Luigi Delle Site (FU Berlin) and **Rupert Klein** (FU Berlin):

Liouville-type equations for the n-particle distribution functions of an open system

Abstract:

We derive a mathematical model for an open system that exchanges particles and momentum with a reservoir from their joint Hamiltonian dynamics. The complexity of this many-particle problem is addressed by introducing a countable set of n-particle phase space distribution functions just for the open subsystem, while accounting for the reservoir only in terms of statistical expectations. From the Liouville equation for the full system we derive a set of coupled Liouville-type equations for the n-particle distributions by marginalization with respect to reservoir states. The resulting equation hierarchy describes the external momentum forcing of the open system by the reservoir across its boundaries, and it covers the effects of particle exchanges, which induce probability transfers between the n- and (n+1)-particle distributions. Similarities and differences with the Bergmann-Lebowitz model of open systems (P.G.Bergmann, J.L. Lebowitz, Phys.Rev., 99:578--587 (1955)) are discussed in the context of the implementation of these guiding principles in a computational scheme for molecular simulations.