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A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modeling of complex fluids

A. Ammar [a,*], B. Mokdad [a], F. Chinesta [b], R. Keunings [c]

[a] *Laboratoire de Rhéologie, INPG, UJF, CNRS (UMR 5520), 1301 rue de la piscine, BP 53 Domaine Universitaire, F-38041 Grenoble Cedex 9, France*
[b] *Laboratoire de Mécanique des Systèmes et des Procédés, UMR 8106 CNRS-ENSAM-ESEM, 151 Boulevard de l'Hôpital, F-75013 Paris, France*
[c] *CESAME, Université Catholique de Louvain, Bat. Euler, Av. Georges Lemaitre 4, B-1348 Louvain-la-Neuve, Belgium*

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Abstract

Kinetic theory models involving the Fokker–Planck equation can be accurately discretized using a mesh support (finite elements, finite differences, finite volumes, spectral techniques, etc.). However, these techniques involve a high number of approximation functions. In the finite element framework, widely used in complex flow simulations, each approximation function is related to a node that defines the associated degree of freedom. When the model involves high dimensional spaces (including physical and conformation spaces and time), standard discretization techniques fail due to an excessive computation time required to perform accurate numerical simulations. One appealing strategy that allows circumventing this limitation is based on the use of reduced approximation basis within an adaptive procedure making use of an efficient separation of variables.

Keywords: Complex fluids; Kinetic theory; Model reduction; Multidimensional problems; Separation of variables; Numerical modeling

1. Introduction

Many natural and synthetic fluids are viscoelastic materials, in the sense that the stress endured by a macroscopic fluid element depends upon the history of the deformation experienced by that element. Notable examples include polymer solutions and melts, liquid crystalline polymers and fibre suspensions. Rheologists thus face a challenging non-linear coupling between flow-induced evolution of molecular configurations, macroscopic rheological response, flow parameters (such as the geometry and boundary conditions) and final properties. Theoretical modeling and methods of computational rheology have an important role to play in elucidating this coupling.

Atomistic modeling is the most detailed level of description that can be applied today in rheological studies, using techniques of non-equilibrium molecular dynamics. Such calculations require enormous computer resources, and they are currently limited to flow geometries of molecular dimensions. Consideration of macroscopic flows found in processing applications calls for less detailed mesoscopic models, such as those of kinetic theory.

Models of kinetic theory provide a coarse-grained description of molecular configurations wherein atomistic processes are ignored. They are meant to display in a more or less accurate fashion the important features that govern the flow-induced evolution of configurations. Over the last few years, different models related to dilute polymers have been evaluated in simple flows by means of stochastic simulation [9] or Brownian dynamics methods.

* Corresponding author. Tel.: +33 4 76 82 52 94; fax: +33 4 76 82 51 64.
E-mail addresses: Amine.Ammar@ujf-grenoble.fr (A. Ammar), Bechir.Mokdad@ujf-grenoble.fr (B. Mokdad), francisco.chinesta@paris.ensam.fr (F. Chinesta), rk@inma.ucl.ac.be (R. Keunings).

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In this context, micro–macro methods of computational rheology that couple the coarse-grained molecular scale of kinetic theory to the macroscopic scale of continuum mechanics have an important role to play (for a review, see [10]). This approach is much more demanding in computer resources than more conventional continuum simulations that integrate a constitutive equation to evaluate the viscoelastic contribution of the stress tensor. On the other hand micro–macro techniques allow the direct use of kinetic theory models and thus avoid the introduction of closure approximations.

Since the early 1990s the field has developed considerably following the introduction of the CONNFFESSIT method by Ottinger and Laso [14]. Being relatively new, micro–macro techniques have been implemented only for models of kinetic theory with few configurational degrees of freedom, such as non-linear dumbbell models of dilute polymer solutions and single-segment tube models of linear entangled polymers.

