Simulations on DPD Thermostat and Standard MD for Different Systems

SUNITA ANDREEA MOGA[1]*, NICOLAE GOGA[2,3], SVETLANA BAOUKINA[4], CATINCA SECUIANU[5,6], ANTON HADAR[1,7]

[1]Politehnica University of Bucharest, Department of Materials Strength, 313 Spl. Independenţei, 060042 Bucharest, Romania

[2] Politehnica University of Bucharest, Department of Engineering in Foreign Languages, 313 Spl. Independenţei, 060042 Bucharest, Romania

[3]University of Groningen, Groningen,the Netherlands, Molecular Dynamics Group

[4] University of Calgary, Department of Biological Sciences,Calgary, Canada

[5] Politehnica University of Bucharest, Department of Inorganic Chemistry, Physical Chemistry & Electrochemistry, 1-7 Gh. Polizu Str., 011061 Bucharest, Romania

[6]Department of Chemical Engineering, Imperial College London, South Kensington Campus, SW7 2AZ London, United Kingdom

[7]Academy of Romanian Scientists, 54 Splaiul Independentei, 50085, Bucharest, Romania

This article presents a benchmark between Dissipative Particle Dynamics (DPD) thermostat and Standard Molecular Dynamics (MD) simulations for three different systems: a water cube, a small dipalmitoylphosphatidylcholine (DPPC) bilayer in water, and a large DPPC bilayer in water. The DPPC phospholipids' molecule consists of a hydrophilic head and two hydrophobic tails. The molecular dynamics simulations results for the three above systems as function of number of cores are shown.

Keywords: molecular dynamics, thermostats, friction

Classical atomistic simulations and, in particular, molecular dynamics (MD) simulation, have become a useful tool for studying the physico-chemical properties of molecular systems. Nowadays, the algorithms of molecular dynamics are considered an important part in the study of the dynamical properties of polymers [1], proteins, lipids, and other systems [2]. One goal of using MD by both academia and industries is investigating systems evolution with time and their properties at high resolutions, on the length and time scales not accessible to the experimental methods.

Ideally, computational algorithms should keep the temperature constant in a molecular dynamics simulation. However, because of numerical errors this is not usually the case. For this reason algorithms (thermostats) to be used in molecular simulations for maintaining the temperature constant are conceived. One recent advance is the development of Dissipative Particle Dynamics (DPD) thermostats that have the property of preserving the total momentum of a molecular system which is important for large scales simulations, hydrodynamics, etc. In a previous article [3] we reported the theory and different properties of new DPD-types of thermostats. The goal of this article is to study computational efficiency of the DPD-like thermostat [3] and compare it to standard molecular dynamics (MD) simulations [4] for different molecular systems. The work was done through a research collaboration consortium between Molecular Dynamics Group, University of Groningen, one of the well-known groups into the MD domain, researchers from University of Calgary, Canada, and University Politehnica of Bucharest, Romania. The simulations were done in GROMACS v. 4.6 [5,6], one of the most popular open software available in the molecular dynamics field.

Theory: Dissipative Particle Dynamics (DPD) thermostat

In this section we will shortly present the Dissipative Particle Dynamics (DPD) thermostat. In this thermostat, Galilean-invariant friction and noise act on velocity differences for a pair of particles, while the time evolution of the system is described by a Hamiltonian. The isotropic case only was considered with friction and noise applied to all three velocity components, and restricted to one neighbour within the given range. For a detailed description we refer to [3]. In the following we will summarize this theory with a special focus on the iso case [3]. For DPD-iso case the friction and noise are applied to relative difference of velocities between pair of particles, isotropically to the velocity difference vector, irrespective of its direction. A full DPD [3] has also two others cases:

- *par*: the velocity difference vector is split into a component parallel to the inter-particle vector.
- *perp*: the velocity difference vector is split into a component perpendicular to the inter-particle vector.

If we consider a pure DPD, like in [7], only the *par* case would be used; the perp case was introduced by Junghans et al. [8]. In all variants a damping rate γ and a velocity factor *f* are taken into consideration.

$$f = 1 - \exp(-\gamma\Delta t)$$

Both f and γ are influenced by the interparticle distance. A cutoff distance should be chosen beyond which the impulsive friction and noise is not applied *(f=0)*. For the computation of forces and also for the computation of the inter-particle distance, usually one uses the short range pair particle list. For reducing the complexity, we use the selection of one neighbor per particle at random.

