Simulating the Dynamics of Entangled Polymers Using the Kinetic Theory Description of the Doi-Edwards Model

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SIMULATING THE DYNAMICS OF ENTANGLED POLYMERS USING THE KINETIC THEORY DESCRIPTION OF THE DOI-EDWARDS MODEL

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ABSTRACT

In this work, the model of Doi-Edwards with independant alignment approximation describing the dynamics of polymer melts is simulated. The main aim of this work is the analysis of some new simulation techniques operating on the Fokker-Planck equation related to that model. For this purpose we consider the kinetic theory description of the Doi-Edwards model, implemented in the 2D and 3D cases under shear and elongational flows. The Fokker Planck equation which governs the evolution of the distribution function involves two variables: the tube orientation (described by a unit vector defining the unit surface in 3D and the unit circle in 2D) and the coordinate that locates the segment tube on the molecular chain, taking values in the unit interval. To separate both variables during the problem resolution we make use of the Alternating Direction Implicit method (ADI) which allows reducing the computation time and efforts.

A model reduction technique is also proposed and analyzed. It consists of considering an optimal representation basis which is constructed during the problem resolution. Thus, a reduced number of approximation functions, now defined in the whole domain, are enough to describe the solution evolution during the entire time interval considered in the simulation, with significant CPU time savings.

Keywords: Polymer melt, Kinetic theory, Doi-Edwards model, Reptation, Alternating Direction Implicit Mehod, Model reduction, Karhunen-Loeve decomposition, Krylov subspaces

INTRODUCTION: DOI-EDWARDS MODEL WITH INDEPENDENT ALIGNMENT APPROXIMATION

In most polymer processing operations such as injection molding, film blowing and extrusion, the polymers are in the molten state. A widely applied class of molecular-based models for concentrated polymer solutions and melts relies on the notion of reptational motion: Doi-Edwards model (M. Doi and S. F. Edwards., 1978) being one a such model.

The key idea of this model is application of the reptation mechanism introduced by De-Gennes (P. G. De Gennes., 1971) to a tube (along which the molecule can move) in order to describe the viscoelastic behaviour of entangled polymers. The molecule is described as sliding or reptating through a tube whose contours are defined by the locus of entanglements with neighbouring molecules. The motion of a molecular chain in any other direction than the one defined by the tube axis is strongly

restricted, except at both tube ends, where it can move in any possible direction. The tube moves itself due to two mechanisms: (i) by means of the motion of the central chain itself, which partially leaves its original tube, for extending it in other directions, and (ii) by the fluctuation induced by the motions of the neighbour chains defining the tube lateral border. In addition to the reptation mechanism, the Doi-Edwards model assumes affine tube deformation induced by the macroscopic flow as well as a complete chain, but neglects other phenomena like the stretch of the chain and the Convective Constraint Release. Within this reptation picture and these assumptions, the dynamics of a single segment is given by:

$$\frac{d\underline{u}}{dt} = (\underline{\underline{I}} - \underline{u} \otimes \underline{u})\ grad \underline{v}\ \underline{u}$$

Where $\underline{u}$ is the unit vector describing the orientation of the tube segment, $grad \underline{v}$ the velocity gradient and $\underline{\underline{I}}$ the unit tensor. The distribution function ψ is such that $\psi(\underline{u}, s, x, t)\ d\underline{u}\ ds$ represents the joint probability that at time t and position x a tube segment has an orientation in the interval $[\underline{u},\ \underline{u} + d\underline{u}]$ and contains the chain segment labelled in the interval $[s, s+ds]$. Thus, the configuration space is Ω=B(0,1)×[0, 1], where B(0,1) is the surface of the unit sphere centered at the origin. The Fokker-Planck equation related to the Doi-Edwards model is the convection-diffusion equation that governs the conservation balance of the distribution function:

$$\frac{d\psi}{dt} = -\frac{\partial}{\partial \underline{u}}\left[\left[(\underline{\underline{I}} - \underline{u} \otimes \underline{u})\ grad \underline{v}\ \underline{u}\right]\psi\right] + \frac{1}{\pi^2 \tau_d}\frac{\partial^2 \psi}{\partial s^2}$$

