DE LA RECHERCHE À L'INDUSTRIE

Séminaire

Vendredi 18 juillet 2014 à 10h30

Salle de réunion du SRMP – Bâtiment 520 - Pièce 109

Computational Modeling of Reaction-Diffusion Systems: From particle to hydrodynamic simulations

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I will discuss several different models for spatially-extended reaction-diffusion models. I will start by summarizing particle-based models and the First Passage Kinetic Monte Carlo (FPKMC) algorithm for simulating such particle models efficiently [A. Donev, V. V. Bulatov, T. Oppelstrup, G. H. Gilmer, B. Sadigh and M. H. Kalos, J. Comp. Phys., 229(9):3214-3236, 2010, arXiv:0905.3576].

I will also review some recent developments of extensions of FPKMC by other groups, which I believe are relevant for modeling of radiation-damage in metals. I will then discuss semi-continuum approaches suitable for modeling systems in which a small fast-diffusing agent reacts with large slow traps (sinks). In these models the concentration of the reactive agent is modeled at the continuum level (PDE) and the sinks are minimally-resolved as explicit particles [A. Pal Singh Bhalla, B. E. Griffith, N. A. Patankar and A. Donev, J. Chem. Phys., 139:214112, 2013, arXiv:1306.3159].

Finally, I will discuss fully-continuum fluctuating hydrodynamics models of chemically-reactive spatially extended systems, in which all reactions and diffusion are modeled at a continuum level (stochastic PDE). I will present some preliminary results for a recent model of bistable systems in which diffusion strongly affects the fluctuations in a steady nonequilibrium state [S. Tanase-Nicola, D. K. Lubensky, Phys. Rev. E 86:040103, 2012].

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