Generalised Energy-Conserving Dissipative Particle Dynamics: a Coarse-Grain Method to Simulate Complex Fluids Through a Locally Defined Fluctuating Thermodynamics

Josep Avalos [C, S]
Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona, Catalonia, Spain
josep.bonet@urv.cat

Martin Lísal
Department of Molecular and Mesoscopic Modelling, Institute of Chemical Process Fundamentals, Praha, 6, Czech Republic

James P. Larentzos
Weapons and Materials Research Directorate, U.S. Army Combat Capabilities Development Command Army Research Laboratory, Aberdeen, Maryland, U.S.A.

Allan Mackie
Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona, Catalonia, Spain

John K Brennan
Weapons and Materials Research Directorate, U.S. Army Combat Capabilities Development Command Army Research Laboratory, Aberdeen, Maryland, U.S.A.

In a recent article we introduced the so-called Generalised energy-conserving Dissipative Particle Dynamics (GenDPDE) method [1,2]. In this simulation method particles are considered as mesoscopic objects for which one can define a particle thermodynamics. However by construction, the variables defining the particle internal state are fluctuating due to the mesoscopic size of the object. In the original DPDE definition[3], particle thermodynamics was restricted to a linear relation between the stored energy u and the particle temperature τ through $u = CV\,\tau$, where CV is the mesoparticle heat capacity. The force between DPDE particles was a function of the distance only, independent of the temperature. Only with the introduction of the GenDPDE method the particle temperature and interparticle forces are entangled, giving rise to temperature-dependent forces.

Unexpectedly, some fundamental questions about what can be referred to as heat and work in small fluctuating systems have been risen. In this presentation we will show the theoretical implications of the definition of a local thermodynamics for fluctuating systems and its application to the construction of a consistent framework for non-equilibrium simulations of complex systems, as the GenDPDE. We show some applications to prove the internal consistency and capacity of the method to be applied to important problems, e.g., the Chemical Engineering domain.

References

[1] J. B. Avalos, M. Lísal, J. P. Larentzos, A. D. Mackie, and J. K. Brennan, Phys. Chem. Chem. Phys. 21, 24891(2019).

[2] J. B. Avalos, M. Lísal, J. P. Larentzos, A. D. Mackie, and J. K. Brennan (submitted)

[3] J. B. Avalos and A. D. Mackie, Europhys. Lett. 40, 141 (1997).