Available online at www.sciencedirect.com
ScienceDirect
C. R. Acad. Sci. Paris, Ser. I 344 (2007) 473–476
COMPTES RENDUS MATHEMATIQUE
http://france.elsevier.com/direct/CRASS1/

Numerical Analysis

Adaptive models for polymeric fluid flow simulation

Alexandre Ern, Tony Lelièvre

CERMICS, École nationale des ponts et chaussées, ParisTech, 6 & 8, avenue Blaise Pascal, 77455 Marne-la-Vallée cedex 2, France

Received 24 January 2007; accepted 5 February 2007

Available online 26 March 2007

Presented by Philippe G. Ciarlet

Abstract

We propose a new adaptive algorithm for multiscale simulations of non-Newtonian fluids. Using a posteriori error indicators, the method can switch dynamically at each timestep between a rough (macroscopic) and a detailed (microscopic) model in each cell of the mesh. The validity of the approach is tested on a plane shear flow for the FENE model of polymeric fluids. ***To cite this article: A. Ern, T. Lelièvre, C. R. Acad. Sci. Paris, Ser. I 344 (2007).***

Résumé

Modèles adaptatifs pour la simulation de fluides polymériques. Nous proposons un nouvel algorithme adaptatif pour la simulation multi-échelles de fluides non-newtoniens. Le principe est d'utiliser soit un modèle simple (macroscopique) soit un modèle plus détaillé (microscopique) dans chaque maille, le choix étant effectué de manière dynamique à chaque pas de temps sur la base d'indicateurs d'erreur a posteriori. Des tests sur un écoulement cisaillé pour le modèle FENE de fluides polymériques démontrent l'intérêt de l'approche. ***Pour citer cet article : A. Ern, T. Lelièvre, C. R. Acad. Sci. Paris, Ser. I 344 (2007).***

1. Introduction

We are interested in multiscale models for dilute polymer solutions, which are fluids containing non-interacting polymer chains. Even if the concentration of the polymer chains is very low, the rheology of the fluid is influenced by the presence of the polymer chains. Indeed, even though the solvent is a Newtonian fluid, the polymeric solution is nevertheless non-Newtonian. To derive models describing the behavior of such fluids is a very difficult task, still in progress.

There are basically two types of models: macroscopic models and microscopic models. Macroscopic models are usually derived starting from the classical conservation laws of mechanics (conservation of momentum and conservation of mass) and then adding a so-called stress–strain relation. This relation is usually a partial differential equation (PDE) or an integral relation. In this case, the model is called *macro–macro*, since only macroscopic quantities (velocity, pressure, stress) are involved.

E-mail addresses: ern@cermics.enpc.fr (A. Ern), lelievre@cermics.enpc.fr (T. Lelièvre).

1631-073X/$ – see front matter
doi:10.1016/j.crma.2007.02.013

The main difficulty with the macro–macro approach is that the obtained results usually compare poorly with experiments. With a view to improve accuracy, the idea then came up to couple the kinetic equations which describe the dynamics of a polymer chain in a flow (see [3]) with the momentum and mass conservation equations (see the CONNFFESSIT approach [5]). Such an approach is referred to as *micro–macro*, since it couples a microscopic description of the microstructures evolving in the fluid with a macroscopic equation for the velocity and pressure. This coupling is made through the computation of the extra stress tensor $\boldsymbol{\tau}$ as a function of the configuration of the polymer chains in the fluid. This micro–macro approach is very promising from the modeling viewpoint: it yields usually better results than macro–macro models and enables numerical explorations of the link between microscopic properties and macroscopic behavior. The main drawback of micro–macro models is their computational cost. Indeed, the introduction of additional microscopic variables implies a substantial increase of computations.

The goal of this Note is to describe a numerical procedure which allows to reduce the computational cost of micro–macro simulations while maintaining accuracy. The key idea, inspired by [2], is to switch dynamically in some cells of the mesh from the microscopic model to an associated macroscopic model, using suitable a posteriori error indicators. This Note is organized as follows. The micro–macro and macro–macro models under scrutiny are presented in Section 2. The adaptive algorithm is described in Section 3. The error indicators are supported by numerical evidence for one-dimensional shear-flow problems; results are discussed in Section 4. Based on these very promising results, further work will deal with the error analysis, the balance between modeling and discretization errors and with multi-dimensional situations.

