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CONSISTENT SCALING OF THERMAL FLUCTUATIONS IN DPD/SPH

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ABSTRACT

Dissipative Particle Dynamics (DPD) as originally invented by Hoogerbrugge and Koelman is a stochastic particle model for the simulation of Newtonian fluids at mesoscopic scales [1,2]. In DPD, a Newtonian fluid is represented by a collection of points with prescribed stochastic interactions that conserve momentum and produce hydrodynamic behavior at a coarse-graining level. Moreover, DPD includes thermal fluctuations in a thermodynamically consistent way [2] and it is thus applicable to mesoscopic scales where diffusive processes are important. Since its development, the method has been applied to a wide class of problems and is now emerging as a powerful numerical technique for simulations in the area of micro/nano science.

Despite its recent success, DPD suffers from a number of conceptual shortcomings which can limit its applicability and physical understanding. In particular, they are related to the following issues:

(i) the resulting **equation of state** turns out to be quadratic in density [3];

(ii) no direct connection between the model parameters and the **transport coefficients** of the simulated fluid (kinetic theory or preliminary runs are necessary to measure the transport coefficients);

(iii) unclear definition of the **particle size**.

The second point (ii) is related to the concept of scalability in DPD, that is: physical properties of the system should not depend on the coarse-graining level in which one operates, i.e *transport coefficients* should be *scale invariants*. As it will be discussed during this talk, this can be enforced in DPD only if a proper scaling of the model parameters is adopted producing, however, numerical artifacts (particle freezing) [4].

The third point (iii) represents an additional problem preventing an "*a priori*" control of the spatio-temporal scales simulated. Indeed, due to the lack of a specific physical size associated to the particles, DPD is unable to characterize in a unambiguous way the external lengths of

the problem under study. This is crucial, for instance, in the case of suspended colloidal particles or in microfluidics applications where the physical dimensions of the external objects determine whether and, more importantly, *to which extent* **thermal fluctuations** come into play.

In this talk, we discuss in detail a modified DPD formalism, in the following denoted as Smoothed Dissipative Particle Dynamics (SDPD), recently proposed by Espanol et al. [5]. The new method is able to solve the problems mentioned above and, in addition, it helps to bridge the gap with another particle approach operating at the macroscopic level: Smoothed Particle Hydrodynamics (SPH) which represents a Lagrangian mesh-less discretisation of partial differential equations [6,7].

In SDPD, the volume of a fluid particle is uniquely specified and the size of thermal fluctuations is given by the typical length size of the fluid particle scaled as the the inverse of its square root, in accordance with usual concepts of equilibrium statistical mechanics. Therefore, for large enough fluid particles, the thermal fluctuations in the momentum and energy equation can be neglected. Of course, this is consistent with the fact that in order to simulate a basket ball in a swimming pool we do not introduce thermal fluctuations in the description. On the other hand, if we want to simulate a sub-micron sized colloidal particle in a microfluidics environment we will need to resolve the solvent liquid with fluid particles of at least one order smaller than the diameter of the colloid, which will produce non-vanishing stochastic terms giving rise to its ultimate Brownian diffusive motion. We show that SDPD turns out to be an SPH version in the limit of vanishing fluctuations. The new method deepens therefore the connection between DPD and SPH, extracting the best of both methods (fluctuations from DPD, connection to Navier-Stokes from SPH) and clarifying the link between the concept of fluid particles in DPD/SPH.

In order to show the advantages of the new technique, the simple case of a rigid **colloidal particle** suspended in a Newtonian solvent will be investigated for different particle resolutions (coarse-graining levels). Finally, the results will be discussed in relation to standard DPD.

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