Where $\frac{d}{dt}$ represents the material derivative, τ_d is the disengagement time, namely the characteristic time for a chain to come out the tube by reptation. We can define the diffusion coefficient related to the s-coordinate as $D_r = \frac{1}{\pi^2 \tau_d}$. To solve the Fokker-Planck equation, one needs to prescribe appropriate boundary conditions at the tube borders s=0 and s=1 (the orientation coordinate being defined on the unit sphere does not require any boundary condition). In general, as previously indicated, an isotropic orientation distribution is prescribed at both ends, which reads:

$$\psi(\underline{u}, s = 0, x, t) = \psi(\underline{u}, s = 1, x, t) = \frac{1}{4\pi}\delta\left(\|\underline{u}\| - 1\right)$$

where δ is the Dirac delta distribution. Knowing the distribution function, the stress can be computed from:

$$\underline{\underline{\tau}}_p = G \int_0^1 \int_{B(0,1)} \underline{u} \otimes \underline{u}\ \psi\ d\underline{u}\ ds$$

where G is an elastic modulus and $\underline{\underline{\tau}}_p$ is the polymer stress tensor.

RESOLUTION STRATEGY: ALTERNATING DIRECTION IMPLICIT

The alternating direction implicit method, ADI, (Jr. J. Douglas and J. E. Gunn.,1964) has been found to be effective for many problems, and generally has a faster convergence rate than SOR strategies. The idea is an alternating resolution of the problems defined in each coordinate. Thus, the ADI strategy instead of solving the 2D (respectively 3D) problem, solves a succession of two (respectively three) one-dimensional problems. The major advantages of the ADI method are: (i) it is unconditionally stable for some operator due to its implicit character; (ii) it can be applied for solving numerous multidimensional problems (in moderate dimensions).

The first step to define a finite-difference scheme for solving a partial differential equation is to discretize the continuous space domain with a grid, whose number of nodes depends on the solution to be approximated. In what follows we are considering only homogeneous flows, which allows to write $\psi(\underline{u}, s, t)$ (that does not depend on the physical coordinates). The degree of freedom related to a grid point (i, j, n) is $\psi(\underline{u}_i, s_j, t_n)$ that is usually denoted by $\psi_{i,j}^n$.

Now, at each time step *n*, the alternating directions method solves (in the 2D case) two steps:

Step I: U-updating:

$$\frac{\psi_{i,j}^{n+\frac{1}{2}} - \psi_{i,j}^{n}}{\Delta t/2} = -E_1(u_i)\left[\beta\left(\frac{\psi_{i,j}^{n+\frac{1}{2}} - \psi_{i-1,j}^{n+\frac{1}{2}}}{\Delta u}\right) + (1-\beta)\left(\frac{\psi_{i+1,j}^{n+\frac{1}{2}} - \psi_{i,j}^{n+\frac{1}{2}}}{\Delta u}\right)\right] - E_0(u_i)\ \psi_{i,j}^{n+\frac{1}{2}} + D_r\left[\frac{\psi_{i,j-1}^{n} - 2\psi_{i,j}^{n} + \psi_{i,j+1}^{n}}{(\Delta s)^2}\right]$$

Step II: S-updating:

$$\frac{\psi_{i,j}^{n+1}-\psi_{i,j}^{n+\frac{1}{2}}}{\Delta t/2}=-E_1(u_i)\left[\beta\left(\frac{\psi_{i,j}^{n+\frac{1}{2}}-\psi_{i-1,j}^{n+\frac{1}{2}}}{\Delta u}\right)+(1-\beta)\left(\frac{\psi_{i+1,j}^{n+\frac{1}{2}}-\psi_{i,j}^{n+\frac{1}{2}}}{\Delta u}\right)\right]$$
$$-E_0(u_i)\ \psi_{i,j}^{n+\frac{1}{2}}+D_r\left[\frac{\psi_{i,j-1}^{n+1}-2\psi_{i,j}^{n+1}+\psi_{i,j+1}^{n+1}}{(\Delta s)^2}\right]$$

