

Adaptive Resolution Molecular Dynamics Simulation with Constant in H

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Abstract— Molecular dynamics simulations are done to observe the behavior of the dynamics at microscopic level of systems during a period of nanoseconds. Advanced computation is done for a large number of degrees of freedom which belong to the atoms. The coarse grained systems have larger components compared to the fine-grained systems. This article outlines an innovative version of the adaptive resolution scheme which connects the coarse-grained system with the fine-grained system based on a force interpolation scheme, taking into consideration a constant which maintains the temperature of the system around the value of 323 K degrees. The Hamiltonian derivation has been used for expressing the interactions which appear inside the system. The novel solution has been tested on the butane system and implemented in the GROMACS molecular dynamics software. The introduction of the constant in the Hamiltonian derivation lead to the creation of a thermostat for the butane system.

Keywords— molecular dynamics, thermostat, Hamiltonian derivation, coarse-grained, fine-grained

I. INTRODUCTION

As technology advanced, molecular dynamics simulations are much more used to outline the events which happen at atomic level during a period of nanoseconds [1].

Computer modeling allows the investigation of physical mechanisms and to assess their properties. The trajectories of the atoms are given by Newton's second law of motion. The properties of systems are studied in physics, material science, nanotechnology, chemistry, molecular biology where temperature represents an important parameter [2].

The system's complexity is given by the mobility of the ions. Due to the large number of particles which are subject to the simulation, the computation of the current state takes a lot of time, even for today's most powerful computers.

The degrees of freedom have to be diminished in order to have a proper physical system. This leads to modeling approaches that consider the coarse-grained (CG) methods at multiscale level [3]. Coarse-graining is bridged by having a fine-grained (FG) model between the two parts of the system. The fine-grained part of the system is based on atom model. The interactions of potentials belonging to the coarse-grained model result from the mapping the fine-grained model to the coarse-grained model [4].

The adaptive resolution scheme (AdResS) is a molecular dynamics simulation based on a multiscale approach that

couple coarse-grained regions with fine-grained regions [5]. The scheme considers that the molecules adjust their resolution based on their current coordinates within the system.

The coupling between several molecules is comprised within one coarse-grained bead. The Martini coarse-grained force field acts upon the computational gains [5]. Atomistic descriptions of the butane are needed at the vicinity of a molecule [6]. The Lennard-Jones interactions appear between ions, as well as electrostatic interactions [6].

In this paper, molecular dynamics simulations are conducted to study the temperature evolution inside a butane system. The temperature is a significant parameter of a system because it characterizes the system's ergodicity, entropy, state and stability [2].

The Hamiltonian version of the adaptive resolution scheme [7, 8] is improved by considering a constant which is scaled by the λ factor. Based on this, the thermodynamic equilibrium is maintained in every region.

The paper is organized as follows. In section 2 is presented the multiscale model based on the adaptive resolution scheme and the details of the simulation. The results and discussions are outlined in section 3. Section 4 presents the conclusions.

II. COMPUTATIONAL METHODS

Molecular dynamics simulations characterize the multiscale model which is tested. The system to be analyzed presents a transition region between the coarse-grained and the fine-grained regions.

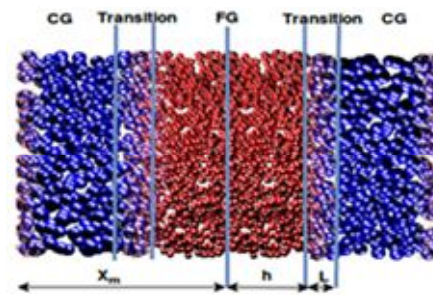


Fig. 1. Molecular system structure

In Figure 1, X_m is the coordinate in the reference system for the center of fine-grained region, h is half of the length of the fine-grained region and L is the length of transition (hybrid) region.

To combine the two systems, FG and CG, it was developed the multiscale simulation technique [9, 10, 11, 12, 13]. This method combines the two resolution by coupling them with an interpolation formula for the force:

$$F = \lambda(X_\alpha)\lambda(X_\beta)F_{\alpha\beta}^{FG} + [1 - \lambda(X_\alpha)\lambda(X_\beta)]F_{\alpha\beta}^{CG} \quad (1)$$

where α and β are the labels of two CG molecules, $F_{\alpha\beta}^{FG}$ and $F_{\alpha\beta}^{CG}$ are the forces derived from the atomistic, respectively coarse-grained, potential, X_α and X_β are the coordinates of the center of CG molecules α and, respectively, β .

