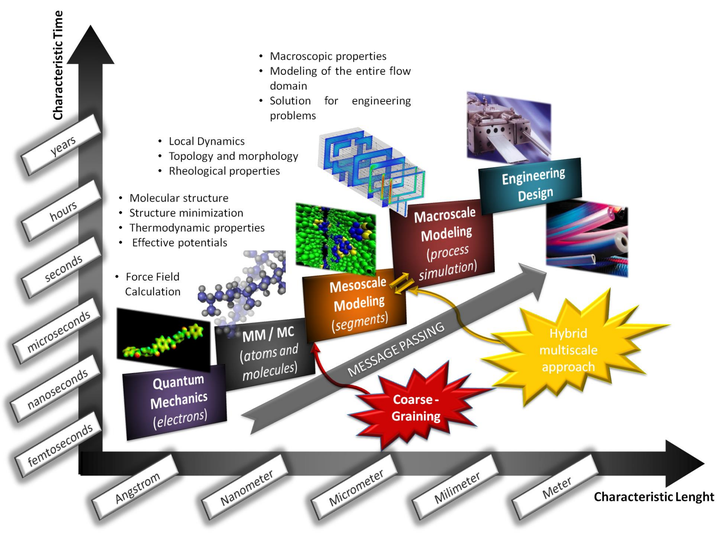
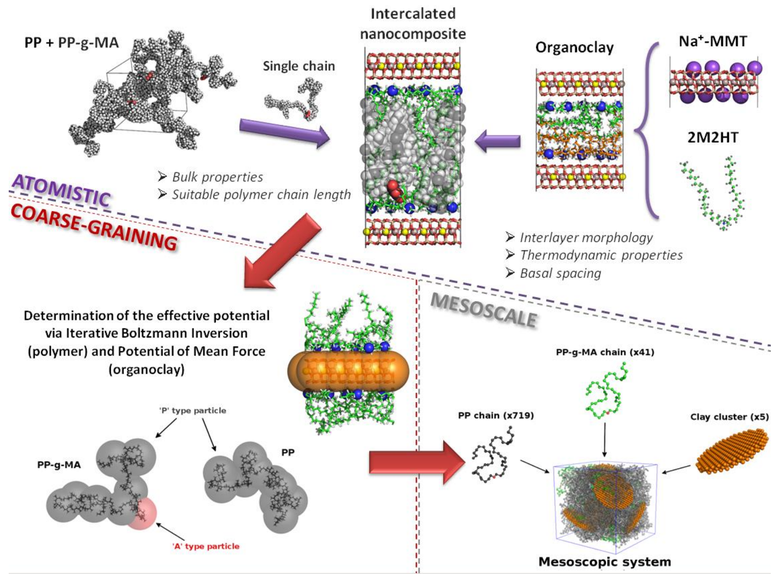
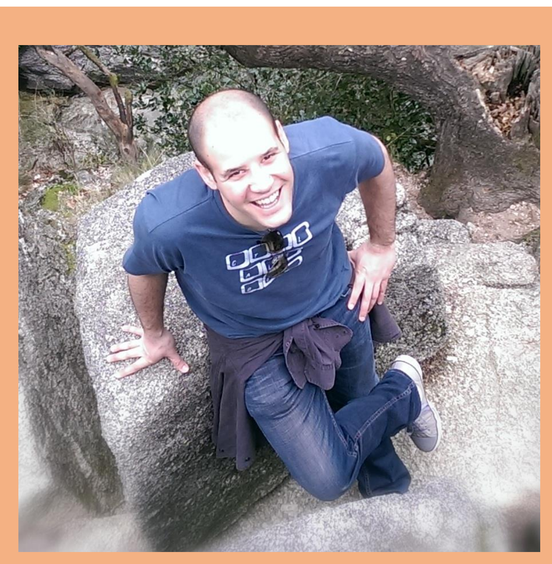
Multiscale modelling of polymer nanocomposites







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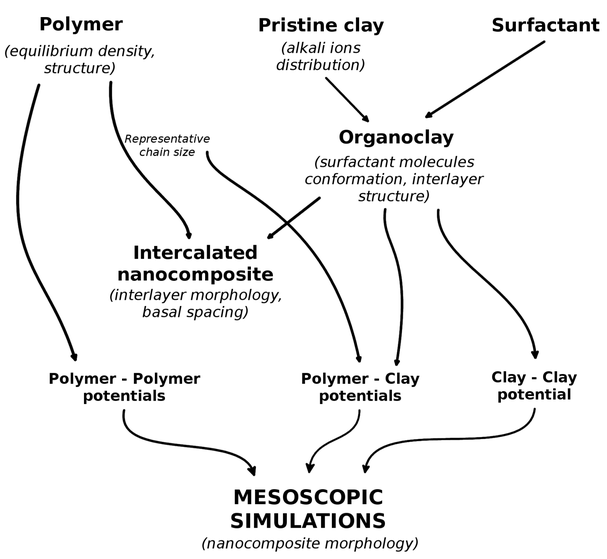
Objectives

- Develop multiscale simulation tools to solve problems of **industrial** interest;
- Assist **material design** and **property prediction**;
- **Correlate** macroscopical behavior with underlying subtleties (e.g., morphology, chemical affinity, local dynamics);
- Derive **constitutive model** abe to describe the rheological nature of polymer nanocomposite systems;l
- Provide complementary information to **experimental** based studies;
- Trace ***"Virtual Screening"*** protocols to optimize material formulations and/or process parameters.

