Procedia Computer Science

Volume 29, 2014, Pages 728–739

ICCS 2014. 14th International Conference on Computational Science

Restrictions in model reduction for polymer chain models in dissipative particle dynamics

Nicolas Moreno[1,2], Suzana Nunes[1], and Victor M. Calo[2,3]

[1] Environmental Science and Engineering, Water Desalination and Reuse Center, King Abdullah University of Science and Technology Thuwal, Saudi Arabia
nicolas.morenochaparro@kaust.edu.sa

[2] Center for Numerical Porous Media NUMPOR, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

[3] Applied Mathematics & Computational Science, Earth Science Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Abstract

We model high molecular weight homopolymers in semidilute concentration via Dissipative Particle Dynamics (DPD). We show that in model reduction methodologies for polymers it is not enough to preserve system properties (i.e., density ρ, pressure p, temperature T, radial distribution function $g(r)$) but preserving also the characteristic shape and length scale of the polymer chain model is necessary. In this work we apply a DPD-model-reduction methodology for linear polymers recently proposed; and demonstrate why the applicability of this methodology is limited upto certain maximum polymer length, and not suitable for solvent coarse graining.

Keywords: Dissipative Particle Dynamics, polymer solutions, coarse graining, chain conformation

1 Introduction

Meso-scale particle-based methods are commonly used in the study of static and dynamic properties of polymers in solution. In bottom-up methodologies (a.k.a *Coarse graining*) the atoms of the polymer molecules are coarse-grained, and their atomic potentials are replaced by effective potentials between beads. Some of the most widespread methods include coarse-grained Molecular Dynamics (cgMD)[1] and Dissipative Particle Dynamics (DPD)[2], among others. In coarse-grained molecular dynamics the effective potentials are constructed to preserve particular properties from molecular dynamics simulations, providing a quantitative analysis of the physical systems. Nevertheless, the derivation of this potentials may require iterative refining stages, and sometimes the shape of the derived potentials can restrict the number of atoms coarse grained in a bead[3]. Rigorous effective potentials can also be derived for DPD[4], however in contrast to cgMD, in dissipative particle dynamics it is generalized the use simplified soft

 Selection and peer-review under responsibility of the Scientific Programme Committee of ICCS 2014
© The Authors. Published by Elsevier B.V.

doi:10.1016/j.procs.2014.05.065

potentials[5] that facilitates the study polymeric systems from a qualitative stand point. In this context DPD appears as an attractive and simple tool in polymer modeling. Indeed, dissipative particle dynamics is widely used in the modelling of biological [6] and synthetic polymers [7]. Many practical applications have been reported for microphase separation [5], amphiphiles [8], self assembly of block copolymers [9, 10], and blood flow [11, 12].

DPD describes a linear polymer as a set of beads connected through bond potentials such as harmonic springs or finite-extensible non-linear elastics potentials. The DPD chain models are constructed by mapping macro or microscopic properties of real polymers to the DPD parameters, and groups of atoms (i.e., monomers, Kuhn segments) are coarse grained into DPD beads.

One of the most relevant problems in the modelling of polymers is the increment of the computational demand as the molecular weight of the polymer increases. Typical mapping methodologies associate the size of a DPD bead with a few solvent molecules or monomers [13] (i.e., three molecules of water per bead), which in turn may require hundreds or even thousand of DPD beads to represent high molecular weight polymers. Indeed, the applicability of DPD to model high molecular weight molecules was questioned [14] based on the mapping methodology proposed by Groot and others [15, 5, 13], where the level of coarse graining exhibits a disappointly low maximum, limiting the use of DPD as a full meso-scale method.

In order to overcome the upper limits in coarse graining, Backer et al.[16], and Füchslin et al., [17] proposed model reduction methodologies for non-connected particles in flow problems. Füchslin [17] showed that the maximum level of coarse graining [14] appears due to the mapping procedure used; in [17] the authors proposed a consistent scaling of DPD parameters that restates DPD as a truly atomistic-to-continuum bridging method. In general these authors proposed a model reduction process that preserves particular properties of the fine-grained representation such as pressure p, temperature T, mass density ρ, and number of interactions.

Regarding the coarse graining of polymer chains, Spaeth et al.[18] generalized the model reduction proposed by Backer et al.,[16]. This model reduction for polymeric systems preserved the relevant characteristics of the polymer-solvent phase diagram. However, large deviations occur when the level coarse graining q was higher than five, furthermore this error also increases when the DPD chains contain more than 40 beads.

Herein we show that model reduction methodologies cannot be arbitrarily extended in the modelling of polymer chain, since the characteristic shape and size of the chain plays an important role in the equilibrium and dynamic properties of the polymer. The upper limits in chain lengths and coarse grain level were identified by [18] based on the construction of the phase diagram for fine- and coarse-grained systems. Since the asymmetry of the phase diagram is dictated by the relative size of the two species, in [18] the authors were able to reproduce the original system if the coarse graining procedure is applied only over the polymer chain (but not in the solvent). In this work we present the particular example of semidilute systems to demonstrate the effect of the inadequate preservation of the characteristic chain size, when the model reduction is applied to polymer chains with larger molecular weight and level of coarse graining

This documents is organized as follows, first, we introduce the conventional DPD governing equations, next the model reduction extended by [18] is presented. Later it is described the

simulation conditions used in our study. Finally we present the analysis of variation in size of polymer chain models; and show how the the polymer-solvent phase equilibria can not be preserved for long polymer chains.