The weight function λ is defined in such a way that it is zero in the CG region and one in the FG region. In the hybrid region, λ is smooth and monotonic [7, 13].

For simplifying the presentation, it is considered that the space factor λ is function only on the X coordinate reference system. On the Y and Z coordinate axis, λ is constant.

Because the chemical potential differs between the fine-grained and coarse-grained systems, the differences are equilibrated by adding a constant into the Hamiltonian expression [14]. The forces at fine-grained and coarse-grained levels are parameterized such that they are compatible, but their integrations, namely the potentials of the interactions between particles, might differ through a constant.

The classical molecular dynamics simulations are represented by the Hamiltonian function [11]:

$$H(r, p) = K(p) + V(r) \quad (2)$$

where K is the kinetic energy, V the interaction energy between the particles, p and r are the generalized momentum and position coordinate of particles.

In multiscale simulation, the interaction energy consists of four individual terms: the fine-grained bonded and non-bonded interactions (V_{FG}^b and V_{FG}^{nb}) and the coarse-grained bonded and non-bonded interactions (V_{CG}^b and V_{CG}^{nb}). With these notations, it is defined the multiscale interaction energy:

$$V^m(x) = \lambda(X(x)) V_{FG}^{nb}(x) + [1 - \lambda(X(x))] V_{CG}^{nb}(X(x)) + V_{FG}^b(x) + V_{CG}^b(X(x)) + \lambda(X(x)) c \quad (3)$$

where it is considered only the X coordinate according to the factor λ . It is noted by $x = x_{ai}$ the X coordinate of

the FG particle with the number i in the CG molecule with the number α . The CG molecule α is described by the $X = X_\alpha$ coordinate of its center of mass.

In Figure 2 more coarse-grained molecules with corresponding fine-grained particles and the parameters x_{ai} and X_α are represented.

It is expressed X_α according to x_{ai} :

$$X_\alpha = \frac{\sum_i m_{ai} x_{ai}}{\sum_i m_{ai}} = \frac{\sum_i m_{ai} x_{ai}}{M_\alpha} \quad (4)$$

where m_{ai} is the mass of the i atom and M_α is the mass of the α molecule.

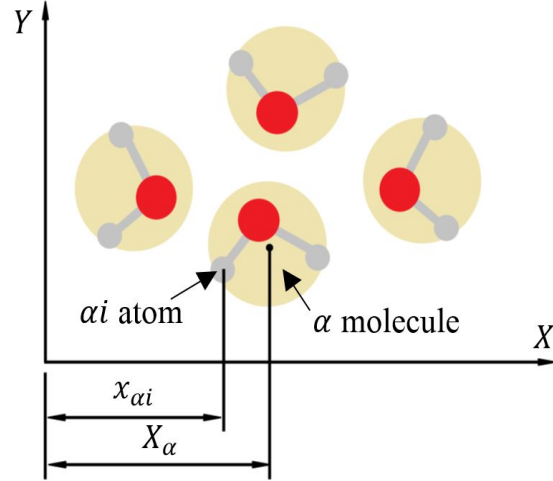


Fig. 2. The coordinates for a FG particle and for a CG molecule

The space factor λ is defined as follows:

$$\lambda(X) = \cos^2 \left[\frac{\sqrt{(X_\alpha - X_m)^2 - h}}{L} \frac{\pi}{2} \right] \quad (5)$$

The X component of force in ai atom is obtained by (3):

$$-F^m(x_{ai}) = \frac{\partial \lambda}{\partial x_{ai}} V_{FG}^{nb} + \lambda \frac{\partial V_{FG}^{nb}}{\partial x_{ai}} + (1 - \lambda) \frac{\partial V_{CG}^{nb}}{\partial x_{ai}} - \frac{\partial \lambda}{\partial x_{ai}} V_{CG}^{nb} + \frac{\partial V_{FG}^b}{\partial x_{ai}} + \frac{\partial V_{CG}^b}{\partial x_{ai}} + c \frac{\partial \lambda}{\partial x_{ai}} \quad (6)$$

The derivative of λ with respect x_{ai} is

$$\frac{\partial \lambda}{\partial x_{ai}} = \frac{\partial \lambda}{\partial X_\alpha} \frac{\partial X_\alpha}{\partial x_{ai}} = \lambda' \frac{\partial X_\alpha}{\partial x_{ai}} \quad (7)$$

with λ' notation for the derivative of λ with respect X_α . Using (4), results

$$\frac{\partial \lambda}{\partial x_{ai}} = \lambda' \frac{m_{ai}}{M_\alpha} \quad (8)$$

Taking into account that

$$F_{ai}^{nb} = -\frac{\partial V_{FG}^{nb}}{\partial x_{ai}}; F_{ai}^b = -\frac{\partial V_{FG}^b}{\partial x_{ai}}; \quad (9)$$

$$F_\alpha^{nb} = -\frac{\partial V_{CG}^{nb}}{\partial X_\alpha}; F_\alpha^b = -\frac{\partial V_{CG}^b}{\partial X_\alpha},$$

are the non-bonded and bonded forces in the atom αi , respectively in the molecule α .