* *emaol: moga.sunita.andreea@gmail.com; Tel.: (+40) 0727741613*

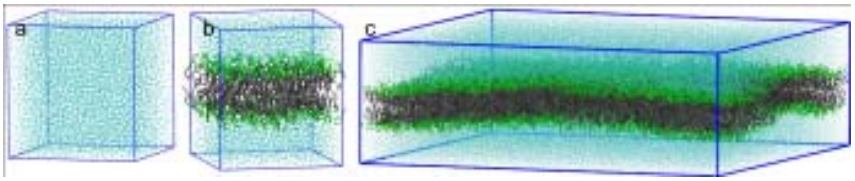


Fig. 1. Simulated systems: a small water cube (a), a small DPPC bilayer in water (b), and a large DPPC bilayer in water (c)

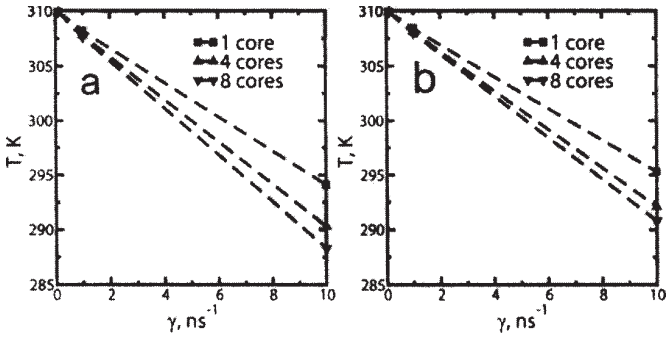


Fig. 2. Temperature deviations in DPD-like simulations: actual temperatures for a small water cube (a) and a small bilayer (b) are shown as a function of friction rate for simulations on different numbers of processors; the reference temperature is 310 K.

- for i, j simulation pair step do:
  - choose the velocity reduction factor – $f = f_{iso}$
  - determine the velocity noise factor – g
  - construct the relative velocity vector – v
  - if iso:
    - choose 3 random numbers $\xi = (\xi_1, \xi_2, \xi_3)$ from a standard normal distribution (mean=1, sd=1)
    - construct the vector - Δv
  - distribute the relative velocity change over the 2 particles:

$$v_i \leftarrow v_i + m_j/m_i+m_j \Delta v$$

$$v_j \leftarrow v_j - m_i/m_i+m_j \Delta v$$

Bellow we will present the algorithm for the *iso* case:

Simulations procedure

The Dissipative Particle Dynamics (DPD) thermostat with pairwise impulsive friction was implemented in the version v.4.6 of GROMACS software. Parallelization is based on domain decomposition.

The system setup included: a small water cube, a small dipalmitoylphosphatidylcholine (DPPC) bilayer in water, and a large DPPC bilayer in water (fig. 1). The coarse-grained (CG) model MARTINI was used for all simulations. In this force-field, molecules are represented by particles that group approximately four heavy atoms together. The water cube contained 8312 CG particles, the small bilayer contained 288 lipids, and 8056 CG particles in total, the large bilayer was composed of 4608 lipids, and 146210 CG particles in total.

We investigated the performance of this DPD-like thermostat, and compared it to the standard molecular dynamics (MD) simulations. For non-bonded interactions, the standard cutoffs for the MARTINI force field were used: the Lennard-Jones potential was shifted to zero between 0.9 and 1.2 nm; the Coulomb potential was shifted to zero between 0 and 1.2 nm with a relative dielectric constant of 15. The cutoff distance for application of the impulsive friction was set to 1.2 nm. The time step was 20 fs with neighbour list updates every 10 steps. The pressure of 1 bar was maintained using the Berendsen barostat with a time constant of 4 ps and a compressibility of $5 \cdot 10^{-5}$ bar^{-1}. Isotropic scheme was used for the water cube, and semi-isotropic scheme for the bilayers. Lipids and water were coupled separately to a reference temperature of 310 K. For standard MD simulations, the velocity rescaling thermostat with a time constant of 1 ps was used. For DPD-like simulations, the friction rates of 0.1, 1, and 10 ps^{-1} were used for small systems (bilayer and water), and of 1 ps^{-1} for the large bilayer. The small systems were simulated on 1, 4, and 8 cores. The large bilayer was simulated on 36, 72, 144, and 288 cores. The simulation time was 100 ns for the water cube, and 200 ns for the bilayers.