2 Dissipative Particle Dynamics

In DPD, the particle dynamics and the balance of linear momentum are written according to Newton's laws as $d\mathbf{r}_i/dt = \mathbf{v}_i$ and $m_i(d\mathbf{v}_i/dt) = \mathbf{f}_i$ respectively. Here, $\mathbf{r}_i$, $\mathbf{v}_i$, m_i are the position, velocity and mass of a particle i, respectively. The force acting over the particles ($\mathbf{f}_i$) is given by

$$\mathbf{f}_i = \sum_{j \neq i} (\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R), \tag{1}$$

where $\mathbf{F}_{ij}^C$ is a conservative force, that models pressure effects between particles. $\mathbf{F}_{ij}^D$, models dissipative interactions in a fluid, and $\mathbf{F}_{ij}^R$ models random collisions between particles (i.e., Brownian motion).

The conservative force typically [15] has the form

$$\mathbf{F}_{ij}^C = \left\{ \begin{array}{rl} a_{ij}\ \omega^C \hat{\mathbf{e}}_{ij}; & (r_{ij} < r_c), \\ 0; & (r_{ij} \geq r_c) \end{array} \right\}, \tag{2}$$

where a_{ij} is the maximum repulsion between particles i and j, $\omega^C = (r_c - r_{ij})$ is a weighting function that sets the range of interaction between particles; r_c is the cut-off radius, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$, $\hat{e}_{ij} = r_{ij}/|r_{ij}|$.

Dissipative and random forces are defined as

$$\mathbf{F}_{ij}^D = -\gamma \omega^D(r_{ij})(\hat{\mathbf{e}}_{ij} \cdot \mathbf{v}_{ij})\hat{\mathbf{e}}_{ij}, \tag{3}$$

$$\mathbf{F}_{ij}^R = \sigma \omega^R(r_{ij}) \zeta \Delta t^{-1/2} \hat{\mathbf{e}}_{ij}, \tag{4}$$

where the weighting functions ω^D and ω^R vanish for $r > r_c$, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$, and ζ is a random number with Gaussian statistics. The parameters γ and σ are the friction coefficient and the noise amplitude, respectively. Espanol and Warren [19] showed that DPD obeys a Gaussian distribution and satisfy the fluctuation-dissipation theorem if $\omega^D(r) = [\omega^R(r)]^2$ and $\sigma^2 = 2\gamma k_B T$, where k_B is the Boltzmann constant and T is the equilibrium temperature. The most common choice of the weighting function $\omega^R(r)$ is

$$\omega^D(r) = [\omega^R(r)]^2 = \left\{ \begin{array}{rl} (1 - r/r_c)^2; & (r < r_c), \\ 0; & (r \geq r_c), \end{array} \right. \tag{5}$$

where $\omega^R(r)$ is assumed to vary linearly away from the particle. In DPD the time scale is given by

$$\tau^2 = r_c^2 \frac{m}{\epsilon}, \tag{6}$$

where the traditional selection $r_c = 1$, $m = 1$ and $\epsilon = k_B T = 1$ leads to a DPD time scale of unity. In this case the time scale is defined once the energy units are chosen. $\epsilon = k_B T$ is adequate in the study of equilibrium states, however the time scale can be also determined by direct comparison of experimental and simulated transport coefficients as discussed by [17].

Polymer chains are constructed in DPD as a sequence of M connected particles interacting through bond potentials (i.e., harmonic springs, finite-extensible-non-linear elastic, etc)[20]. When harmonic spring are used, the force contribution F_{ij}^S (in addition to F^C, F^D and F^R) between connected particles i and j is given by

$$F_{ij}^S = K_s(r_{ij} - r_o), \tag{7}$$

where K_s is the force spring constant, and r_o is the equilibrium bond distance between them.

The equilibrium distribution of particles along the chains models and therefore the chain size is governed by enthalpic and entropic interactions between beads. The entropic contribution can be associated with the configuration of the polymer, such as linear, star, branched, etc. While the enthalpic contributions are in general driven by the polymer-polymer and/or polymer-solvent interactions in solutions. In this paper we restrict our study to linear polymers, in order to facilitate the discussion of the coarse graining restrictions stressed.

2.1 Coarse Graining methodology

Herein we use the coarse graining approach proposed by [18] to reduce the number of degrees of freedom of a polymer solution. In this paper we apply the coarse graining over the whole system (polymer and solvent). At the high level of coarse graining that we use, the relative size of the species is not preserved, therefore, there is not practical relevance to coarse grain only the polymer chains.

