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Numerical simulation of a micro–macro model of *concentrated suspensions*

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SUMMARY

We deal here with the numerical simulation of a multiscale model of concentrated suspensions. We compare the deterministic solution procedure for the Fokker Planck equation with the Monte Carlo simulation of the stochastic differential equation. In particular, we examine questions of variance reduction.

KEY WORDS: micro–macro model; deterministic approach; stochastic approach; variance reduction

1. INTRODUCTION

We simulate here the mesoscopic model proposed by Hébraud and Lequeux in Reference [4] for simple shear flows of concentrated suspensions. Let a sample of material be divided into blocks carrying a stress σ. Then, the probability $P(t,\sigma)$ of finding a stress σ in a block, at time t, evolves as follows:

$$\frac{\partial}{\partial t}P(\sigma,t) = -G_0\,\partial_y u(t)\,\frac{\partial}{\partial\sigma}P(\sigma,t) + D(t)\,\frac{\partial^2}{\partial\sigma^2}P(\sigma,t) - \frac{H(|\sigma|>\sigma_C)}{T_0}P(\sigma,t) + \frac{1}{T_0}\left(\int_{|\sigma'|>\sigma_C} P(\sigma',t)\,\mathrm{d}\sigma'\right)\delta_0(\sigma) \tag{1}$$

Here $D(t)=\int_{|\sigma|>\sigma_C} P(\sigma,t)\,\mathrm{d}\sigma$, $H(|\sigma|>\sigma_C)$ denotes the characteristic function of the open set $\mathbb{R}\backslash[-\sigma_C,\sigma_C]$ and δ_0 the Dirac mass. Each term arising in Equation (1) (HL equation in short)

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has a clear physical interpretation. When a block is sheared, the stress of this block evolves with a variation rate proportional to the shear rate $\partial_y u$ (G_0 is an elasticity constant). When the modulus of the stress overcomes a critical value σ_C, the block becomes unstable and may relax into a state with zero stress after a characteristic relaxation time T_0. This phenomenon induces a rearrangement of the blocks that is modelled through the diffusion term $D(p(t))\partial^2_{\sigma\sigma} p$. The diffusion coefficient $D(p(t))$ is assumed to be proportional to the amount of stress that has to be redistributed by time unit and the positive parameter α is supposed to represent the 'mechanical fragility' of the material. In practice, the shear rate is not uniform in space. We therefore introduce the following micro–macro model to better describe the coupling between the macroscopic flow and the microstructure of concentrated suspensions:

$$\begin{aligned}
\rho\partial_t u(y,t) &= \partial_y \tau(y,t)\\
\partial_t P(y,\sigma,t) &= -G_0\partial_y u(y,t)\partial_\sigma P(y,\sigma,t) + D(t,y)\partial^2_{\sigma\sigma} P(y,\sigma,t)\\
&\quad - \frac{H(|\sigma|>\sigma_C)}{T_0} P(y,\sigma,t) + \frac{1}{T_0}\left(\int_{|\sigma'|>\sigma_C} P(\sigma',y,t)\,\mathrm{d}\sigma'\right)\delta_0(\sigma)\\
\tau(y,t) &= \int_{\mathbb{R}} \sigma P(t,y,\sigma)\,\mathrm{d}\sigma
\end{aligned}$$

This system is supplied with the following initial and boundary conditions:

$$\begin{aligned}
u(0,y) &= 0 \quad \text{for all } y \in (0,L)\\
P(0,y,\sigma) &= P^0(y,\sigma) \quad \text{for all}(y,\sigma) \in (0,L)\times\mathbb{R}\\
u(t,0) &= 0 \quad \text{for all } t \in [0,T]\\
u(t,L) &= V(t) \quad \text{for all } t \in [0,T]
\end{aligned}$$

Existence and uniqueness of solutions to this system are studied in Reference [1]. We focus here on computational issues.

