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FIRST STEPS TOWARDS A MULTISCALE MODEL FOR FLUID FLOW

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KEYWORDS

Multiscale modelling, molecular dynamics, dissipative particle dynamics, coarse-graining, rheology.

INTRODUCTION

Taking a closer look over the wide range of our daily life products, we realize that most of them are based on soft matter materials. Good examples of these types of materials are polymeric liquids, colloidal dispersions, liquid crystals and nanocomposite systems. The complexity to model and simulate these materials stands on their peculiar macroscopic flow behaviors dependent on their internal degrees of freedom (e.g., molecular orientation, molecular weight) which governs their local dynamics (e.g., viscoelasticity, shear thinning, relaxation times). Although, Computational Fluid Dynamics (CFD) has been used exhaustively to simulate complex fluid systems at their characteristic length and time scales, it still lacks on reliability since most of the constitutive equations for such systems are still to be developed. On the other hand, atomistic and mesoscale simulations are capable to predict the interactions and dynamics of the system explored, but they are computationally prohibitive when coped to large-scale motions far beyond the molecular size. In order to tackle this problem, many authors adopted multiscale schemes to couple the wide range of length and time scales, combining the advantages of each method [1]. The message passing procedure that characterizes the bridge between scales will be according to the type of problem to be solved and the properties to be studied, i.e, there is no general multiscale recipe that applies to all situations.

THE MULTISCALE APPROACH

The multiscale approach proposed in this work can be understood as a bottom-up scheme where the relevant coupling properties of the material are pipelined from lower scales towards the upper scales:

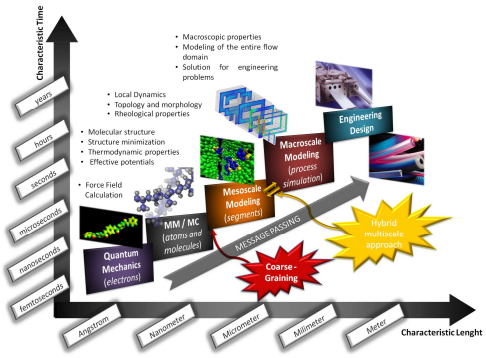

Figure 1. Multiscale pipeline scheme

This concept is not a novelty, some authors followed the same procedure to estimate the mechanical properties of nanostructured materials [2]. It was proven that accurate results can be obtained when the intention is to predict bulk properties of complex systems. Although, things start to get more complicated when the desired properties are time-dependent, such as what happen in rheological studies. Bridging the information between scales is still a challenge in this field [3], assumptions need to be made and some features need to be relaxed.

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RESULTS

Atomistic simulations using molecular dynamics were performed in order to obtain the interaction potentials that will be mapped into the mesoscale.
Table 1 shows the ensemble averages computed from the MD simulations:

Table 1. Energy calculations from MD-NVT simulations (kcal/mol)

	PE (450K, 1bar)	PA6 (550K, 1 bar)	PC (550K, 1 bar)
E_p	-3552.811 (±68.47)	-3481.879 (±80.09)	-982.212 (±86.33)
E_k	8102.815 (±46.09)	7801.799 (±51.18)	10830.637 (±61.80)
E_T	4550.003 (±47.92)	4319.920 (±58.23)	9848.424 (±56.39)

As a means of validating the MD results, Table 2 shows the density for each system obtained from MD-NPT simulations compared with experimental results found on the literature:

Table 2. Densities obtained from MD-NPT simulations

POLYMER	ρ (g/cm^3)	ρ_{EXP} (g/cm^3)
PE	0.7435	0.766 [4]
PA6	0.904	0.9392 [5]
PC	1.147	1.14-1.2 [5]

Structural properties can also be sketched through the radial distribution function. This property will be used further to estimate the interaction potentials that will be used at the mesoscale through a coarse-graining technique called Iterative Boltzmann Inversion [6]:

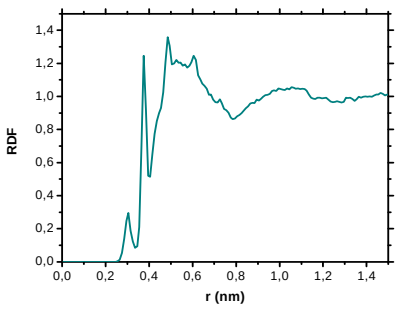

Figure 2. Pair correlation function of C-C in polyethylene

CONCLUSIONS

- A multiscale approach from atomistic to mesoscale was precisely traced and ready to be tested;
- Atomistic simulations for three different systems were performed. The density values obtained perfectly match experimental results found in the literature;
- Coarse-graining simulations are being undertaken;
- Study the shear limits of DPD and the local dynamics of the systems;
- Developed a mapping procedure to macroscale simulation.

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SACHA T. MOULD was boned in São Paulo, Brazil, on the year of 1983. He obtained the BEng degree in Polymer Engineering at the University of Minho (Guimarães, Portugal) in the year of 2006. In 2008 he became an MSc at the same institution. His diploma thesis was related with the development of new on-line rheological devices for extrusion process monitoring. During the years of 2007-2009 he worked as a researched for the European project MultiHybrids and in February 2009 he became a PhD student at Uninversity of Minho supported by the Portuguese Foundation for Science and Technology (FCT).