



**Skalenkaskaden in komplexen Systemen**

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## **Hydrodynamics from dynamical non-equilibrium Molecular Dynamics**

Abstract:

We present a way to extend stationary state (equilibrium and nonequilibrium) Molecular Dynamics to time dependent nonequilibrium situations, including the dynamical processes of response and relaxation. The procedure, which we have called Dynamical Non-Equilibrium Molecular Dynamics (D-NEMD), to distinguish it from standard NEMD, only used to simulate stationary nonequilibrium states, is based on a generalization of linear response theory. The idea has been formulated by Onsager in the thirties in metaphysical language; given a solid foundation in the fifties by Green and Kubo (in the linear and nonlinear regime); and adapted to MD simulations by the present author (in collaboration with G.Jacucci and I.R.Mac Donald) in the seventies. It has been called the nonlinear Kubo-Onsager relation, connecting dynamical nonequilibrium averages or dynamical relaxations to stationary probability distribution functions (initial distribution) suitably sampled. To show the power of the method we apply it to study the onset of nonlinear behavior in transport processes of simple fluids, by looking at the convective circulation in liquids which establishes, as stationary asymptotic state, convective rolls. Moreover we will also apply the method to get the hydrodynamic.