2. NUMERICAL SIMULATIONS

The system we look at has no analytical solution (except in the case when $\sigma_C = 0$). We then make use of numerical simulation in order to check if the model correctly reproduces some physical features of suspensions. We consider first a discretization of the momentum conservation equation. Let $n\,\mathrm{d}t$ be the number of time steps, Δt the time step, $n\,\mathrm{d}y$ the number of finite elements in the interval $(0,L)$ and Δy the space step. In the following, the indices n and j, respectively, denote the time index and the space index. Using a $\mathbb{P}_1$ finite element approximation for u and a $\mathbb{P}_0$ one for τ, we find the algebraic form

$$\rho\,\frac{\mathrm{d}}{\mathrm{d}t} MU(t) = -LT(t) - AV(t)$$

where M is the matrix $(M_{ij})_{1\leqslant i,j\leqslant n\,\mathrm{d}y-1}$ with $M_{ij}=\int_0^L \varphi_i\varphi_j\,\mathrm{d}y$, A is the vector $(A_k)_{1\leqslant k\leqslant n\,\mathrm{d}y-1}$ with $A_k=\int_0^L \varphi_K\varphi_k\,\mathrm{d}y$, and L is the matrix $(L_{jk})_{1\leqslant j,k\leqslant n\,\mathrm{d}y}$ with $L_{jk}=\int_0^L \varphi_j'\chi_k\,\mathrm{d}y$. The vector $U(t)$ and $T(t)$ are, respectively, the velocity and the stress vector. For giving U^n, T^n and V^n, a discretization of this equation by an explicit Euler method gives

$$U^{n+1}=U^n+\frac{\Delta t}{\rho}M^{-1}\cdot B^n$$

with $B^n=-LT(n\Delta t)-AV(n\Delta t)$. We are now, interested by the discretization of Equation (1) and the approximation of $T(t)$. Let us first fix Equation (1) on space. Two approaches will be used for this purpose: a deterministic approach and a stochastic approach. Let us only recall that stochastic simulation techniques provide efficient alternatives to deterministic techniques and are powerful tools for solving the usually non-linear equations describing polymer dynamics [6].

2.1. Deterministic approach

Let as assume that P^n, $\partial_y u^n$ and D^n are given. We apply an operator splitting method [8] to approximate the solution at time $(n+1)\Delta t$ of (1)

$$P((n+1)\Delta t)=\mathrm{e}^{(\Delta t/2\,\mathscr{A}(n\mathrm{d}t))}\,\mathrm{e}^{(\Delta t/2\,\mathscr{D})}\,\mathrm{e}^{(S\,\Delta t)}\,\mathrm{e}^{(\Delta t/2\,\mathscr{D})}\,\mathrm{e}^{(\Delta t/2\,\mathscr{A}(n\mathrm{d}t))}\cdot P(n\mathrm{d}t) \tag{2}$$

with $\mathscr{A}(t)=-G_0\partial_y u^n\partial_\sigma$ being the advection operator, $\mathscr{D}=D^n\partial_{\sigma\sigma}$ the diffusion operator and

$$S=-\frac{H(|\sigma|>\sigma_C)}{T_0}+\frac{1}{T_0}\left(\int_{|\sigma'|>\sigma_C}\bullet(\sigma',y,t)\,\mathrm{d}\sigma'\right)\delta_0(\sigma)$$

the 'sources' operator. This allows us to treat separately these three operators. Standard schemes will be used to discretize each one. We use the Lax Friedrich scheme to approximate the solution of the advection problem. This scheme is stable provided that the CFL condition $|G_0\partial_y u^n\Delta t/\Delta\sigma|<1$ is satisfied. The source problem is solved analytically in the case when $|\sigma|\neq 0$. We use the fact that $\int_{\mathbb{R}} P\,\mathrm{d}\sigma=1$ to approach $P_{k,0}^{n+1}$ by $1/\Delta\sigma-\sum_{m\neq 0}P_{k,m}^{n+1}$. The diffusion problem is discretized as follows: if $D\Delta t/\Delta\sigma^2<\frac{1}{2}$, we use a finite difference method on σ and an explicit Euler scheme on time. Else, we use a finite element method on σ and an implicit Euler method on time. Finally, we approach the global stress vector τ_k^n by interpolation as follows:

$$\tau_k(n\Delta t)=\int_{\mathbb{R}}\sigma P_h((k+1/2)\Delta y,\sigma,n\Delta t)\,\mathrm{d}\sigma \tag{3}$$

