

Lecture

Sara Bonella

CECAM, EPF Lausanne

Welcome to the MaZe, a new approach for simulating adiabatic systems

Tuesday, March 7, 2023

at 13:15 h

ESI, Boltzmann Lecture Hall

Abstract: In several domains of physics, including first principles simulations and classical models for polarizable systems, the minimization of an energy function with respect to a set of auxiliary variables must be performed to define the dynamics of physical degrees of freedom. In this talk, a recent and effective formalism to simulate this type of systems will be discussed: the Mass-Zero (MaZe) Constrained Dynamics [1]. In MaZe the minimum condition is imposed as a constraint on the auxiliary variables treated as degrees of freedom of zero inertia driven by the physical system. The method is formulated in the Lagrangian framework, enabling the properties of the approach to emerge naturally from a fully consistent dynamical and statistical viewpoint [2].

Several examples of current uses of MaZe will be rapidly presented, including first principles molecular dynamics based on orbital-free density functional theory (in which $N\log N$ scaling and exact Born-Oppenheimer dynamics are demonstrated) [3] and classical polarizable models [4]. A recent development enabling to study ionic transport for classical polarizable systems in the presence of an external magnetic field will also be discussed [5].

[1] A. Coretti, S. Bonella, G. Ciccotti, "Constrained molecular dynamics for polarizable models", *The Journal of Chemical Physics Communications*, 149 (2018) 191102

[2] S. Bonella, A. Coretti, R. Vuilleumier, G. Ciccotti, "Adiabatic motion and statistical mechanics via mass-zero constrained dynamics", *PCCP*, 22 (2020) 10775 [3] A. Coretti, T. Baird, R. Vuilleumier, and S. Bonella, "Mass-zero constrained dynamics for simulations based on orbital-free density functional theory", *The Journal of Chemical Physics*, 157 (2022) 214110 [4] A. Coretti, L. Scalfi, C. Bacon, B. Rotenberg, R. Vuilleumier, G. Ciccotti, M. Salanne, and S. Bonella, "Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems", *The Journal of Chemical Physics*, 152 (2020) 194701

[5] D. Girardier, A. Coretti, G. Ciccotti, S. Bonella "Mass-Zero constrained dynamics and statistics for the shell model in magnetic field", *The European Physical Journal B*, 94 (2021) art. N. 158

Ch. Dellago

February 16, 2023