Coarse-graining dynamics by telescoping down time-scales: comment for Faraday FD144

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I briefly review some concepts related to coarse-graining methods for the dynamics of soft matter systems and argue that such schemes will almost always need to telescope down the physical hierarchy of time-scales to a more compressed, but more computationally manageable, separation.

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The question of how to properly coarse-grain a dynamical simulation is a very interesting one. I think there is no single answer, but want to use an example here from our simulations of colloidal hydrodynamics to make some points that I believe are of more general relevance.

Consider a buoyant colloid of mass M_c and a radius $a = 1\mu m$ in H_2O. As described in more detail in [1], its behaviour is governed by a series of different timescales shown in table I. If you are only interested in the behaviour of the colloids, then the two fastest time-scales, the solvent collision time τ_{col} and the solvent relaxation time τ_f, can be ignored as long as they are shorter than any other colloidal time-scales. The first physically relevant time-scale is the Fokker Planck time-scale $\tau_{FP} \approx 10^{-13}$ over which the colloid loses memory of the short-time forces acting on it [2]. For the example colloid, the next time-scale up is the sonic time $t_{cs} \approx 6.7{\times}10^{-10}s$. Then comes the Langevin time $\tau_B \approx 2.2 \times 10^{-7}s$ that measures the exponential decay time of the velocity autocorrelation function within the Langevin approximation. Interestingly, for colloids this time-scale is artificial and does not have direct physical meaning (see appendix of [1]). Next up is the kinematic time $\tau_\nu \approx 10^{-6}s$ over which vorticity diffuses away from the colloid. If your colloid moves a significant fraction of its radius within the time τ_ν, then the colloid will feel the effects of its own motion from a time τ_ν back, and finite Reynolds number (Re) effects start to kick in. For that reason, it needs to be kept small compared to time-scales of colloidal diffusion or advection. The largest time-scale we consider here is the diffusion time $\tau_D \approx 5s$. However, if the colloid also moves under an external force with a velocity v_s, then there is an additional time-scale $t_s = a/v_s$ that measures how long it takes to advect over its radius, and you can then also define a related Peclet number $Pe = t_s/\tau_D$ that measures the relative importance of convection over diffusion.

From the Fokker Planck time on up to the diffusion time covers 13 orders of magnitude. It is clearly not possible to capture all of these in a simulation. Instead, what is needed is time-scale separation. As long as the time-scales are properly separated, you should still be simulating the correct underlying physics. This process can visualized in Figure 1 (taken from ref. [1]) which shows an example of how the hierarchy of time-scales is telescoped down to a more computationally manageable separation in order maximise simulation efficiency, but in such a way that the times are still sufficiently separated to correctly resolve the underlying physical behaviour. A good example of the rationale behind this thinking can be illustrated with the sonic time t_{cs}. Physically it needs to be much smaller than the diffusion time, or else locally you have supersonic behaviour. But if it is too small, the simulation will spend most of its time resolving sound waves that may not be that interesting for the colloidal behaviour you are trying to reproduce, making the simulation very inefficient.

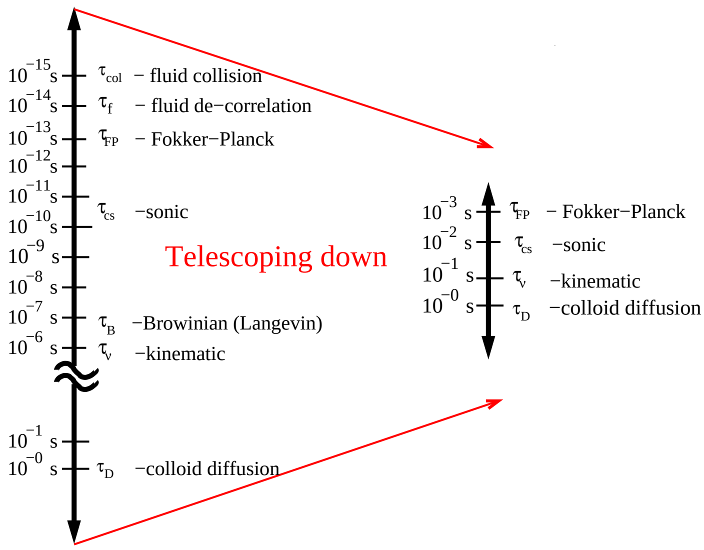

FIG. 1: Telescoping down: The hierarchy of time-scales for a colloid (here the example taken is for a colloid of radius 1 μm in H_20) is compressed in the coarse-grained simulations to a more manageable separation. As long as the physically important times are clearly separated, the simulation should still generate the correct physical picture. Once the simulations are completed, they can be related in more detail to particular experiments by telescoping back out to the relevant experimental time-scales.

In order to correctly interpret the physical meaning of you simulation you need to telescope the time-scale hierarchy back out to the physical one you want to study. For example, if you are interested in physics that is dom-