2.2. Stochastic approach

As in the CONNFFESSIT approach [7], which was introduced to perform flows calculations for polymeric liquids, we can combine the finite elements method used to discretize Equation (2) with stochastic simulation techniques to discretize (1). The stochastic process associated to the partial differential Equation (1) is a non-linear jump-diffusion stochastic process in the sense of McKean, which is produced with the rate $1/T_0$ when $|\sigma|>\sigma_C$. Let us

assign N particles to each point $(k+1/2)\Delta y$. The particles evolve then, as follows:

$$\text{If } |\Sigma_{k,i}^n| < \sigma_C \quad \text{then} \quad \Sigma_{k,i}^{n+1} = \Sigma_{k,i}^n + G_0\,(U_{k+1}^n - U_k^n)/\Delta y)\Delta t + v_k\sqrt{\Delta t}G_i^n$$

$$\text{else} \quad \text{if } \omega_i^n \in \left[0, \frac{\Delta t}{T_0}\right] \text{ then } \Sigma_{k,i}^{n+1} = 0$$

$$\text{else } \Sigma_{k,i}^{n+1} = \Sigma_{k,i}^n + G_0\,(U_{k+1}^n - U_k^n)/\Delta y)\,\Delta t + v_k\sqrt{\Delta t}G_i^n$$

with $\Sigma_{k,i}^n$ the stress on time $n\Delta t$ and at $(k+1/2)\Delta y$ of the ith particle, $v_k^n = \sqrt{2D_k^n}$, with $D_k^n = 1/N\,\text{Cardinal}\{i; |\Sigma_{k,i}^n| > \sigma_C\}$ and G_i^n and ω_i^n are random variables which, respectively, follow the Gaussian law and the uniform law on [0,1]. The global stress is then approximated by the empirical mean

$$\tau_k^n \simeq \frac{1}{N}\sum_{i=1}^{N} \Sigma_{k,i}^n$$

2.3. Comparison between deterministic simulations and stochastic simulations

Let us analyse the numerical results (see Figure 1) obtained by the two approaches (deterministic and stochastic) described above, for a start-up shear flow between parallel plates. The physical parameters are: $\rho = \alpha = L = 1$, $T_0 = 0.5$, $\sigma_C = G_0 = 2$. The numerical parameters are: $T = 10$, $n\,\mathrm{d}t = 10\,000$, $n\,\mathrm{d}y = 200$, $N = 1000$ for the stochastic approach and $\sigma \in [-5, 5]$ and $n\,\mathrm{d}s = 1000$ in the deterministic approach. The computation was carried out on a Pentium IV, 2.4 Ghz with 512 Mb RAM and run with Linux. The CPU with the stochastic approach was about 1h35 and the memory required was 15 Mbytes. The CPU with deterministic approach was about 1h27 and the memory required was 14.8 Mbytes. Clearly, results given by the two methods are similar. The advantage of the stochastic simulation method is its simplicity. Therefore, this method will be useful especially for high dimensions. Let us, finally, note the overshoot of the velocity (see Figure 2), which is a typical behaviour of concentrated suspensions.

2.3.1. Remark. Adjust the parameters α, G_0 and σ_C, and T_0 is necessary to validate the model. This can be carried out using optimization techniques (see Reference [3]) by comparing the numerical results with the experimental one recently obtained by NMR techniques [2].

3. VARIANCE REDUCTION METHODS

As often, is necessary to make use of variance reduction techniques. In the present context, the techniques were introduced in References [5] and [7].

3.1. Brownian configuration fields

The main idea here is to correlate the Brownian motion in space. For this, let us simply consider that at the initial time, all particles founded at the same point k in space, have the same value and that at every time step, all particles in the same point k experience the same