Kinetic theory provides two basic building blocks: the diffusion or Fokker–Planck equation that governs the evolution of the distribution function (giving the probability distribution of configurations) and an expression relating the viscoelastic stress to the distribution function. The Fokker–Planck equation has the general form

$$\frac{\mathrm{D}\psi}{\mathrm{D}t} + \frac{\partial}{\partial \underline{X}}(\underline{A}\psi) = \frac{1}{2}\frac{\partial}{\partial \underline{X}}\frac{\partial}{\partial \underline{X}} : (\underline{\underline{D}}\psi) \tag{1}$$

where $\mathrm{D}/\mathrm{D}t$ is the material derivative, vector $\underline{X}$ defines the coarse-grained configuration and has dimensions N. Factor $\underline{A}$ is a N-dimensional vector that defines the drift or deterministic component of the molecular model. Finally $\underline{\underline{D}}$ is a symmetric, positive definite $N \times N$ matrix that embodies the diffusive or stochastic component of molecular model. In general both $\underline{A}$ and $\underline{\underline{D}}$ (and in consequence the distribution function ψ) depend on the physical coordinates $\underline{x}$, on the configuration coordinates $\underline{X}$ and on the time t.

The second building block of a kinetic theory model is an expression relating the distribution function and the stress. It takes the form

$$\underline{\underline{\tau}}_p = \int_C \underline{\underline{g}}(\underline{X})\psi \,\mathrm{d}\underline{X} \tag{2}$$

where C represents the configuration space and $\underline{\underline{g}}$ is a model-dependent tensorial function of configuration. In a complex flow, the velocity field is a priori unknown and stress fields are coupled through the conservation laws. In the isothermal and incompressible case the conservation of mass and momentum balance are then expressed (neglecting the body forces)

$$\begin{cases} \mathrm{Div}\,\underline{v} = 0 \\ \rho\frac{\mathrm{D}\underline{v}}{\mathrm{D}t} = \mathrm{Div}(-p\underline{\underline{I}} + \underline{\underline{\tau}}_p + \eta_s\underline{\underline{d}}) \end{cases} \tag{3}$$

where ρ is the fluid density, p the pressure and $\eta_s\underline{\underline{d}}$ a purely viscous component ($\underline{\underline{d}}$ being the strain rate tensor). The set of coupled Eqs. (1)–(3), supplemented with suitable initial and boundary conditions in both physical and configuration spaces, is the generic multiscale formulation.

Kinetic theory models involving the Fokker–Planck equation, can be accurately discretized using a mesh support (finite elements, finite differences, finite volumes, spectral techniques, etc.). However these techniques involve a high number of approximation functions. In the finite element framework, widely used in complex flow simulations, each approximation function (also known as shape function) is related to a node that defines the associated degree of freedom. When the model involves high dimensional spaces (including physical and conformation spaces and time) standard discretization techniques fail due to an excessive computation time required to perform accurate numerical simulations.

To alleviate the computational effort some reduction strategies have been proposed, as is the case of the partial solution of the cyclic reduction (PSCR) [11,16] which solves linear systems by using techniques of separation of variables, partial solution and projection techniques [1,12,17] and [19]. Despite the significant reduction of the computational effort this technique can only be applied for solving particular partial differential equations and it fails also in the multidimensional case.

Another appealing strategy that allows alleviating the computational effort is based on the use of reduced approximation bases within an adaptive procedure. The new approximation functions are defined in the whole domain and they contain the most representative information of the problem solution. Thus, the number of degrees of freedom involved in the solution of the Fokker–Planck equation is drastically reduced. The construction of those new approximation functions is done with an ‘a priori’ approach, which combines a basis reduction (using the Karhunen–Loève decomposition) with a basis enrichment based on the use of some Krylov’s subspaces. This strategy has been successfully applied, in some of our former works, to solve kinetic theory models defined on the surface of the unit sphere (for simulating short fibers suspensions) as well as 3D models describing some molecular models [3,15]. The main conclusion of our former works was the fact that an accurate description of a complex system evolution can, in general, be performed from the linear combination of a reduced number of space functions (defined in the whole space domain), the coefficients of that linear combination evolving in time. Thus, during the solution of the evolution problem the coefficients of the approximation are computed at the same time that the numerical algorithm constructs the reduced approximation basis. An important drawback of one such approach is the fact that the approximation functions are defined in the space domain, and until now, the simplest form to represent one such function is given its value in some points of the domain of interest, being its value defined in any other point