WARWICK
THE UNIVERSITY OF WARWICK

# WCPM/CSC joint seminar

## Multiscale modelling of polymer aggregates

Paola Carbone

School of Chemical Engineering and Analytical Science,
University of Manchester

Monday, 31st October, 1 p.m.
D202 Seminar room, School of Engineering, 2nd Floor

**Abstract:** The ability to combine a detailed description of the chemistry of a molecular model with an efficient exploration of the conformation space is a key point and a real challenge in material science. This is particularly true in the case of soft materials where phenomena taking place at different length scales (ranging from few picoseconds to microseconds and beyond) are responsible for their global properties. Due to the current computational power, all-atom (AA) simulations, which naturally describe the chemical details, are often constrained in time scale up to hundreds of nanoseconds and limited in the number of atoms. In order to overcome this problem, coarser or continuous models can be developed to expand at the same time the size and the time scale of the simulations. [1]

In this talk we will present two different approaches to combine continuous (specifically Computational Fluid Dynamics) or systematic CG with all-atoms force fields to efficiently model polymer aggregates in melt and solutions keeping the atomistic details only where they should be explicitly modelled. We will present results on test models of polyacaprolactone [2], polyethylene and polystyrene [3] and recent developments on nylon [4]. We will also present a simple method to implement a multiple time step algorithm for the simulation of such models. [5]

[1] H. A. Karimi-Varzaneh, N. van der Vegt, F. Müller-Plathe and P. Carbone, ChemPhysChem, 13, 3428-3439 (2012)
[2] N Di Pasquale, DL Marchisio, P Carbone, AA Barresi, Chemical Engineering Research and Design 91, 2275-2290 (2013)
[3] N. DiPasquale, D. Marchisio, P. Carbone, J. Chem. Phys. 137: 164111-164119 (2012)
[4] R. Gowers, P. Carbone, J. Chem. Phys 142: 224907 (2015)
[5] N. DiPasquale, R. Gowers, P. Carbone, J. Comp. Chem., 35, 16, 1199-1207 (2014)

More info: http://warwick.ac.uk/wcpm/seminars

WCPM
Warwick Centre for Predictive Modelling