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Grassmann Extrapolation of Density Matrices for Born-Oppenheimer Molecular Dynamics

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Résumé — Ab-initio molecular dynamics simulations are powerful but require expensive calculations. In general, the most costly part of the computation consists of the many resolutions of the Kohn-Sham equations arising at each time-step of the simulation. Proposing good initial guesses of the density matrix for the Self-Consistent Field procedure is therefore key to reduce the overall computational cost of the simulation.

In this talk, I will first present a method to provide such guesses based on previous calculations, exploiting the geometrical structure of the manifold to which the density matrix belongs, in order to perform linear extrapolation in a vector space, while at the same time, retaining the correct physical properties of the extrapolated density. I will also show how the time-reversibility of the simulation can be obtained. I will then illustrate the performance of the method by showing numerical results on a few real-life, multiscale, polarizable QM/MM simulations. Third, I will provide a theoretical analysis of the method for a better understanding of the observed results.

Mots clés — Ab initio ; molecular dynamics ; Grassmann manifold ; molecular descriptors