

MULTISCALE METHODS FOR MOLECULAR DYNAMICS

The goal is to construct computational methods with error estimates for molecular dynamics, based on neural network approximations of the molecular dynamics potential and of constitutive relations for the stress tensor and heat flux in fluid dynamics.

On the smallest sub-atomic quantum scale, matter properties formed by interaction of nuclei and electrons are described by the Schrödinger equation. This equation has the attractive property that it includes all physical information about the nuclei-electron system without any empirical parameters (i.e. it is an *ab initio* model), thereby being an essential part of computational chemistry and physics. To solve the Schrödinger equation for several nuclei and electrons means to approximate the solution in several variables which is computationally feasible only for small systems. On the other hand, the Schrödinger equation is also used to derive more tractable approximations in the case of large nuclei-electron systems. For instance, *ab initio* molecular dynamics simulations for the nuclei, with electrons in their ground state, can be performed with ten thousand particles [2]. *Ab initio* molecular dynamics is derived by the Born-Oppenheimer approximation, which is valid for large nuclei-electron mass ratio and a ground state electron eigenvalue that is well separated from the other eigenvalues of the electron operator at fixed nuclei positions. The starting point for this project is the work [1] and [3]. The work [1] extends the semi-classical analysis to small eigenvalue gaps in the canonical ensemble, i.e. when the eigenvalue gap is not large compared to the temperature. The work [3] derives molecular dynamics expressions to determine the constitutive relations for the stress tensor and the heat flux in compressible fluids, for any temperature.

Molecular dynamics can be based on empirical potentials or *ab initio* potentials. In the case of empirical potentials substantial scientific work has been performed to determine force fields for chemical substances, see [4]. One advantage with such empirical potentials is that they are computational inexpensive to evaluate so that relative many particles and long simulation times are feasible. *Ab initio* potentials on the other hand have an advantage to capture general nuclei configurations and reactions including bond breaking. The drawback is the relative high computational cost to solve the electron eigenvalue problem in each time step of the nuclei dynamics. Recent research has shown that machine learning techniques can be used to approximate *ab initio* molecular dynamics potentials, see e.g. [6, 5].

The aim of this project is to analyze the accuracy for *ab initio* molecular dynamics using machine learning and neural network approximations.

REFERENCES

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