Coarse-graining molecular dynamics

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Models at the molecular scale usually involve a huge number of particles. In many practical situations, the behavior of interest occurs in a very localized region, while the rest of the particles merely act as the surrounding environment. The direct approach of treating these excessive particles explicitly would either introduce finite size effect, or lead to a rather large system, which makes the computation prohibitably expensive. Therefore it is of considerable practical interest to develop an alternative approach in which the effect of these particles is incorporated implicitly.

This talk will present a coarse-graining strategy for molecular dynamics in which the excess degrees of freedom are removed and effective equations are derived for the representative variables. A variational approach to obtain the effective equations will be discussed. Other issues, such as the stability, energy dissipation, sampling the random noise, and application to dynamic fractures will be addressed as well.

References

[1] Li X., E W., *Boundary conditions for molecular dynamics simulations of solids: Treatment of the heat bath*, Phys. Rev. B, vol 76, 2007, 104107.

[2] Li X., E W., *Boundary conditions for molecular dynamics simulations of solids at low temperature*, Comm. Com. Phys., 1 (2006), 136–176.