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Hybrid Molecular Dynamics/hydrodynamics modelling of liquid solutions of complex molecular systems: 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. The framework is based on the analogy with two-phase hydrodynamics that has been extended to dynamically tracking the feature of interest at all-atom resolution. 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 (Fig. 1). 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 $0 \leq s \leq 1$. 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 (Fig. 1). The approach is implemented in a popular Molecular Dynamics package GROMACS.

As an example, a virus PCV2 is modelled as 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 (Fig. 1). The simulations were performed with the focus on the reconstructed N-terminals of the capsid's proteins inside it that are believed to interact with the DNA, and that are invisible in experiment. We compared the results of two simulations at same conditions: the empty capsid with N-terminals and without them, (Fig. 1). Investigating the effect of the N-terminals on the properties of the capsid we found that they play a key role in the stability of the capsid, their absence leads to the collapse of the capsid, while in their presence the symmetry of the capsid is preserved. Also our simulations have demonstrated that the N-terminals are aligned along the internal wall of the capsid to conserve the space in its centre.

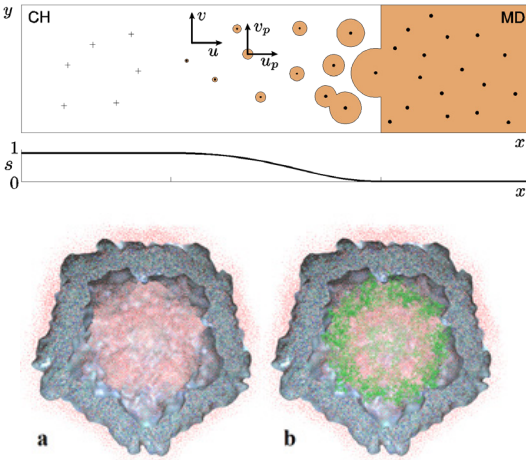

Fig. 1 *Top*: A schematic representation of the hybrid simulation framework; purely MD particles on the right are gradually transformed into passive traces that follow the hydrodynamics flows on the left.

Bottom: All-atom model of a virus capsid without (a) and with (b) internal parts of the proteins invisible in experiment (shown in green); explicit water (red) is also included.

REFERENCES

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