A Seamless Multiscale Method and Some Applications

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Abstract: In many areas of science and engineering, we face the problem that we are interested in analyzing the macroscale behavior of a given system, but we do not have an explicit and accurate macroscopic model for the macroscale quantities that we are interested in. On the other hand, we do have at our disposal a microscopic model (e.g. molecular dynamics) with satisfactory accuracy - the difficulty being that solving the full microscopic model is far too inefficient.

In this talk, I present a seamless multiscale method, which captures the macroscale behavior of a system with the help of a microscale model. In the seamless algorithm, the micro model supplies the data which is needed but missing in the macro model. The two models evolve simultaneously using their intrinsic time steps, and they exchange data at every time step. We illustrate the multiscale method using two examples. One is modeling complex fluids. In this example, the macroscopic conservation laws for the mass and momentum are coupled with molecular dynamics of polymer chains; the later supplies the stress tensor for the macroscale model. In the second example, we apply the seamless algorithm to compute transition states and minimum free-energy pathways (MFEP) in the space of collective variables. The transition pathways are represented using a string, i.e. a continuous curve parameterized by normalized arc-length. The string is evolved on the free energy landscape according to the steepest descent dynamics (the macro model). The mean force needed to evolve the string is computed on-the-fly from molecular dynamics (the micro model). We apply the algorithm to study conformational changes of alanine dipeptide and wetting transitions on patterned solid surfaces.

References

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