Due to the convection-diffusion character of the equation to be solved in the first step an appropriate stabilization is needed to avoid numerical instabilities induced by the convection term. In our simulations we considered a streamline upwinding, where the upwinding parameter β approaches to 1 when advection becomes dominant and $E_1(u_i)>0$ (respectively to zero for dominant advection and $E_1(u_i)<0$). When the diffusion term is dominant β approaches to 0.5 and then, both terms affected by the beta coefficients are equivalent to the centred finite difference.

In the 2D case, step I, requires the resolution of a system of equations. This resolution must be done as many times as the number of nodes of s-axis discretization (we exclude the nodes located at the border where the boundary condition is prescribed). The linear system can be expressed by:

$$\underline{\underline{M}}\ \dot{\underline{\psi}}+\underline{\underline{G}}\ \underline{\psi}=\underline{S}$$

The difference between the 2D and the 3D cases is that in the first case, vector $\underline{u}$ can be easily described by the scalar φ ($0\le\varphi\le 2\pi$) whereas in the 3D case $\underline{u}$ needs two scalars, φ and θ if one considers polar coordinates ($0\le\varphi\le 2\pi$ and $0\le\theta\le\pi$).

NUMERICAL RESULTS

The distribution function is represented in the space of configurations and shows a periodic evolution according to the space orientation ($\underline{u}(\varphi)$ in the 2D case and $\underline{u}(\varphi,\theta)$ in the 3D case) and a parabolic evolution according to the curvilinear coordinate (s), see Figures 1, 2, 3 and 4, proving, as expected, that segments located in the central region are more stretched, and their orientations more constrained, than the ones located in the borders neighbourhood.

2D simulations:

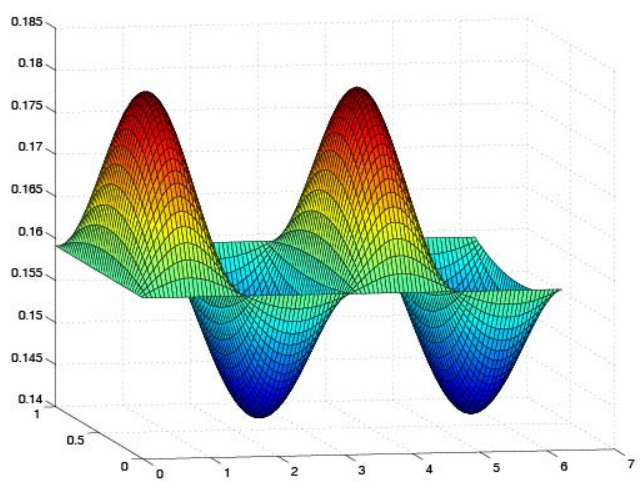

Figure 1 Evolution of the distribution function in a 2D shear flow case with Dr=1 and We=1.

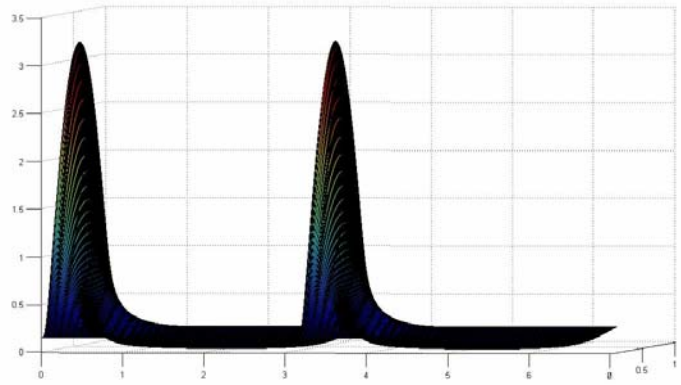

Figure 2 Evolution of the distribution function in a 2D shear flow case with Dr=1 and We=100.

