On the Simulation of Kinetic Theory Models of Complex Fluids Using the Fokker-Planck Approach

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Abstract:
Models of kinetic theory provide a coarse-grained description of molecular configurations wherein atomistic processes are ignored. The Fokker-Planck equation related to the kinetic theory descriptions must be solved for the distribution function in both physical and configuration spaces. When the model involves high dimensional spaces (including physical and conformation spaces and time) standard discretization techniques fail due to excessive computation requirements. In this paper, we revisit some model reduction techniques recently proposed to circumvent those difficulties, exploring other new application areas related to entangled polymer models as well as the use of such reduced models for treating complex flows in which the distribution function involves both the physical and the conformation coordinates.

Zusammenfassung:
Modelle der kinetischen Theorie stellen eine vergröberte Beschreibung molekularer Konfigurationen zur Verfügung, bei der atomistische Details vernachlässigt werden. Die zur kinetischen Theorie gehörende Fokker-Planck-Gleichung muss für eine Verteilungsfunktion sowohl im physikalischen als auch im Konfigurationsraum gelöst werden. Wenn das Modell dabei einen hochdimensionalen Raum erfordert (einschlisslich physikalischer Raum, Konfigurationsraum und Zeit) versagen konventionelle Diskretisierungstechniken aufgrund ihrer sehr hohen Anforderungen an die Rechenzeit. Mit diesem Beitrag geben wir einen Überblick über kürzlich vorgeschlagene Modell-Reduktionstechniken, die in der Lage sind, diese Schwierigkeiten zu überwinden, und mithilfe derer neue Anwendungsgebiete, in denen die Verteilungsfunktionen sowohl die physikalische als auch konfigurelle Dimension beschreiben muss, angegangen werden können. Dazu zählen insbesondere verschlaufte Polymersysteme in komplexen Strömungen.

Résumé:
Les modèles de théorie cinétique définissent une description globale de la configuration moléculaire dans laquelle l'échelle atomistique est ignorée. L'équation de Fokker-Planck relative à la théorie cinétique doit être résolue en donnant la fonction de distribution aussi bien sur l'espace physique que de configuration. Quand le modèle se définit sur un espace de dimension élevée (en superposant l'espace physique, de configuration et temporel) les techniques usuelles de discrétisation se heurtent à la difficulté du traitement numérique excessivement gourmant en temps de calcul et en stockage. Dans ce travail, on présente une revue de quelques techniques de réduction en explorant des nouvelles applications liées à la reptation des polymères fondus et également aux traitements d'écoulements complexes dans lesquels la fonction de distribution s'exprime sur l'espace physique et de configuration.

Key words: kinetic theory, Fokker-Planck equation, model reduction, separated representation, Karhunen-Loève decomposition

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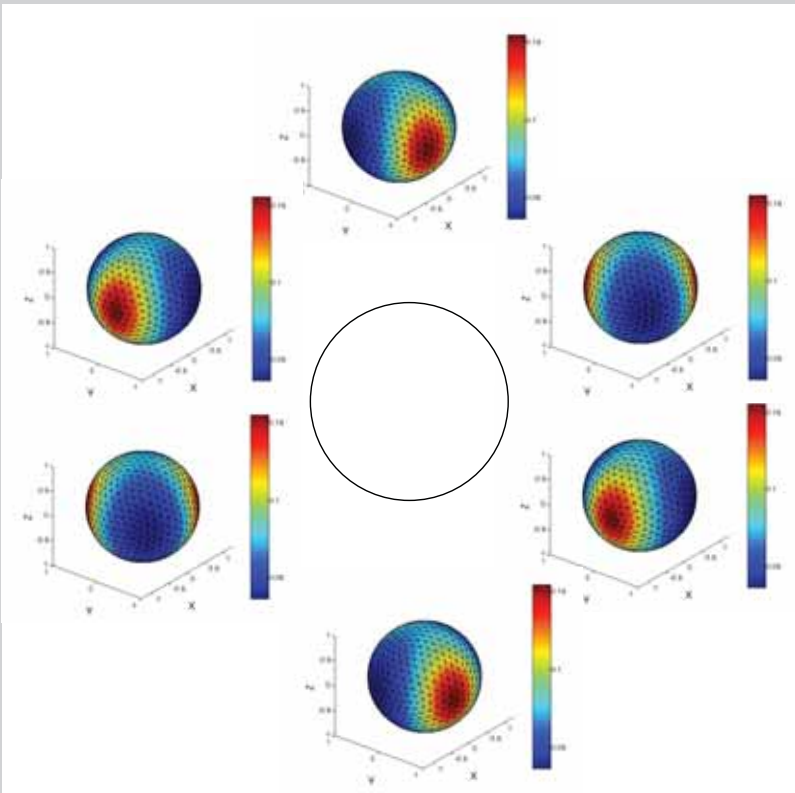


Figure 10 depicts the computed results and Figure 11 the 9 orientation approximation functions used for computing the distribution evolution along the whole circular trajectory. The computed solution is in good agreement with the ones computed by using the standard finite element technique.

