



A semi-analytical approach to molecular dynamics



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ARTICLE INFO

Article history:

Received 12 July 2014
Received in revised form 28 September 2015
Accepted 2 October 2015
Available online 13 October 2015

Keywords:

Energy conservation
Explicit integration
Exponential integrators
Fast Multipole Method
Krylov subspace projection
Molecular dynamics
Momentum conservation
Symplectic integrators

ABSTRACT

Despite numerous computational advances over the last few decades, molecular dynamics still favors explicit (and thus easily-parallelizable) time integrators for large scale numerical simulation. As a consequence, computational efficiency in solving its typically stiff oscillatory equations of motion is hampered by stringent stability requirements on the time step size. In this paper, we present a semi-analytical integration scheme that offers a total speedup of a factor 30 compared to the Verlet method on typical MD simulation by allowing over three orders of magnitude larger step sizes. By efficiently approximating the exact integration of the strong (harmonic) forces of covalent bonds through matrix functions, far improved stability with respect to time step size is achieved without sacrificing the explicit, symplectic, time-reversible, or fine-grained parallelizable nature of the integration scheme. We demonstrate the efficiency and scalability of our integrator on simulations ranging from DNA strand unbinding and protein folding to nanotube resonators.

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1. Introduction

With an ever-increasing need to understand complex behavior at the molecular level comes a high demand for computational methods that can simulate the macroscopic properties of systems from models describing the geometry and the interactions of their molecules. Molecular Dynamics (MD), in particular, has been proven helpful in nanomaterials and bio-engineering, as it allows to understand observed phenomena and predict observations that would be difficult or costly to make experimentally. The drastic improvements in computational power witnessed in recent years have allowed to investigate the structure, dynamics, and even thermodynamics of increasingly complex biological molecules. Yet, only modest progress has been made in extending the size of the time step used in numerical schemes: since explicit time integrators are favored for their ease of parallelization, the time step size remains restricted by the highest frequency components of the intrinsic dynamics of the nuclei—typically arising from stiff bonding between atoms.

This paper tackles this long-standing issue, and proposes the use of a semi-analytical integrator derived from [16,11] to reliably produce three orders of magnitude larger time steps in MD than regular integrators [60], for a resulting 30-fold speedup on average. We demonstrate the efficiency and scalability of our explicit, structure-preserving, and easily

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parallelizable approach on various typical MD simulation runs, varying from DNA unfolding and protein folding to nanotube resonators.

1.1. Related work

Classical versus Quantum Molecular Dynamics. While the motion of atoms and molecules can be obtained in principle by solving the time-dependent Schrödinger equation simultaneously for both electrons and nuclei, such a quantum mechanics approach remains too computationally prohibitive in practice to investigate large molecular systems (see [29] for recent advances). Instead, classical Molecular Dynamics uses Newtonian mechanics: it treats the nuclei (which are much heavier than electrons) as point particles in a force field that accounts for both their mutual interaction as well as the electronic interactions. This force field derives from a potential energy function that is formulated either from expectation values of the quantum system (see Section 2), or using empirical laws.

Numerical integration schemes. Given the typically large number of molecules involved in MD simulations, a fully analytical solution of the resulting Newtonian mechanical system is out of reach. Consequently, numerical methods that evaluate the position of each nucleus at (fixed or adaptive) time intervals are used to find computational approximations to the solutions, given proper initial conditions [28]. Established molecular dynamics simulators (e.g., *LAMMPS* [36]) often make use of the “velocity Verlet” integration scheme [60]—a simple, explicit integrator that can easily be parallelized and whose symplectic nature provides numerical benefits including exact momenta preservation and excellent energy behavior. However, solving for this initial value MD problem is particularly challenging due to the strong covalent bonds between nuclei, requiring painfully small time steps to properly capture the dynamics without generating instability. Turning these covalent bonds into rigid constraints (using RATTLE [4], SHAKE [51], or through internal variables [58] for instance) alleviates the most stringent time step restrictions, but at the cost of having to solve non-linear systems and a significant decrease in parallelizability. Computational efficiency has further increased over the past few years, either through algorithmic improvements (e.g., by computing the more distant interactions less often), or by leveraging specialized hardware for parallel computing (GPU computing). However, the ability to achieve longer time steps efficiently remains a major computational challenge.

1.2. Contributions

In this paper, we present a practical approach to computational molecular dynamics. We propose an efficient (explicit, second-order, and linear-time), structure-preserving (symplectic), and semi-analytical (exponential, or Gautschi-type¹) integration scheme that allows the use of significantly larger time steps than usual methods through its closed-form treatment of the strongest bonding forces deriving from harmonic potentials.

The key ingredient of our approach, i.e., the use of an exponential integrator combined with a Krylov-based evaluation of matrix functions, has been proposed in the context of quantum molecular dynamics [29]; but hasn’t gained acceptance in classical MD so far. Yet, we will demonstrate that its use is particularly appropriate for Hamiltonian systems involving a potential energy with a strong harmonic part, such as the harmonic potentials of bounded atoms in combination with regular non-bonded potentials in MD, or in coarse-graining methods [34]. Moreover, our algorithm scales linearly with the number of atoms and exhibits excellent long-term preservation of momenta and energy, which are hallmarks of symplectic and time-reversible integrators. Finally, our scheme is easily parallelizable as it involves sparse matrix and vector operations, rendering it particularly attractive as a basis for large-scale MD computations.

2. Background

For completeness, we begin our exposition by reviewing the forces involved in molecular dynamics, then discussing the resulting stiffness of the differential equations that we wish to numerically simulate.

2.1. Ehrenfest potential

To bypass the difficulty of solving the time-dependent Schrödinger equation simultaneously for both electrons and nuclei, Ehrenfest was the first to describe the evolution in time of a molecular system using Newtonian (classical) dynamics where nuclei are simply submitted to a force field deriving from a single, effective potential, given as the mean expectation value

¹ The history of so-called *exponential integrators* [30] goes back to the late 1950s, when Joseph Hersch pointed out that traditional numerical integrators do not compute the correct solution even if the differential equation is analytically solvable. He then proposed an exact integration scheme for linear ordinary differential equations with constant coefficients, see [24]. Three years later, Walter Gautschi proposed the integration of the non-linear part of the variation of parameters formula with trigonometric polynomials, see [16]. Almost 20 years later, this approach was combined with the trapezoidal rule [11] and a significant improvement was achieved in the late 1990s by Bosco García-Archilla, who introduced *filter functions* for the non-linear part arguments in this context [15]. Today, there exists a variety of exponential integrators, like multistep integrators of this type (cf. [9]), Rosenbrock methods (cf. [50]), and Runge–Kutta-based methods of simple (cf. [37]) and higher orders (cf. [14]) aiming at finding an efficient approximation of the solutions of stiff differential equations.

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