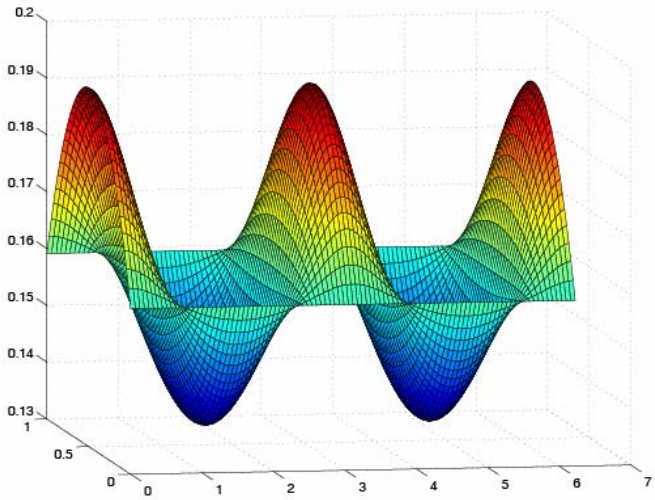

Figure 3 Evolution of the distribution function in a 2D elongation flow case with Dr=1 and We=1.

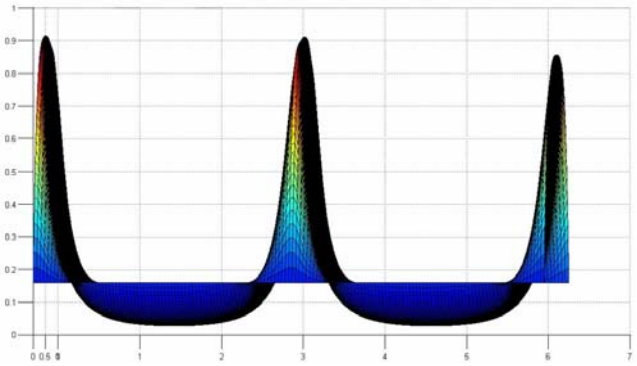

Figure 4 Evolution of the distribution function in a 2D elongation flow case with Dr=1 and We=50.

We can also notice at these figures that as the Weissenberg number increases the peaks become more prominent and more localized noticing that the chain is the more and more sollicitated.

3D simulations:

In this case, due to the symmetry of the chain, we consider only a half, Figure 5.

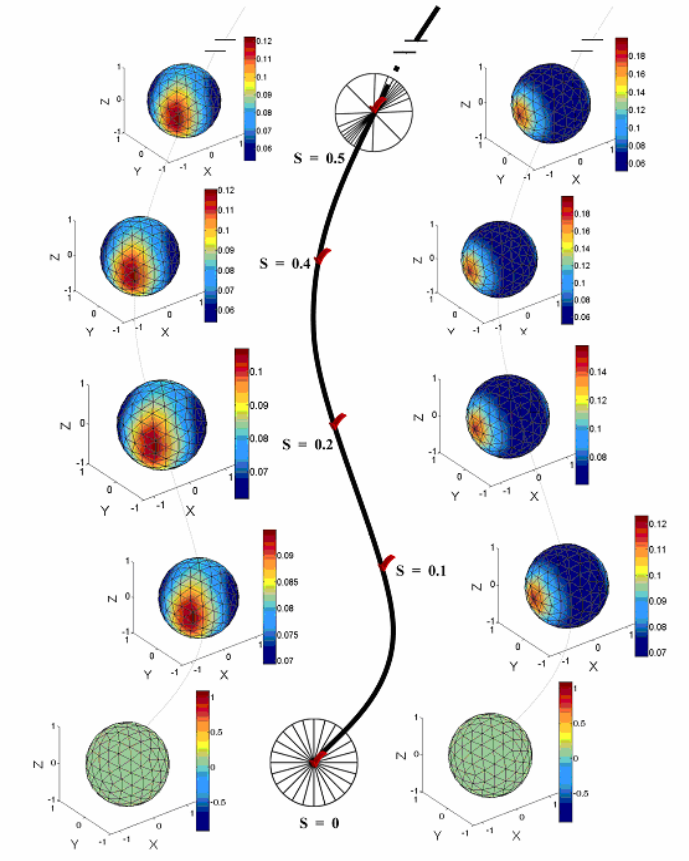

Figure 5 Evolution of the distribution function in a 3D case with Dr=1 and We=1: (left) Shear flow (right) Elongation flow.