4 CONCLUSIONS AND PERSPECTIVES

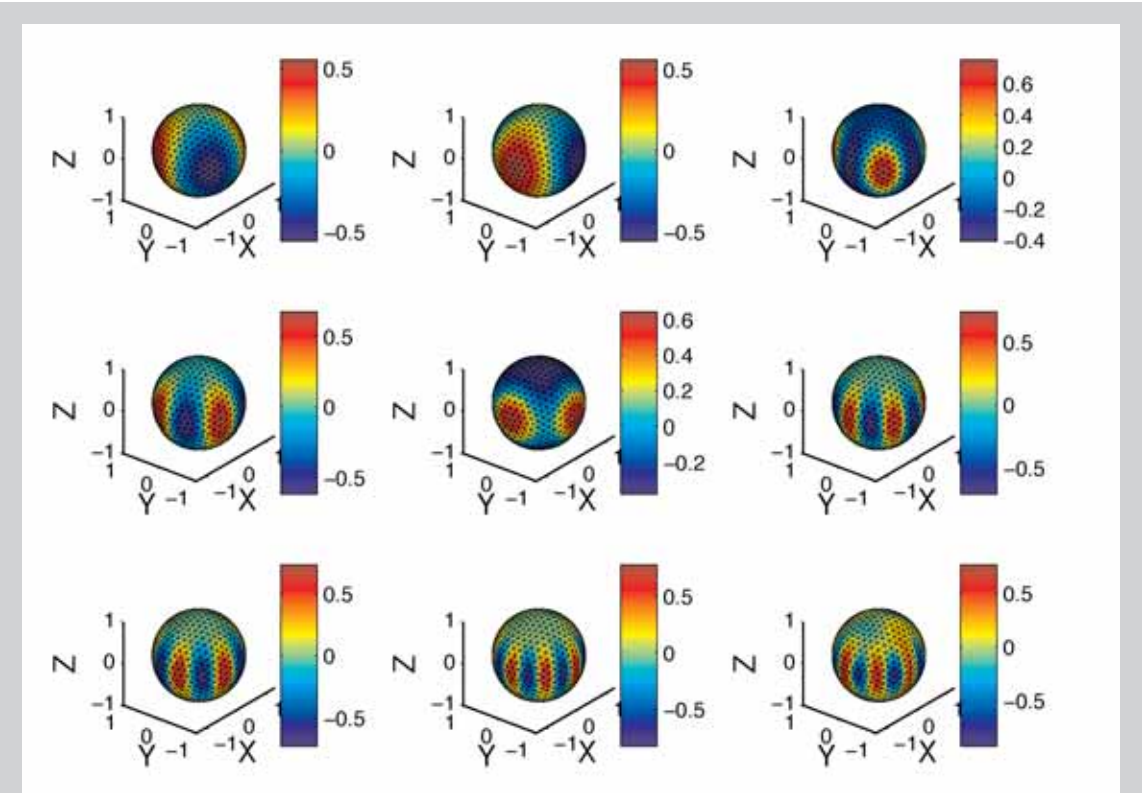
In this paper we explored the ability of some recent numerical strategies for solving steady or transient multidimensional partial differential equations as the ones encountered in the kinetic theory description of complex fluids. The technique based on the use of reduced approximation bases constructed from the application of the Karhunen-Loève decomposition can be successfully applied to simulate kinetic theory models defined in spaces of moderate dimension, but it fails in highly dimensional spaces. In highly dimensional problems, the technique based on a separated representation of the solution seems to be an excellent candidate for treating this kind of complex models, as proved in this paper throughout several examples.

Figure 10 (above): Steady 3D fiber orientation distribution at some locations on the circular trajectory.

Figure 11: 3D orientation approximation functions $F_j(\mathbf{p})$.

defined on the unit surface. Thus, the separated representation reads:

$$\psi(s,\mathbf{p}) = \sum_{j=1}^{\infty} \alpha_j F_j(\mathbf{p}) G_j(s) \qquad (49)$$



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The main challenge in the simulation of complex flows is the coupling between the physical and the conformation discretization spaces. The separated representation of the advective stabilization terms requires further developments. On the other hand, fully coupled models, coupling the macroscopic flow kinematics and the microscopic fluid description, deserve additional works.

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