**Abstract of the Habilitation thesis** defended the 3rd June 2009
by **Tony Lelièvre**, with title
**Mathematical and numerical analysis of some models for materials, from the microscopic scale to the macroscopic scale.**

The first part of the manuscript concerns multiscale (or micro-macro) models for complex fluids. The interest of these models is to avoid the assumption of a phenomenological constitutive law, by coupling a macroscopic description (momentum and mass conservation laws) on the velocity and pressure, with microscopic models for the evolution of the microstructures in the fluid at the origin of the non-Newtonian features of the fluid. The constitutive law consists in a formula giving the stress tensor as a function of the conformation of the microstructures. During my PhD thesis, we obtained some existence and uniqueness results, and proved the convergence of numerical methods adapted to these models. More recently, we propose a numerical method to couple micro-macro models (very precise but computationally expensive) with macroscopic models (coarser but much cheaper). Besides, we analyze a numerical method recently proposed to solve high dimensional partial differential equations in the context of the discretization of micro-macro models for polymeric fluids.

Our recent works on the subject essential deal with the longtime behaviour of these models. The aim is twofold: theoretically, the understanding of the physical content of a model typically requires a fine study of the stability of its stationary solutions, and the convergence to equilibrium ; numerically, the longtime stability of the numerical schemes is often crucial, since longtime simulations are typically used to compute stationary solutions. We show how to analyze the longtime behaviour of micro-macro models using entropy methods. This is then generalized to macroscopic models (like the Oldroyd-B model), and to numerical schemes used to discretize macroscopic models.

The second part of the manuscript summarizes recent works in molecular simulation, at the quantum level, or at the molecular level. At the quantum level, we are interested in Quantum Monte Carlo methods. These are probabilistic methods to compute the ground state of a molecule (the smallest eigenvalue of a Schrödinger operator). It consists in deriving Feynman-Kac representation formulae to apply Monte Carlo methods which are well-suited for this high-dimensional setting. We first propose a theoretical study of the Diffusion Monte Carlo method, and in particular of a bias introduced by the probabilistic representation called the fixed node approximation. Then, we analyze numerical methods used for the Diffusion Monte Carlo method, and propose a new strategy to enhance the sampling for the Variational Monte Carlo method.

In molecular dynamics, we study numerical methods to compute free energy differences. The configuration of a system is described through the positions (and sometimes also the momenta) of the particules (typically the nuclei of a molecular system), interacting through a so-called potential (which would ideally come from a computation at the quantum level to determine the ground state of the electrons, for a given position of the nuclei). The aim is to compute some averages with respect to the Boltzmann-Gibbs measure associated to this potential (averages in the canonical ensemble). Mathematically, this is a high-dimensional sampling problem of metastable (or multimodal) probability measures. The peculiarity of molecular dynamics is that some information is given on the "metastability direction" through the reaction coordinate. Using this data, many methods have been proposed for an efficient sampling of the Boltzmann-Gibbs measure. In a series of works, we analyze methods based on stochastic differential equations with constraints (whose solutions live on submanifolds which are level sets of the reaction coordinate). These are techniques to sample probability measures with support a high-dimensional submanifold. More recently,

we analyze adaptive methods which have been proposed to get rid of metastabilities. Mathematically, these are importance sampling method, with an importance function which is adaptively computed. We study the rate of convergence to equilibrium for such methods, using entropy methods. New discretization methods are proposed to enhance the efficiency.

The third and last part of the manuscript summarizes works coming from a collaboration with the company Rio Tinto (formerly Pechiney and Alcan), world leader for the technology of aluminium electrolysis cells. This collaboration started many years ago with C. Le Bris, and especially through the PhD thesis of J-F. Gerbeau. Mathematically, it amounts to analyzing and discretizing the magnetohydrodynamics equations for two immiscible incompressible fluids, separated by a free interface. We explain the industrial context and the modelling assumptions, we summarize the numerical approach we use (Arbitrary Lagrangin Eulerian method) and we give some properties satisfied by the numerical scheme (stability, mass conservation). We then show how this model can be used to study the metal pad rolling, which is a well known phenomenon leading to instabilities in the cells. Most of these results have been obtained during the PhD thesis.

More recently, we have been interested in a fundamental modelling problem, namely the moving contact line problem. The question is how to model correctly the dynamics of the boundary of the free surface (or free interface). Our two contributions are: (i) We propose a variational interpretation of the Generalized Navier Boundary Condition which has been recently proposed to model the moving contact line. This leads to a very natural implementation within an Arbitrary Lagrangian Eulerian method ; (ii) We analyze the stability of the numerical scheme.