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Boltzmann inversion: Measuring forces from watching movies

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In the context of Simons Collaboration "Cracking the Glass Problem" (https://scglass.uchicago.edu/**) and the ANR project THEMA involving L2C (Montpellier), LPTHE Jussieu and MSC (Paris)**

Scientific context: Statistical mechanics traditionally deals with predicting phase transitions and microscopic dynamics for systems that are both at thermal equilibrium or evolve far from equilibrium. Given some microscopic rules, interactions, equations of motion, researchers have tried for decades to make predictions about the physical behaviour emerging from a given set of rules.

It is sometimes useful to work backwards and ask the reverse 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 its observed physical behaviour.

As an example one can ask if the image below taken from a confocal microscopy experiment can be used to measure the actual interactions between the particles.

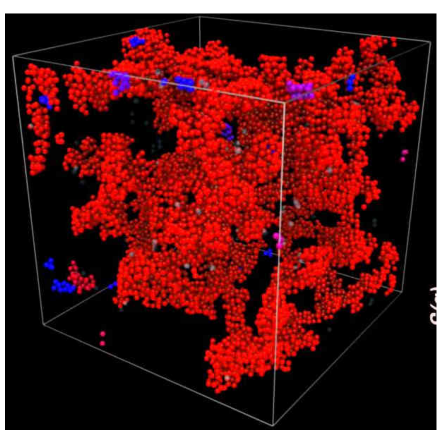

Figure: Confocal microscopy image of a colloidal gel [1]. The goal is to infer from the observed structure the forces between the particles that allow the formation of this beautiful structure.

The inverse problem has of course a long history across various fields from statistical mechanics to soft matter and computational studies of complex systems with many applications from self-assembly to non-equilibrium phase transitions in driven systems.

In this context, our broad goal is to develop a rapid, efficient method to guess the interaction between elementary particles of a broad range of physical systems simply from watching movies of those systems.

Description: Our primary goal is to develop a robust method to infer from the simple observation of microscopic particle configurations the forces between them. Earlier works have mainly used techniques such as Iterative Boltzmann Inversion [2] which requires a painful iterative process involving a new computer simulation for each step of the iteration until convergence of the structure is achieved.

Here 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.

Supervision: The work will take place mainly at the Laboratoire Charles Coulomb (CNRS and Université de Montpellier) and will be supervised by L. Berthier (DR1, CNRS, HDR) inside the team "Statistical Physics" of the Theoretical Physics Department. If the covid situation allows, visits to the University of Cambridge will be possible, since L. Berthier is currently on sabbatical there.

Références :

[1] P. Lu *et al.*, Nature 453, 499 (2008).

[2] D. Reith *et al.*, J. Comput. Chem. 24, 1624 (2003).