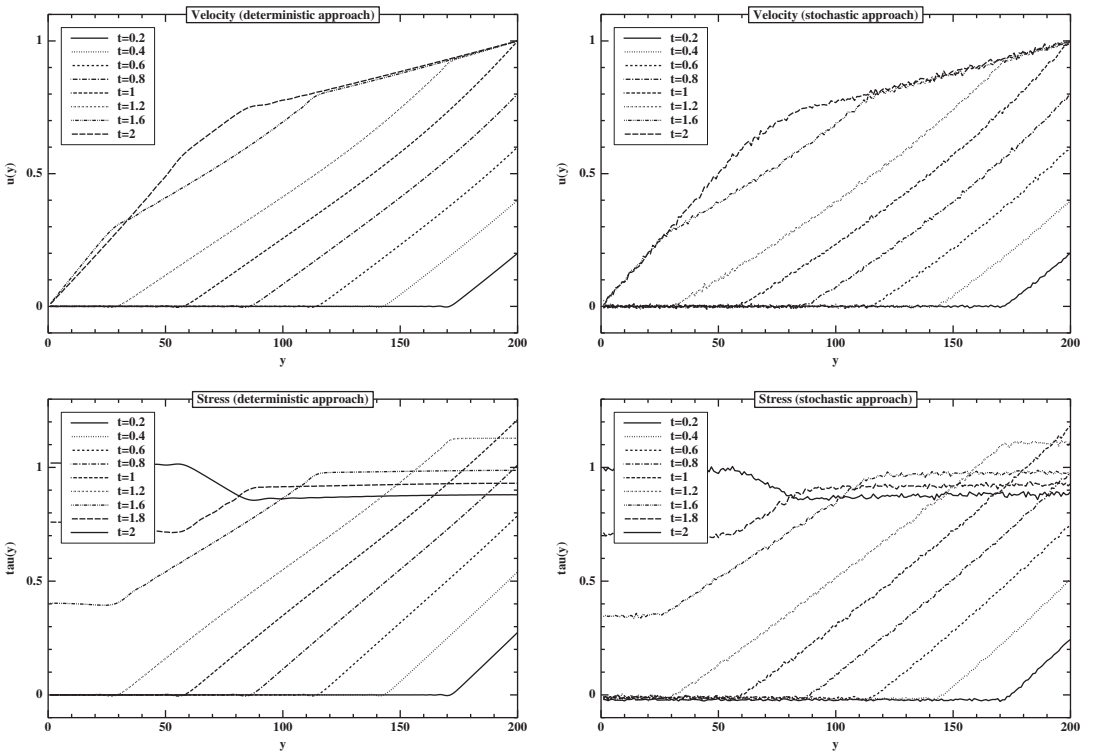

Figure 1. Deterministic (left) and stochastic (right) computations of start-up Couette flow: velocity profiles $u(y)$ and stress profiles $tau(y)$ at various time steps.

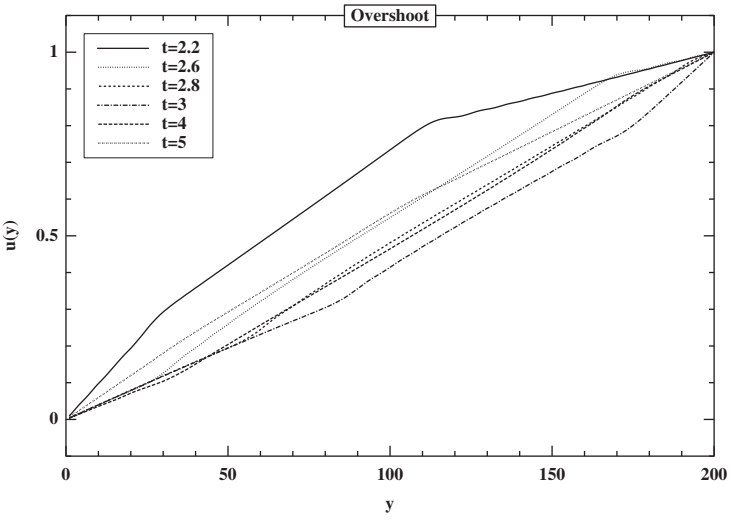

Figure 2. Overshoot of the velocity.