Using (8) and (9) in (6), results

$$F^m(x_{ai}) = \left(\frac{-m_{ai}}{M_\alpha} \lambda' V_{FG}^{nb} + \lambda F_{ai}^{nb} + F_{ai}^b \right) + \frac{m_{ai}}{M_\alpha} \left[\lambda' (V_{CG}^{nb} - c) + (1 - \lambda) F_\alpha^{nb} + F_\alpha^b \right] \quad (10)$$

The terms that contain the energy are separated:

$$F^m(x_{ai}) = \lambda F_{ai}^{nb} + F_{ai}^b + (1 - \lambda) \frac{m_{ai}}{M_\alpha} F_\alpha^{nb} + \frac{m_{ai}}{M_\alpha} F_\alpha^b + \frac{m_{ai}}{M_\alpha} \lambda' (V_{CG}^{nb} - V_{FG}^{nb} - c) \quad (11)$$

III. RESULTS AND DISCUSSION

The system was tested using the molecular dynamics simulation package, GROMACS. Message passing interface (MPI) is used for parallelizing the processes, resulting in a shorter execution time.

The simulation was done on an Asus ZenBook Pro UX501VW computer with an Intel Core i7-6700HQ processor. It has 8 threads at a frequency of 2.6 GHz. The butane simulation environment has been used. This comprises 36900 atoms. 323K is the reference temperature.

The adaptive resolution molecular dynamics simulation having a constant in H is done in parallel, where the

computation involves the all the computer's processors. Each simulation has 10,000 steps.

Every processor computes firstly the bonded fine-grain and course-grain interactions. The multiscaling forces depend on the constant c which varies as in Table 1. They are computed using formula (11). After this step the velocities and the positions get computed again.

TABLE I. TEMPERATURE VARIATION ACCORDING TO THE CONSTANT

Test No.	Simulation parameters	
	Constant	Temperature [K]
1	- 1.0	330.313
2	- 0.8	329.013
3	- 0.6	327.952
4	- 0.4	327.178
5	- 0.2	326.661
6	0.0	326.487
7	0.2	326.624
8	0.4	326.854
9	0.6	327.254
10	0.8	327.482
11	1	327.832

Gromacs Energies

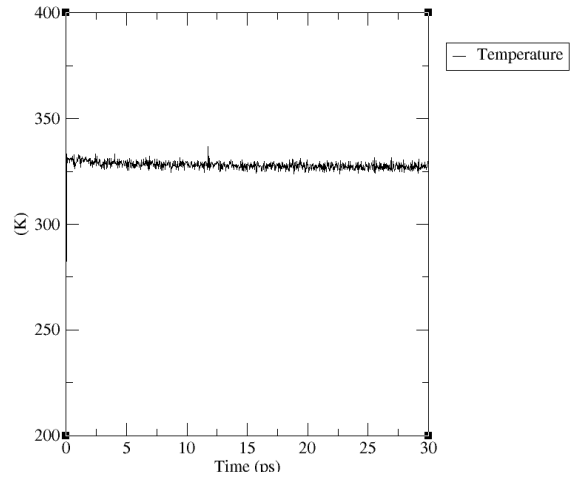


Fig. 3. Temperature evolution when the constant is equal to 1

Compared to the reference temperature of 323 K, the system temperature varied around ± 7 K. Due to this, the feasibility of the Hamiltonian adaptive resolution molecular system is demonstrated.

The evolution of the temperature where the constant for computing the forces is involved can be observed in Figure 3. The temperature varied around the value of 327 K, where the difference of 4 K compared to the reference value is statistically acceptable.

IV. CONCLUSIONS

The butane is used as a test case to validate the proposed Hamiltonian adaptive resolution molecular system with constant. The studied system presents the adequate results, being studied for different situations where the constant varied. The temperature varied inside a reasonable range of ± 7 K, demonstrating that the proposed calculations are feasible.

The system is intended to be tested on several systems for generalizing the theory.

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