Methods and techniques

The procedure combines models and simulation techniques intrinsic to each scale. While, molecular dynamics simulations are used to cope with the fine *atomistic* subtleties (e.g., local structure at the interlayer, thermodynamics considerations), the correlations between state of dispersion and macroscopic properties are accessed through *mesoscopic* simulations. A structure based coarse-graining technique (*Iterative Boltzmann Inversion* protocol) is used to estimate the effective potentials describing the free-energy of the mesoscopic system.



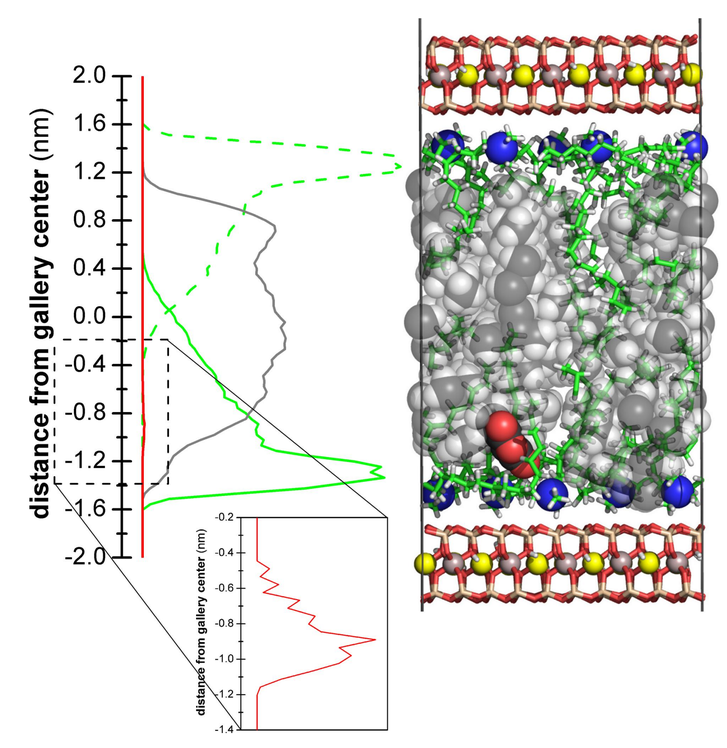


Fig 1. Intercalated PP-g-MA between organoclay layers; surfactants in green, PP in gray, MA oxygens in red.

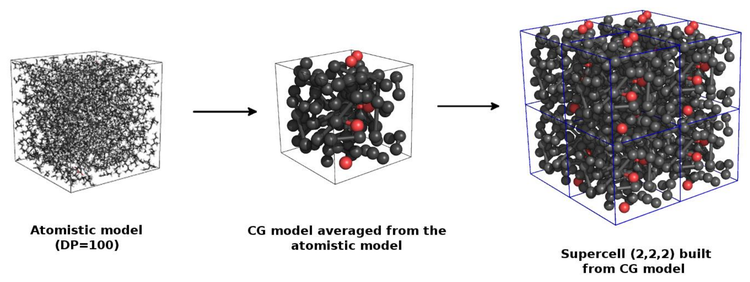


Fig 2. Coarse-grained system built from an atomistic trajectory.

Results

- The favorable $E_{bind}^{PP-g-MA}$ (due to coulombic interactions) demonstrates the importance of using a compatibilizer, while the dispersion forces are responsible for the favorable interaction between quats and the polymer (see Fig. 1);
- The mesoscopic simulations shows that the set of non-bonded interactions estimated coherently reproduces the expected equilibrium features of the system (Fig. 2).

$$E_{bind} = -E_{nb} = -(E_{VdW} + E_{Coul})$$

	PP-g-MA/MMT	quat/MMT	PP-g-MA/quat
E_{bind}^{VdW}	-687.76	288.56	129.32
E_{bind}^{Coul}	46532.79	38474.91	-47.78
E_{bind}^{tot}	45845.05	38766.83	81.54

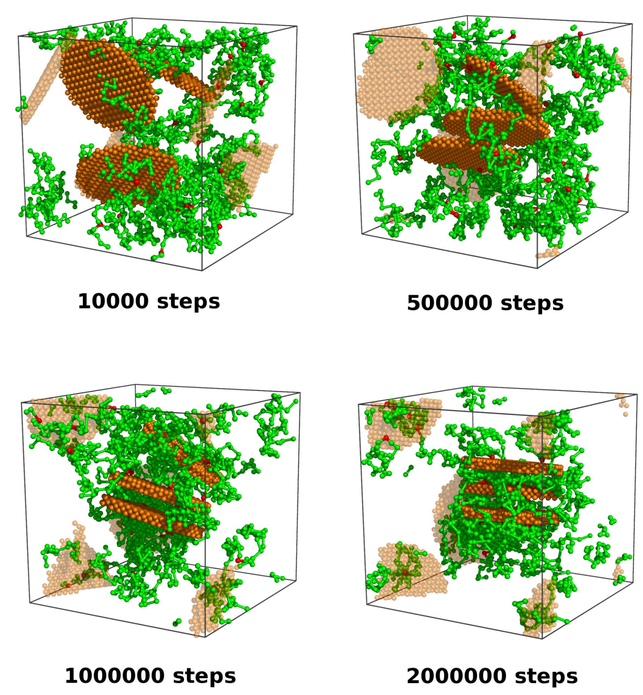


Fig 3. Evolution of nanoclay particles during an equilibrium mesoscopic simulation.

Acknowledgements

✓ The Portuguese Foundation for Science and Technology (FCT) for the financial support given through the PhD grant SFRH/48512/2008;
✓ Matepro – Optimizing Materials and Processes project (Ref. NORTE-07-0124-FEDER-000037);
✓ SeARCH supercomputing facility at the Department of Informatics, University of Minho.

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