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The computational and mathematical challenges of simulating non-equilibrium molecular systems

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Statistical physics gives a probabilistic description of the microscopic dynamics of a system allowing one to deduce its macroscopic properties. The numerical realization of this idea: molecular dynamics, i.e the simulation of the dynamics of molecular and atomistic systems, provides scientists a "numerical microscopic" to conduct computer experiments allowing them to test physical theories and to make precise quantitative measurements of simulated systems. The static or equilibrium case is well understood and consequently powerful methods permit computing quantities of interest to high precision in the matter of hours in most cases. Furthermore, we have strong theoretical guarantees on the convergence. The dynamic or non-equilibrium case is much less well understood in contrast. Standard simulation methods of take weeks if not months of computation time and practitioner mostly have to guess if their simulation converges.

We give a brief introduction to non–equilibrium molecular dynamics with special focus on the computation of transport coefficients. Our talk will highlight why the non–equilibrium case is so much more difficult than the equilibrium case as well as some attempts at accelerating certain non–equilibrium methods.

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