Results and discussions

Temperature deviations from to the reference temperature of 310 K for different friction rates and different numbers of processors are presented in figure 2. For both the water cube and the bilayer, the actual temperature in simulations decreases strongly with increasing the friction rate. This result is consistent with previously reported DPD-like simulations. For both systems, the temperature slightly decreases for parallel simulations compared to serial simulations. This decrease is pronounced for larger friction rates, and smaller for lower friction rates. Temperature deviations become negligible for larger systems simulated on the large number of cores (fig. 3).

The computational efficiency of parallel simulations using the DPD-like thermostat is comparable to the standard GROMACS MD simulations (fig. 4). The software with the DPD-like thermostat performance is somewhat

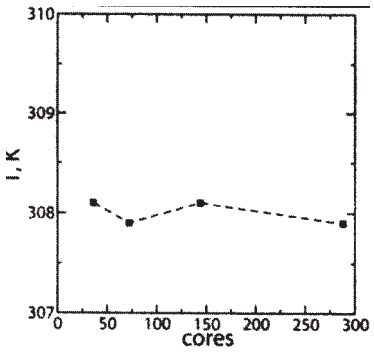
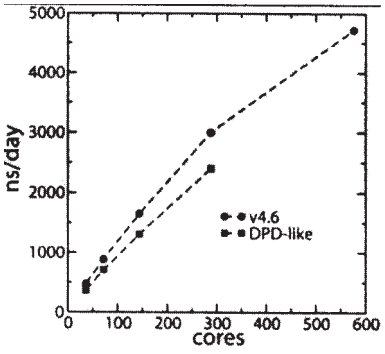


Fig. 3. Temperature deviations in DPD-like simulations. Actual temperature for a large system (fig. 1c) simulated on a large numbers of cores at a friction rate of $1ps^{-1}$. The reference temperature is 310 K.



Fig,4. Gromacs scaling. Simulations of the large bilayer (fig. 1c) on different numbers of processors in DPD-like simulations compared to the standard Gromacs (v.4.6) simulations.

lower compared to standard MD, however, the scaling remains high when used on a large number of cores (up to 288).

Conclusions

This article presents the theoretical background and a benchmark comparison between the DPD thermostat and standard molecular dynamic simulation. Some properties like temperature were analyzed on three different systems: a small water cube, a small DPPC bilayer in water, and a large DPPC bilayer in water. For the studied property, the temperature, the thermostat results provide a predictable behaviour in all three systems. Another important conclusion is that the computational efficiency of parallel simulations using the DPD thermostat is comparable with the standard molecular dynamics simulations. Also, the scaling remains high when a large numbers of cores are used.

Future work includes applying DPD-type algorithms for studying the characteristics and properties of different polymers with the scope of defining novel ones.

In [9] has been studied the combining Berendsen Thermostat with DPO for polymer simulation.

Acknowledgement: The work has been funded by the Sectoral Operational Programme Human Resources Development 2007-2013 of the Ministry of European Funds through the Financial Agreement POSDRU/159/1.5/S/132395.

References

1. REITH, D., MILCHEV, A., VIRNAU, P., BINDER, K., Macromolecules, **45**(10), 2012, p. 4381
2. AUFFINGER, P., LOUISE-MAY, S., WESTHOF, E., J. Am. Chem. Soc., **117**, 1995, p. 6720
3.GOGA, N., RZEPIELA, A. J., DE VRIES A. H., MARRINK, S. J., BERENDSEN, J. C., J. Chem. Th. Comp., **8** (10), 2012, p. 3637
4. BERENDSEN, H. J. C., VAN DER SPOEL, D., VAN DRUNEN, R., Comput. Phys. Commun., **91** (1-3), 1995, p. 43
5. GROMACS tool and documentation, www.gromacs.org
6. VAN DER SPOEL, D., LINDAHL, E., HESS,B., GROENHOF, G., MARK, A.E., BERENDSEN, H. J. C.,
J. Comput. Chem., **26** (16), 2005, p. 1701
7. ESPANOL, P., WARREN, P., Europhys. Lett., **30**, 1995, p. 191
8. JUNGHANS, C., PRAPOTNIK, M., KREMER, K., Soft Matter, **4**, 2008, p. 156
9. MOGA, A.S., GOGA, N., HADAR, A., Mat. Plast. **50**, no. 3, 2103, p. 196

Manuscript received: 26.06.2014