Boltzmann inversion : measuring forces by watching movies

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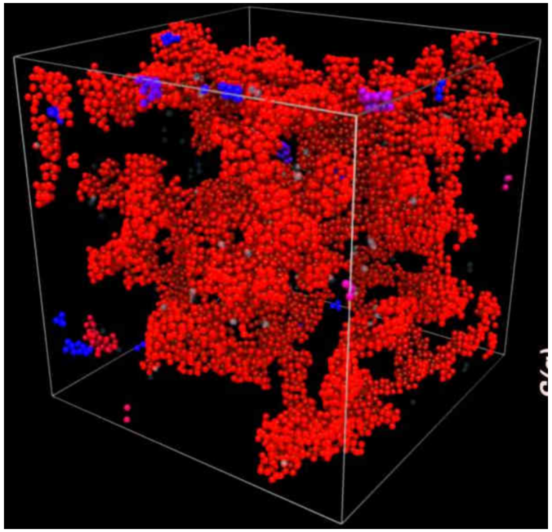

Confocal microscopy image of a colloidal gel. The goal is to infer directly from these images the particle interactions leading to the formation of this material.

Résumé

Statistical mechanics traditionally starts from microscopic interactions: given microscopic rules, interactions, equations of motion, one tries to make predictions about the emerging physical behaviour. It is sometimes useful to work backwards and ask the opposite question. Given a specific experimental system, say a complex fluid or a biological system, what are the rules governing the behaviour of that particular system? This amounts to addressing the inverse problem of guessing the model from the observed physics.

The inverse problem has a long history across various fields from statistical mechanics to soft matter and computational studies of complex systems with applications from self-assembly to non-equilibrium phase transitions in driven systems. Our broad goal is to develop an efficient method to guess particle interactions of a broad range of physical systems simply from watching movies. Earlier work mainly used techniques such as Iterative Boltzmann Inversion which requires a painful iterative process involving a new Monte Carlo simulation for each step of the iteration until convergence.

We will develop a method based on formal but straightforward manipulations of the pair correlation function to efficiently iterate towards the correct result. Mathematically, the method is well-defined and simple and necessarily leads to the correct solution. Preliminary results show that robustly inferring forces from a set of images involves solving a number of practical obstacles when only a finite number of data is available. Several exciting applications of the method will then be explored, involving both equilibrium and non-equilibrium physics with applications to active matter, biological systems and disordered systems.

The work will make use of basic concepts of statistical mechanics, and will explore different physical systems in colloidal physics and active matter. Watching lots of movies will also be required.

Keywords: statistical mechanics, colloids, active matter