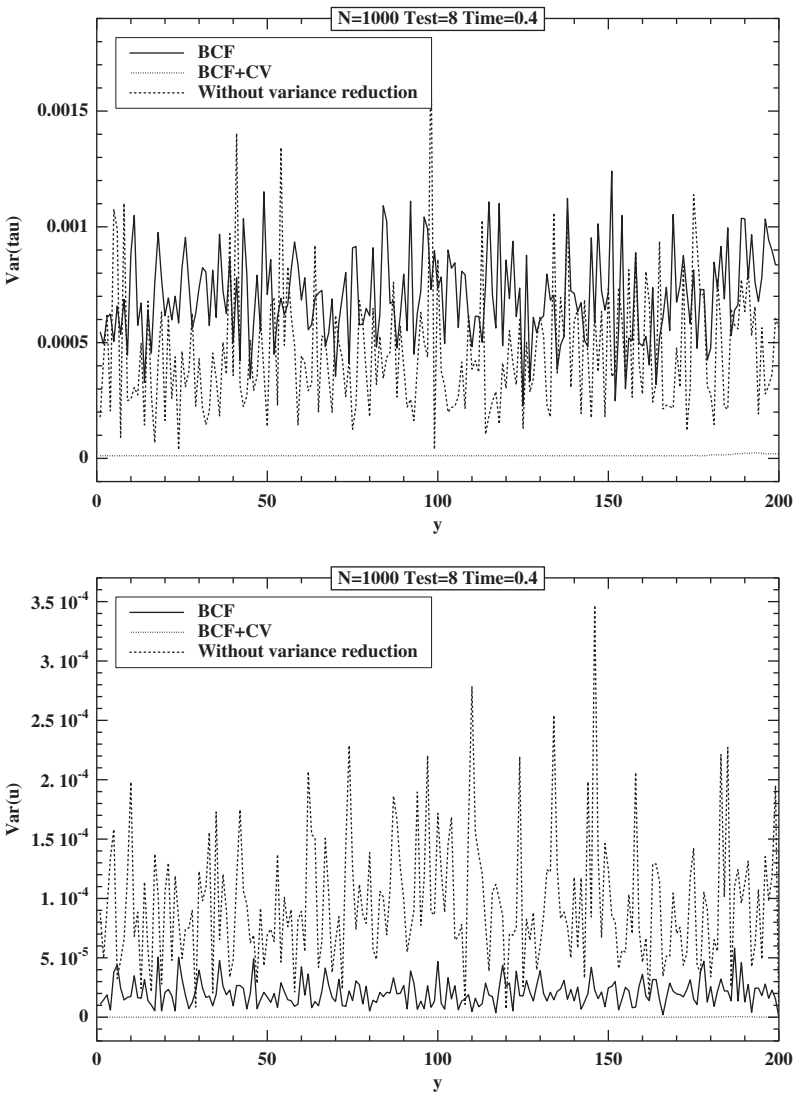

Figure 3. Variances of u and τ (versus space) for simulations without variance reduction, with Brownian configuration fields (BCF) and with BCF and Control variates (BCF+CV).

Brownian motion. As it is shown in Figure 3, this technique reduces the variance on u and increases it for τ.

3.2. *Control variates*

The basic idea here is to write τ_k^n as $\tau_k^n = \mathbb{E}(\Sigma_k^n - \tilde{\Sigma}_k^n) + \mathbb{E}(\tilde{\Sigma}_k^n)$, with $\mathbb{E}(\tilde{\Sigma}_k^n)$ easy to calculate and such that $\mathrm{Var}(\Sigma_k^n - \tilde{\Sigma}_k^n) < \mathrm{Var}(\Sigma_k^n)$. Let us, as in References [5, 7] set $\tilde{\Sigma}_k^n$ equal to Σ_k^n at

equilibrium (that is when $\partial_y u = 0$). The equation verified by $\tilde{\Sigma}_k^n$ is discretized as Equation (1). We use at each time step n the same random numbers to calculate $\tilde{\Sigma}_k^n$ and Σ_k^n. The spatial fluctuations of both velocity and stress are strongly reduced as shown in Figure 3.

4. CONCLUSION

In this work, we have presented a micro–macro model describing the Couette flow of concentrated suspensions. Two different methods were performed to simulate numerically the problem. Numerical results of a simulation of a start-up test given by the two methods were compared and were shown to be similar. Finally, variance reduction schemes were developed to reduce the noise when the stochastic approach is used. The validity of the algorithms was confirmed by numerical results.

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Details of this work and further numerical simulations of rheological tests can be found in Reference [3].

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