The micro-macro modeling is done by the calculation of the stress tensor, and then the shear and elongation viscosities. The steady shear viscosity, depicted in Figure 6, decreases as the shear rate increases (shear thinning behaviour). At high shear rates, the asymptotic viscosity curve related to the Doi-Edwards model possesses a slope of –3/2 (in the double logarithmic presentation), higher than the –1 slope (also indicated in that plot) noticing for the instability of that model.

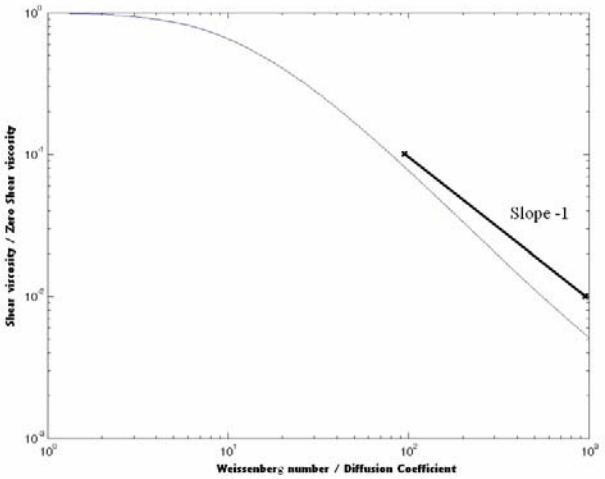

Figure 6 Steady shear viscosity, 2D case.

Besides, we observe that the shear stress shows transient overshoots in the start-up shear flow at low shear rates, which is one of the major features that the Doi-Edwards model is not able to predict.

MODEL REDUCTION

The goal of the reduction model is to define an optimal approximation subspace able to represent accurately the whole field evolution, in our case the time evolution of the distribution function. As the number of approximation function is much lower than the number of grid points, the associated linear system is of low dimension and significant CPU time savings can be attained. The new shape functions are defined in the whole domain in an appropriate manner (the most characteristic functions related to the model solution) (A.Ammar et al., 2005). The construction of those new approximation functions is done with ‘a priori’ approach.

In this section we are going to apply the ideas just introduced to the discrete problem resulting from the discretisation of the Fokker-Planck equation that we can express in the matrix form:

$$\underline{\underline{M}}\ \dot{\underline{\psi}} + \underline{\underline{G}}\ \underline{\psi} = \underline{S}$$

whose implicit time discretization results:

$$\underline{\psi}_{t+\Delta t} = \left(\underline{\underline{M}} + \Delta t \underline{\underline{G}}\right)^{-1} \underline{\underline{M}}\ \underline{\psi}_t + \Delta t \left(\underline{\underline{M}} + \Delta t \underline{\underline{G}}\right)^{-1} \underline{S}$$

We consider that the probability distribution have been accurately described in [0, t_α]. We assume that at time t_α the reduced approximation basis is given by $\underline{\underline{B}}^{(n)}$. Moreover, at certain times t_p, with $t_p \le t_\alpha$, the solution is assumed known and defined by the reduced vectors $\underline{\xi}_p^{(n)}$. Knowing $\underline{\xi}_p^{(n)}$, the finite element description of ψ at time t_p results: $\underline{\psi}^p = \underline{\underline{B}}^{(n)} \underline{\xi}_p^{(n)}$. We can assume that the first approximation basis $\underline{\underline{B}}^{(0)}$ contains a single vector that corresponds with the initial probability $\underline{\psi}^0$. Now, we compute the evolution of ψ in $\left[t_\alpha, t_\beta\right]$ solving the reduced form related to implicit scheme:

