

Molecular dynamics algorithm for multiple time scales: Systems with disparate masses

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A frequently encountered problem in molecular dynamics is how to treat the long times that are required to simulate condensed systems consisting of mixtures of light and heavy particles. Standard methods require the choice of time step sufficiently small to guarantee stable solution for the low mass component with the consequence that these simulations require a very large number of central processing unit cycles to treat the relaxation of the heavier component. In this note, we present a new method that allows one to use a time step appropriate for the heavy particles. This method uses a similar idea to numerical analytical propagator algorithm, an algorithm we invented to treat high frequency oscillators interacting with low frequency baths and is based on a choice of a reference system for the light particle motions. The method is applied to the case of a liquid containing 864 Lennard-Jones spheres, 824 of these particles having a mass, $M = 100$ and 40 spheres picked at random have a mass $m = 1$. It is shown that molecular dynamics using the new algorithm runs seven to ten times faster than standard methods and this approach as well as suitable generalizations should be very useful for future simulations of quantum and classical condensed matter systems.

I. INTRODUCTION

Consider a system consisting of a mixture of light (mass = m) and heavy spheres (mass = M). In such systems, there is a disparity in the molecular dynamic time scales. If one wishes to simulate such systems using the standard integrators of molecular dynamics, then the maximum time step that can be used to integrate the equations of motion must be chosen to insure accurate integration of the low mass component with the consequence that a very small time step is needed. When a large disparity in time scales exists, a very large number of central processing unit (CPU) cycles will be required to allow the slow degrees of freedom to fluctuate enough to obtain converged time averages for the whole system.

In this paper, a method for accelerating the simulation of such systems is presented. This method, called RESPA (reference system propagator algorithm), is a variant of the numerical analytical propagator algorithm (NAPA), algorithm that we invented for treating the problem of high frequency oscillators coupled to low frequency oscillators.¹ The RESPA method is based on numerical solutions of the reference system equations. The gist of the method is to define a dynamical reference system for the fast motion and to derive equations of motion for the deviation $\delta(t)$ of the fast coordinates from the reference system coordinates. These deviations are coupled to the equations of motion of the slow coordinates. The fast dynamical system is integrated for n small time steps $\omega\delta t$ holding the slow coordinates fixed. The time dependence of the reference system is then fed into the coupled equations for $\delta(t)$ and the slow coordinates and the resulting equations are integrated for one large time step

$\Delta t = n\delta t$. The initial conditions for each large time step are then chosen so that this deviation $\delta(t)$ is zero with the consequence that the deviation is always kept small. The only approximation in this algorithm springs from the numerical integrator used to integrate the equations of motion of the reference system and the coupled equations. Otherwise, the method is self-correcting and exact. For simplicity, the reference system is taken to be the Hamiltonian of the original system with the slow coordinates held fixed at their values at the beginning of the time step.

Teleman and Jönsson² have proposed a multiple time-step (TJMTS) method in which the forces are separated into slow and fast components. This separation yields a set of coupled equations of motion for the slow and fast degrees of freedom. TJMTS uses a small step δt to advance the fast degrees of freedom n steps holding the slow variables fixed. The slow degrees of freedom are then updated using a time step $\Delta t = n\delta t$. This method does not correct for the errors incurred in the approximate factorization of the equations of motion, a fact which shows up in poor energy conservation. This is well illustrated when we compare the results of RESPA, TJMTS, and velocity Verlet³ (using a small time step). Swindoll and Halle⁴ have proposed a more accurate multiple time-step method than Teleman and Jönsson, but their method requires high-order spatial derivatives of the potential and is therefore more computationally intensive than RESPA.

For simplicity, we apply this new method to the simulation of a mixture of Lennard-Jones spheres consisting of 824 heavy spheres of mass $M = 100$ and 40 light spheres of mass $m = 1$. For Lennard-Jones (LJ) spheres, the two time scales are $\Delta t_f = \sqrt{m\sigma^2}/\epsilon_1$ and $\Delta t_s = \sqrt{M\sigma^2}/\epsilon_2$, where σ_i and ϵ_i are the Lennard-Jones parameters for component i . For il-

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web jul 27 2020 chizuko brought some origami folding paper and told sadako of a legend she explained that the crane a sacred bird in japan lives for a hundred years and if a sick person folds 1 000 paper cranes then that person would soon get well after hearing the legend sadako decided to fold 1 000 cranes and pray that she would get well again

sadako and the thousand paper cranes litcharts - Dec 06 2022

web after sadako s death in october of 1955 her classmates at school folded the remaining 356 cranes needed to reach one thousand after her funeral her class collected sadako s letters and journals and published them as a book which they called kokeshi

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web sep 30 2021 one thousand paper cranes will tell sasaki s true story from her time in hiroshima to her diagnosis to her message of hope raymond described the film saying it shows for the first time the untold truth behind these two remarkable women sasaki and coerr and how their lives are intricately connected

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web jan 9 2001 sadako and the thousand paper cranes tells the true story of a young girl named sadako sasaki who died in 1955 of leukemia resulting from radiation poisoning eleven year old sadako chan was a fast strong runner her dream was to become the best runner in school one afternoon after finishing first in school race sodako chan felt

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web sadako and the thousand paper cranes is a children s historical novel written by canadian american author eleanor coerr and published in 1977 it is based on the story of sadako sasaki the book has been translated into many languages and published in many places to be used for peace education programs in primary schools

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web jan 28 2020 sadako and the thousand paper cranes is a work of historical fiction based on the life of a real girl who fell ill with leukemia caused by radiation from the atomic bombing of hiroshima by the united states author eleanor coerr first learned about sadako sasaki when she traveled to japan in 1949

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web as the rainy season settles in sadako grows pale and listless and is unable to eat though her mother brings her some of her favorite foods in a special care package sadako s swollen gums prevent her from enjoying them sadako s mother hopes that when the sun comes back out sadako will be feeling better

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