Efficient Stabilization of Advection Terms Involved in Separated Representations of Boltzmann and Fokker-Planck Equations

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Abstract. The fine description of complex fluids can be carried out by describing the evolution of each individual constituent (e.g. each particle, each macromolecule, etc.). This procedure, despite its conceptual simplicity, involves many numerical issues, the most challenging one being that related to the computing time required to update the system configuration by describing all the interactions between the different individuals. Coarse grained approaches allow alleviating the just referred issue: the system is described by a distribution function providing the fraction of entities that at certain time and position have a particular conformation. Thus, mesoscale models involve many different coordinates, standard space and time, and different conformational coordinates whose number and nature depend on the particular system considered. Balance equation describing the evolution of such distribution function consists of an advection-diffusion partial differential equation defined in a high dimensional space. Standard mesh-based discretization techniques fail at solving high-dimensional models because of the curse of dimensionality. Recently the authors proposed an alternative route based on the use of separated representations. However, until now these approaches were unable to address the case of advection dominated models due to stabilization issues. In this paper this issue is revisited and efficient procedures for stabilizing the advection operators involved in the Boltzmann and Fokker-Planck equation within the PGD framework are proposed.

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1 Introduction

The fine description of the behavior of a system composed by a series of microscopic entities, e.g. particles or molecules dispersed into a solvent, requires the consideration of all the entities as well as taking into account all existing interactions.

Despite the nowadays computational capabilities, the population of particles or macro-molecules in a system of industrial interest is too large to be described in a discrete manner by considering all the involved individuals.

One possibility to reduce the size of the discrete models lies in considering only the particles of interest (that is, the suspended particles or the macromolecules), being the others (solvent particles) taken into account indirectly from their averaged effects on the particles of interest [26].

Thus for example, in the case of suspensions involving small rigid spherical particles, the motion equation of a particle whose position is described by $\mathbf{x}_i(t)$, is given by the Langevin's equation

$$m\frac{d^2\mathbf{x}_i}{dt^2} = \xi\left(\frac{d\mathbf{x}_i}{dt} - \mathbf{V}(\mathbf{x}_i)\right) + \mathbf{F}_i^{ext}(t); \quad \forall i, \tag{1.1}$$

where m denotes the particle mass, $\mathbf{x}_i$ the position of particle i, ξ the friction coefficient, $\mathbf{V}(\mathbf{x}_i)$ the fluid velocity at position $\mathbf{x}_i$ and $\mathbf{F}_i^{ext}(t)$ the other forces acting on particle i (coming from an external potential or from solvent particles bombardment). We can notice that even if this model does not incorporate explicitly the solvent particles population, their effects are taken into account from the drift term $\xi\left(\frac{d\mathbf{x}_i}{dt} - \mathbf{V}(\mathbf{x}_i)\right)$ as well as by the impact forces of stochastic nature included into the term $\mathbf{F}_i^{ext}(t)$.

In the case of inertialess particles this description was traditionally substituted by continuous approaches involving the macroscopic field $C(\mathbf{x},t)$ given the number of particles per unit of volume at position $\mathbf{x}$ and time t. The balance equation results in this case the classical advection-diffusion equation

$$\frac{\partial C}{\partial t} + \mathbf{V}\cdot\nabla C = \nabla\cdot(\mathbf{D}\nabla C) + \mathcal{S}(\mathbf{x},t), \tag{1.2}$$

where the diffusion term involving the diffusivity tensor $\mathbf{D}$ is related to the stochastic interaction effects, $\mathbf{V}$ is the medium velocity and $\mathcal{S}(\mathbf{x},t)$ an eventual source term. Now, standard discretization techniques can be applied for solving the resulting transient 3D advection-diffusion equation (e.g. finite differences or finite elements among many other possibilities). Since the use of discretization techniques applying on the continuous partial differential equation requires the use of a mesh of the domain in which the model is defined, and then the solution of a linear system (many in the case of transient nonlinear models) in order to calculate the solution at any node of the mesh or grid, as soon as the domain becomes too large, the solution of such linear systems can become a real bottleneck. To circumvent this issue an alternative is to come back to the stochastic discrete approach that proceeds by tracking a large enough population of particles, whose path-