$$\left(\underline{\underline{B}}^{(n)}\right)^T \underline{\underline{B}}^{(n)} \underline{\xi}_{t+\Delta t}^{(n)} =$$

$$= \left(\underline{\underline{B}}^{(n)}\right)^T \left(\underline{\underline{M}} + \Delta t \underline{\underline{G}}\right)^{-1} \underline{\underline{M}}\,\underline{\underline{B}}^{(n)} \underline{\xi}_t^{(n)} + \Delta t \left(\underline{\underline{B}}^{(n)}\right)^T \left(\underline{\underline{M}} + \Delta t \underline{\underline{G}}\right)^{-1} \underline{S}$$

The new reduced approximation basis $\underline{\underline{B}}^{(n+1)}$ is defined by adding to the significant information extracted from $\underline{\xi}_p^{(n)}$, $\forall p \le \alpha$, some Krylov's subspaces computed at t_β. We are going to explicit the construction of $\underline{\underline{B}}^{(n+1)}$.

We define the matrix $\underline{\underline{Q}}$ which contains the reduced vectors $\underline{\xi}_p^{(n)}$, $\forall p \le \alpha$. Now, we solve the eigenproblem related to the Karhunen-Loeve decomposition, given by:

$$\underline{\underline{Q}}\ \underline{\underline{Q}}^T \underline{\vartheta} = \lambda \underline{\vartheta}$$

Whose solution results in α couples ($\underline{\vartheta}_k$, λ_k), where we assume that eigenvalues are ordered $\lambda_1 \ge \lambda_2 .... \ge \lambda_k$, and we select the eigenvectors $\underline{\vartheta}_k$ related to the eigenvalues verifying $\lambda_k \ge 10^{-8} \lambda_1$, that constitute the columns of matrix $\underline{\underline{V}}$. Now we can write:

$$\tilde{\underline{\underline{B}}}^{(n+1)} = \left(\underline{\underline{V}}\ \underline{\underline{B}}^{(n+1)}\right)$$

Obviously, the change in the reduced approximation basis implies a change in the expression of the reduced vectors $\underline{\xi}_p^{(n)}$, $\forall p \le \alpha$. For this purpose one could enforce:

$$\tilde{\underline{\underline{B}}}^{(n+1)} \tilde{\underline{\xi}}_p^{(n+1)} = \underline{\underline{B}}^{(n)} \underline{\xi}_p^{(n)}$$

which it results:

$$\left(\tilde{\underline{\underline{B}}}^{(n+1)}\right)^T \tilde{\underline{\underline{B}}}^{(n+1)} \tilde{\underline{\xi}}_p^{(n+1)} = \left(\tilde{\underline{\underline{B}}}^{(n+1)}\right)^T \underline{\underline{B}}^{(n)} \underline{\xi}_p^{(n)} \Rightarrow$$

$$\tilde{\underline{\xi}}_p^{(n+1)} = \left(\left(\tilde{\underline{\underline{B}}}^{(n+1)}\right)^T \tilde{\underline{\underline{B}}}^{(n+1)}\right)^{-1} \left(\tilde{\underline{\underline{B}}}^{(n+1)}\right)^T \underline{\underline{B}}^{(n)} \underline{\xi}_p^{(n)}$$

$$\forall p \le \alpha$$

Now, the updated basis consist of $\tilde{\underline{\underline{B}}}^{(n+1)}$ completed with some Krylov subspaces generated from the residual $\underline{R}$ at time t_β:

$$\underline{\underline{B}}^{(n+1)} = \left(\underline{\underline{V}}\,\underline{\underline{B}}^{(n)}, \underline{R}, \cdots\right)$$

where the residual is computed according to:

$$\underline{R} = \underline{\underline{B}}^{(n)} \underline{\xi}_{t_\beta}^{(n)} -$$

$$-\left(\underline{\underline{M}} + \Delta t \underline{\underline{G}}\right)^{-1} \underline{\underline{M}}\,\underline{\underline{B}}^{(n)} \underline{\xi}_t^{(n)} + \Delta t \left(\underline{\underline{B}}^{(n)}\right)^T \left(\underline{\underline{M}} + \Delta t \underline{\underline{G}}\right)^{-1} \underline{S}$$

