus PCV2 is modelled at all-atom resolution for the protein shell of the virus, surrounded by a layer of atomistic water (any model of water such as TIP3P, SPC, etc can be used) that gradually changes to hydrodynamic continuum away from the virus. We analyse the connection between the number of ions inside an empty capsid of PCV2 virus and its stability. We compare the crystallographic structures of the capsids with unresolved N-termini and without them at physiological conditions and show that the structure is preserved. We find that the chloride ions play a key role in the stability of the capsid. A low number of chloride ions results in loss of the native icosahedral symmetry, while an optimal number of chloride ions creates a neutralising layer next to the positively charged inner surface of the capsid. Understanding the dependence of the capsid stability on the distribution of the ions will help clarify the details of the viral life cycle that is ultimately connected to the role of packaged viral genome inside the capsid.