2. The micro–macro and macro–macro models

The simplest model to describe the configuration of the polymer chains at the microscopic level is the dumbbell model. It consists of approximating the polymer chain by two beads linked by the end-to-end vector $\boldsymbol{X}_t$ for which a kinetic equation, i.e. a stochastic differential equation (SDE), can be derived. The process $\boldsymbol{X}_t$ depends on the time t, the space variable $\boldsymbol{x}$ and the variable ω in the underlying probability space. In non-dimensional form, the complete micro–macro system couples the Navier–Stokes equations $Re(\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}) = (1-\epsilon)\Delta\boldsymbol{u} - \nabla p + \operatorname{div}\boldsymbol{\tau}$ and $\operatorname{div}(\boldsymbol{u}) = 0$ for the velocity $\boldsymbol{u}$ and pressure p to the following equations allowing to determine the stress tensor $\boldsymbol{\tau}$ as a mean of a functional of the stochastic process $\boldsymbol{X}_t$:

$$\boldsymbol{\tau} = \frac{\epsilon}{We}\big(\mathbb{E}\big(\boldsymbol{X}_t \otimes \boldsymbol{F}(\boldsymbol{X}_t)\big) - \mathrm{Id}\big), \tag{1}$$

$$\mathrm{d}\boldsymbol{X}_t + \boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{X}_t\,\mathrm{d}t = \left(\nabla_{\boldsymbol{x}}\boldsymbol{u}\boldsymbol{X}_t - \frac{1}{2We}\boldsymbol{F}(\boldsymbol{X}_t)\right)\mathrm{d}t + \frac{1}{\sqrt{We}}\,\mathrm{d}\boldsymbol{W}_t, \tag{2}$$

where $\boldsymbol{W}_t$ denotes a d-dimensional standard Brownian motion. The above system is supplemented with initial conditions on $(\boldsymbol{u}, \boldsymbol{X}_t)$ and boundary conditions on $\boldsymbol{u}$. The Reynolds number $Re > 0$, the Weissenberg number $We > 0$ and $\epsilon \in (0, 1)$ are non-dimensional parameters. The vector $\boldsymbol{F}(\boldsymbol{X}_t)$ in (1)–(2) is the force (of entropic origin) between the two beads. In the sequel we consider the FENE model for which $\boldsymbol{F}(\boldsymbol{X}_t) = (1 - \|\boldsymbol{X}_t\|^2/b)^{-1}\boldsymbol{X}_t$. The non-dimensional parameter b is related to the maximal length of the polymer chain. The FENE model accounts for the finite extensibility of the polymer chain, through an explosive force when $\|\boldsymbol{X}_t\| \to \sqrt{b}$.

The above micro–macro model can be discretized using the CONNFFESSIT method. The principle is to use a finite element method in space, a time discretization by an Euler scheme, and a Monte Carlo method to compute the stress tensor as an empirical mean. Thus, in each cell of the mesh, it is necessary to keep track of the configuration of an ensemble of dumbbells, whence the high computational costs.

A macro–macro model, the so-called FENE-P model, can be obtained from the micro–macro FENE model through a closure approximation which consists of replacing the square of the polymer length in the definition of $\boldsymbol{F}(\boldsymbol{X}_t)$ by its expectation, yielding $\boldsymbol{F}(\boldsymbol{X}_t) = (1 - \mathbb{E}(\|\boldsymbol{X}_t\|^2)/\tilde{b})^{-1}\boldsymbol{X}_t$. Using this expression in (1), (2), the stress tensor $\boldsymbol{\tau}$ can be obtained by solving a non-linear PDE. Indeed, letting $\boldsymbol{A} = \mathbb{E}(\boldsymbol{X}_t \otimes \boldsymbol{X}_t)$, it is inferred that

