Water flow in nanotubes: hybrid multiscale simulation for future membrane design”
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The transport of liquids through nanotubes is of considerable scientific and technological interest, in particular for selective filtration applications. In membranes of aligned nanotubes, the flow paths may be very long relative to their diameter and this presents challenges to molecular/continuum (MD/CFD) multiscale simulations. In this talk I discuss our new hybrid approach – now available as open source software – that exploits scale separation in space to enable MD/CFD simulations of water flow in carbon nanotubes that have diameters of ~1-2 nm and lengths (i.e. the membrane thickness) some 2-6 orders of magnitude larger. Our results compare well with full MD simulations of flow cases up to a membrane thickness of 150 nm, beyond which any full MD simulation is computationally intractable. We proceed to use the hybrid method to predict the flow in membranes of thicknesses from 150 nm up to 1 mm, and compare these results with available experimental results. The hybrid simulation is orders of magnitude quicker than a full MD simulation would be.