

A compressible fluid particle model based on the Voronoi tessellation

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Based on the geometrical construction of the Voronoi tessellation, we have formulated a Lagrangian fluid particle method. The *fluid particles* are considered as small thermodynamic subsystems defined in terms of the usual extensive variables (mass, internal energy, entropy and volume) as well as its position and velocity [1]. The volume is a dependent variable on the positions of the particles.

The main attractive point of the Voronoi model is the so called thermodynamic consistency [2,3]. It has been built up via the thermodynamic GENERIC formalism (General Equation for Non Equilibrium Reversible Irreversible Coupling) ([1],[2]) that guarantees the First and Second Law of Thermodynamics and offers a clear guide for including correctly thermal fluctuations. The discrete model can be interpreted as a finite volume discretization of the continuum Lagrangian fluctuating hydrodynamics through the Voronoi tessellation, that is thermodynamically consistent. Our present model is the synthesis of a theoretical analysis and a combination of two other Lagrangian techniques for fluids: the Dissipative Particle Dynamics (DPD) and the Smoothed Particle Hydrodynamics (SPH). The different definitions of the fluid volume (soft sphere or Voronoi) and different ways of introducing the fluctuations (pair-wise or a la Landau Lifshitz) with their respective dissipative terms, can give rise to different particle fluid models like SPH and DPD.

Another important point of the Voronoi model is its Lagrangian character (the interacting fluid particles transport the fluid properties as the flow evolves). This is the reason why the method is very flexible for the treatment of boundary conditions in changing geometries, something crucial when dealing with complex fluids. This technique allows to couple the solvent fluid and the suspended microstructure (like colloidal particles or polymers) adapting the moving mesh in a natural way. Some simulation results in two dimensions will be presented.

References

- [1] M. Serrano and P. Español, *Phys. Rev. E* **64**, 046115 (2001).
- [2] P. Español, M. Serrano and H.C. Öttinger, *Phys. Rev. Lett.* **83**, 4542 (1999).
- [3] M. Serrano, G. de Fabritiis, P. Español, E. G. Flekkøy and P. V. Coveney, *J. Phys. A: Math. Gen.* **35**, 1605-1625 (2002).
- [4] M. Grmela and H.C. Öttinger, *Phys. Rev. E* **56**, 6620 (1997).
- [5] H.C. Öttinger and M. Grmela, *Phys. Rev. E* **56**, 6633 (1997).