$$\boldsymbol{\tau} = \frac{\epsilon}{We}\left(\frac{\boldsymbol{A}}{1 - \operatorname{tr}(\boldsymbol{A})/\tilde{b}} - \mathrm{Id}\right), \tag{3}$$

$$\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t} + \boldsymbol{u}\cdot\nabla\boldsymbol{A} - \nabla\boldsymbol{u}\boldsymbol{A} - \boldsymbol{A}\nabla\boldsymbol{u}^{\mathrm{T}} = -\frac{1}{We}\frac{\boldsymbol{A}}{1 - \operatorname{tr}(\boldsymbol{A})/\tilde{b}} + \frac{1}{We}\,\mathrm{Id}. \tag{4}$$

The parameter $\tilde{b}$ used in the FENE-P model is different from the parameter b used in the FENE model. Typically, $\tilde{b}$ should be chosen smaller than b to obtain consistent results between the FENE and FENE-P models (see [4]). The FENE-P model is a macro–macro model which can be simulated by standard deterministic methods.

3. The adaptive algorithm

This section describes the main contribution of this Note, namely the adaptive algorithm in which a posteriori error indicators are used to switch at every timestep from the micro–macro FENE model to the macro–macro FENE-P model (or conversely) in order to reduce substantially simulation costs of polymeric fluid flow simulations. In each cell of the mesh, either the rough (FENE-P) model or the detailed (FENE) model is used. At each timestep, three tasks are performed:

(i) Compute stress tensor and velocity field for current timestep in each mesh cell using the local model at hand;
(ii) Compute error indicators;
(iii) Based on these indicators, decide in each cell whether to adapt the model or not.

Let us now give some details on the implementation of tasks (ii) and (iii). When the detailed model is used, the Monte Carlo method requires to let an ensemble of M dumbbells evolve in each cell of the mesh. When the rough model is used, we also let an ensemble of M_{err} dumbbells in the cell evolve. The reason for considering these dumbbells is to compute an estimate of the results that would have been obtained if the detailed model had been used instead. Of course, the algorithm is efficient if it is possible to choose $M_{\mathrm{err}} \ll M$. Task (ii) above consists of the following:

– if the rough model is being used locally, estimate the stress tensor and the velocity field at the next time step by the CONNFFESSIT method using the small ensemble of M_{err} dumbbells;
– if the detailed model is being used locally, estimate the stress tensor and the velocity field at the next time step by the deterministic method using (3)–(4).

In both cases, the relative error on the velocity or on the stress tensor can then be used as a local error indicator, and a threshold value is used to flag cells for model adaption.

– If the error is large and the model in the cell is the rough one, the detailed model is selected locally for the next timestep. This requires to initialize an ensemble of $M - M_{\mathrm{err}}$ dumbbells; this is accomplished by replicating the ensemble of M_{err} dumbbells M/M_{err} times.
– If the error is small and the model in the cell is the detailed one, the rough model is selected locally for the next timestep; an ensemble average is simply evaluated to initialize the stress tensor (or the covariance tensor $\boldsymbol{A}$).

4. Numerical experiment

To assess the validity of the approach, we consider a plane shear flow in dimension $d = 2$. In this case, $\boldsymbol{u}(t, \boldsymbol{x}) = (u(t, y), 0)$, where $\boldsymbol{x} = (0, y)$ and all the variables only depend on y. We suppose that $y \in \mathcal{D} = (0, 1)$. We discretize the problem by P_1 finite elements for u, and P_0 finite elements for $\boldsymbol{X}_t$ and $\boldsymbol{A}$. In practice, we use a variance reduction method (see [1]), the FENE-P model being the control variate. Initially, the fluid is at rest, the dumbbells are at equilibrium according to the law $(2\pi b)^{-1}(b+2)(1 - \|\boldsymbol{X}\|^2/b)^{b/2} 1_{\|\boldsymbol{X}\|^2<b}\,\mathrm{d}\boldsymbol{X}$, and the model is the rough model in each cell. We then progressively apply a velocity at $y = 0$: $u(t, 0) = \inf(100\,t/T, 1)V$, where T denotes the final time of the simulation, and V the velocity at the boundary. At $y = 1$, the velocity is zero: $u(t, 1) = 0$. The parameters are: number of space intervals $I = 10$, number of timesteps $N = 2000$, number of dumbbells $M = 10\,000$, number of dumbbells to measure the errors $M_{\mathrm{err}} = 100$ (observe that $M_{\mathrm{err}}/M \ll 1$), $T = 2$, $V = 1$, $Re = 0.1$, $\epsilon = 0.9$, $We = 0.5$, $b = 20$ and $\tilde{b} = 0.4b$.

