

Prospective Merger Between Car-Parrinello and Lattice Boltzmann Methods for Quantum Many-Body Simulations

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Abstract. Formal analogies between the Car-Parrinello (CP) ab-initio molecular dynamics for quantum many-body systems, and the Lattice Boltzmann (LB) method for classical and quantum fluids, are pointed out. A theoretical scenario, whereby the quantum LB would be coupled to the CP framework to speed-up many-body quantum simulations, is also discussed, together with accompanying considerations on the computational efficiency of the prospective CP-LB scheme.

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1 Introduction

Most successful methods in computational physics usually result from a clever resonance between physical intuition and mathematical transparency. This is certainly the case for the celebrated ab-initio molecular dynamics Car-Parrinello method (CPMD), which combines a very elegant field-theoretically modified Lagrangian with the mathematical/computational principles of dynamical optimization [1]. The result is the "magic" capability of tailoring the dynamic optimization in such a way that the fictitious dynamics of the electronic degrees of freedom leaves them on the desired Born-Oppenheimer surface associated with the actual ionic position at the end of the optimization procedure. This spawns a dramatic boost in the capabilities of computer simulation of molecular system including the electronic degrees of freedom (*ab initio*), which has taken the

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solid state community by storm for the last 25 years. Although on a very different domain, fluid-dynamics, the lattice Boltzmann method also offers a remarkable example of a powerful combination of physical intuition and mathematical transparency. The main idea of LB is to formulate hydrodynamics in terms of minimal Boltzmann kinetic equation, in which the dynamics of the fictitious molecules (populations) consists of a simple sequence of free-streaming and local relaxation on a regular lattice [2]. The main advantages over standard discretization of the partial differential equations of continuum fluid mechanics (Navier-Stokes) are space-time locality, easy handling of highly irregular boundaries, transparent inclusion of mesoscopic physics beyond the realm of continuum hydrodynamics. Rather than boosting the CFD frontier by orders of magnitude, the LB has greatly facilitated the simulation of an amazingly broad spectrum of fluid-related problems, ranging from the numerical simulation of turbulent flows of industrial relevance, all the way down to the multiscale translocation of biopolymers across biological membranes [3], and lately extended also to quantum and relativistic fluids [4].

The goal of this paper is twofold. First, we wish to point out a few mathematical analogies between CP and LB, which are well rooted into the physics of the problems dealt with by the two methods. Second, we venture on a speculative ground, and envisage a way of putting the LB technique at work to speed-up CP calculations. Although the viability of such speculative thoughts can only be judged by actual practice, we hope that the present considerations may offer a useful guideline for future development of combined CP-LB schemes.

2 Density functional theory for electronic structure simulation

The ab-initio calculation of the energy levels of molecules, including the self-consistent electronic configuration, requires the solution of the N -body Schrödinger equation. Unfortunately, this equation is literally untractable using conventional grid-discretization methods, the blocking hurdle being memory demand: encoding the N -body quantum wavefunction on a spatial grid with L^3 grid points, requires L^{3N} variables. The result is that even small molecules with, say $N=10$ atoms, on a mere $L=10$ grid points per linear dimension, would entail a totally unfeasible (10^{30}) number of variables. The infamous curse of dimensionality.

Fortunately, back in the early 60's, Kohn and Hohenberg were able to show that the molecular ground state is unambiguously fixed by the total electron density $n(\vec{r})$, i.e., a *single* scalar field [5,6]. This result paved way to effective one-body techniques for electronic structure calculations, i.e., the celebrated Kohn-Sham equations for the electronic orbitals, $\psi_k(\vec{r})$,

$$H_{KS}[n;R_I]\psi_k = E_k\psi_k, \quad (2.1)$$

where $H_{KS}[n;R]$ is the effective Kohn-Sham Hamiltonian, which depends on the total electron density $n(\vec{r}) = 2\sum_k |\psi_k|^2(\vec{r})$, as well as on the set of nuclear (ions) coordinates, here denoted collectively by the symbol R_I .