## *CYCLE DE CONFÉRENCES DE CHIMIE*

*Avec le concours de : Manufacture Française des Pneumatiques MICHELIN*
*Ecole Nationale Supérieure de Chimie de Clermont-Ferrand*
*Institut de Chimie de Clermont-Ferrand (ICCF UMR 6296)*
*U.F.R.S.T. Département de Chimie*

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# Jeudi 28 Novembre 2013 à 10h

Amphi de Chimie Paul REMI - (Site des Cézeaux)

# Pr. William R. Smith

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## Some Unique Monte Carlo Molecular Simulation Algorithms and Their Applications

The development of molecular simulation algorithms for predicting the thermodynamic properties of classical fluids and their mixtures began over 50 years ago. An ultimate goal is to predict system properties at both the macroscopic and molecular levels with the minimal need for experimental data. The two main approaches are Molecular Dynamics (MD) and Monte Carlo (MC); both are based on specifying an underlying mathematical model for the molecular interactions (force fields). MD has the advantage that it can calculate some thermodynamic properties and can also calculate transport properties and study systems away from equilibrium. Since its implementation is relatively straightforward, many commercial and public domain MD computer packages exist. On the other hand, MC is limited to the calculation of thermodynamic properties, for some of which it is in principle much more powerful than MD. However, implementations are often complex and both system and property dependent, and as a result only a few general computer packages exist. In this talk, I will describe three MC algorithms developed in my research group, which are making their way into simulation packages. These have expanded the application of MC methods to new classes of problems of both fundamental scientific interest and practical significance. The algorithms relate to the following calculations: (1) multi-species multiphase chemical reaction equilibria; (2) iso-energetic processes such as those involved in Joule-Thomson expansion and in the determination of adiabatic flame temperatures; and (3) chemical potentials for electrolyte solutions and the direct calculation of electrolyte solubility. No MD algorithms currently exist for the first two problems, and are computationally inefficient for the third. The practical importance of these algorithms is as follows: (1) many systems involving chemical reactions are modelled by assuming equilibrium behaviour; (2) iso-energetic processes are important in the design of refrigeration cycles, and hence can be used to screen for new environmentally benign refrigerants; they are also important in the design of explosives; (3) Electrolyte solutions are important in biological and geochemical systems, and for many industrially important systems.

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