The error indicator is the relative error on the velocity with threshold η being set to 10^{-1}, 10^{-2} or 10^{-3}. With respect to using the detailed model everywhere, the adaptive method yields speedups in execution times of 81, 37 and 18, respectively, for $\eta = 10^{-1}$, 10^{-2} or 10^{-3}. In Fig. 1, we compare on the left the error on the velocity for different values of the threshold parameter (the reference velocity being obtained by the simulation with the detailed

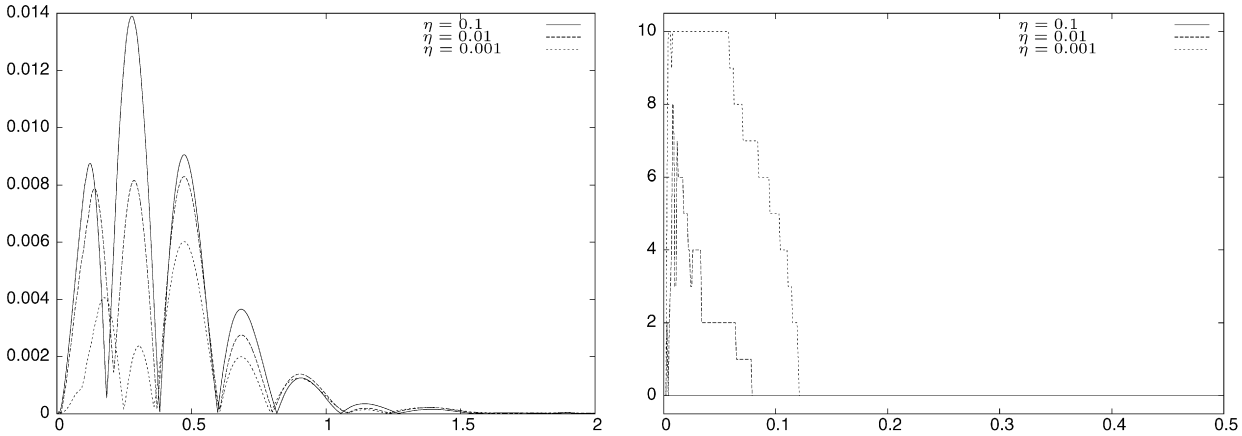

Fig. 1. Left: error on the velocity as a function of time. Right: number of cells where the detailed model is used as a function of time.

model everywhere), and we represent on the right the number of cells where the detailed model is used as a function of time. We observe that for a threshold $\eta = 10^{-3}$, the computational time is divided by 18 and the maximum of the error is only 4×10^{-3}.

References

[1] J. Bonvin, M. Picasso, Variance reduction methods for CONNFFESSIT-like simulations, J. Non-Newtonian Fluid Mech. 84 (1999) 191–215.
[2] M. Braack, A. Ern, A posteriori control of modeling errors and discretization errors, Multiscale Model. Simul. 1 (2) (2003) 221–238.
[3] M. Doi, S.F. Edwards, The Theory of Polymer Dynamics, International Series of Monographs on Physics, Oxford University Press, 1988.
[4] R. Keunings, On the Peterlin approximation for finitely extensible dumbbells, J. Non-Newtonian Fluid Mech. 68 (1997) 85–100.
[5] M. Laso, H.C. Öttinger, Calculation of viscoelastic flow using molecular models: The CONNFFESSIT approach, J. Non-Newtonian Fluid Mech. 47 (1993) 1–20.