GRASSMANN EXTRAPOLATION AS A TOOL TO ACCELERATE BORN-OPPENHEIMER MOLECULAR DYNAMICS

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Born-Oppenheimer molecular dynamics (BOMD), is a powerful, yet expensive computational tool, where the system's nuclei are propagated classically on a potential energy surface generated on the fly with Density Functional Theory (DFT). The iterative solution to the DFT non-linear equations is the most computationally demanding step in BOMD: to speed up such calculations, various extrapolation strategies have been developed to use information available at previous simulation steps as a guess for the iterative procedure.

In this contribution, we present an approach to extrapolate density matrices, rank n projectors that codify the quantum mechanical information, by using computable maps between the Grassmann manifold where they are defined to its tangent space and back [1]. After comparing the new approach to the state of the art, we discuss its current limitations, with particular focus on energy conservation problems. We introduce a time-reversible extrapolation and an approximately reversible one, that exhibits optimal performance and good numerical stability.

References

[1] É Polack et al., *Grassmann Extrapolation of Density Matrices for Born–Oppenheimer Molecular Dynamics*, J. Chem. Theory Comput. 17 (2021), pp. 6965–6973.