In order to analyze the capabilities of this technique we consider the 3D Doi-Edwards model. The technique just described allows to define a reduced approximation basis that is able to represent the entire time evolution of the distribution using only 8 functions, and then only 8 degrees of freedom (at each time step one needs to perform the inversion of a matrix of size 8x8) instead the 642 nodes considered in the coarse mesh illustrated in Figure 7. The computed results are in agreement with the ones obtained using the ADI strategy.

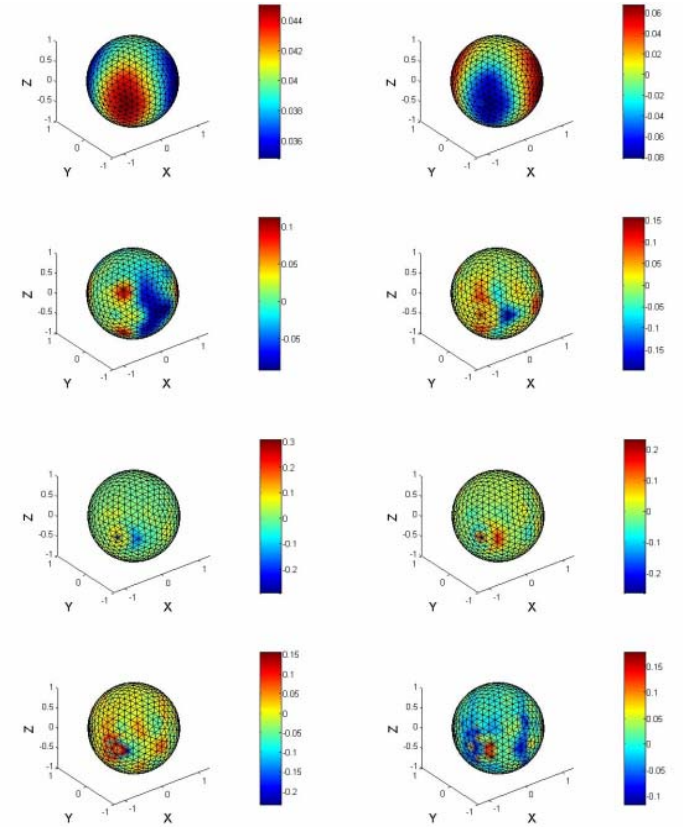

Figure 7 The eight most significatives reduced basis functions:3D case.(up-left) First most significative reduced basis function; (up-right) Second most significative reduced basis function ;...; (down-left) Seventh most significative reduced basis function;(down-right) Eighth most significative reduced basis function.

CONCLUSIONS

In this paper, the Doi-Edwards model with independant alignment approximation has been analyzed, by solving the associated Fokker-Planck equation using two different numerical strategies that combine great accuracy and significant CPU time savings. The first strategy makes use a decoupling between the different model coordinates during the discretization, and the second one is based on the construction of a reduced approximation basis able to represent accurately the entire time evolution of the distribution function.

At present we are developing a second generation of model reduction techniques based on the use of separated representations of fields combined with tensor product approximation spaces. These techniques have been applied in some of our former works (A.Ammar et al., 2006) for solving dumbbells modes (FENE, MBS, …) and seem to be excellent candidates for treating models describing entangled polymers based on the reptation motion or in the molecular networks.

In any case, more realistic models are being considered to avoid the previously referred overshoot in the shear viscosity, being an appealing model the one propose by Ottinger (H. C. Ottinger., 2000).

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