Following the notation used in [18], the properties of systems containing only fine-grained particles are identified with the subscript zero (0), while fully coarse-grained systems are denoted with the subscript one (1). In addition, subscripts "00", "11" and "10" refer to interactions between fine, coarse and mixed particles respectively. Similarly to other authors[16, 17] they use a scaling factor q, that indicates the level of coarse graining. In [18] the authors define the scaling factor as

$$q = \frac{r_{c,11}}{r_{c,00}}, \tag{8}$$

where r_c is the cutoff radius. In order to preserve the mass density, the mass of the particle scales with the volume as

$$m_1 = q^3 m_0, \tag{9}$$

Conserving the number of interaction per particle N_{int} in the coarse-grained representation, and assuming uniform mixing, the particle number density $n = \rho/m$ scales as $n_1 = n_0/q^3$. The pressure, p, of the system is preserved if the proper scaling of the interaction parameters, a_{ij} is adopted [18, 17]. Starting with the virial theorem, assuming the integral of the radial distribution function $g(r)$ of the system is approximately equal to one; the pressure is kept in the coarse-grained system, when the interaction parameter a_{11} scales

$$a_{11} = (q^6 - q^3)\frac{30}{\pi}\frac{k_B T}{n_0 r_{c,11}^4} + q^6 a_{00}\frac{r_{c,00}^4}{r_{c,11}^4}. \tag{10}$$

The scaling of the friction coefficient (and therefore the noise term) are chosen to preserve the shear viscosity ν_0 [21]

$$\nu_0^D = \frac{2\pi}{1575} n_0^2 \gamma_{00} \frac{r_{c,00}^5}{r_{c,11}^5}. \tag{11}$$

Therefore, the expression of the friction coefficient for coarse particles, similarly to Füchslin[17] becomes

$$\gamma_{11} = q\gamma_{00}. \tag{12}$$

If the temperature of the system is conserved after the model reduction, the noise parameter of the DPD random force; satisfying the fluctuation-dissipation theorem scales as

$$\sigma_{11} = (2\gamma_{11} k_B T)^{1/2} \tag{13}$$

In the Table 1 the scaling factors proposed in the model reduction of [18], are summarized.

Table 1: Coarse parameters A_{coarse} and scaling function $\psi(q)$ proposed for coarse graining of systems with chains models.

A_{coarse}	$\psi(q)$
m_1	q^3
$N_{T,11}$	q^{-3}
$r_{c,11}$	q
v_1	q^3
τ_1	1
ϵ_1	1
$a_{ij,1}$	q
γ_1	q
σ_1	$(2\gamma_{11} k_B T)^{1/2}$

3 Simulation Details

The DPD simulations were conducted using the software LAMMPS [22]. We initially study effect of the number of beads and polymer-solvent interaction for single fine-grained chain models to elucidate why the size of the chain is a relevant restriction in the model reduction. We then constructed non-reduced semidilute solutions containing 30% of polymer beads, with DPD chains of 160 beads.

In all the fine-grained systems it was used a particle density $\hat{\rho} = 3$ particles$/r_c^3$, and the traditional scales of energy $\epsilon = k_B T = 1$, length $r_c = 1$, and mass $m = 1$, leading from equation 6 a time unit $\tau = 1$. The simulations conducted include an athermal ($a_{ii} - a_{ij} = 0$) stabilization stage of 20000 time steps, and a production stage of 500000 time steps; the position of the chain particles was stored every 500 steps. The time step $\Delta\tau = 0.04$ was adopted to reduce thermal fluctuations. Similarly to Moreno et. al., [23] the size of the simulation domain L_{box} is defined based on the expected end-to-end distance of the polymer chain, in order to avoid finite size effects, such that

$$L_{box} = 2R_{f,expect} = 2(0.85N^b), \tag{14}$$

where, N is the number of bonds per chain. For highly diluted systems $b = 0.65$ for interaction parameters polymer-solvent $a_{ps} < 29.0$, and $b = 0.4$ otherwise.

Following the scaling functions presented in Table 1, equivalent reduced systems were constructed, and the size of the aggregates in semidilute solutions was compared with its original fine representation.

In [18] the polymer chains are constructed based the spring force used by Schlijper et al.[24], and the magnitude of the spring constant K_s is tuned in order to make the average bond length r_o equal to the distance at which the pair-correlation function $g(r)$ for pure monomers exhibit the first maximum ($0.85r_c$). Here we also procure $r_o = 0.85r_c$, but instead of following Schlijper, our spring force is given by the equation (7).

We characterize the chain size computing the mean-square radius $\mathbf{R}^2$, the radius of gyration R_g, and the contour length l_c of the DPD chains. The mean-square radius can be written as

$$R^2 = \mathbf{R}_N \cdot \mathbf{R}_N = \sum_{i=1}^{N} \sum_{j=1}^{N} \mathbf{s}_i \cdot \mathbf{s}_j, \tag{15}$$

where $\mathbf{s}_i$ is the bond vector pointing from $(i-1)$th to ith segment in the chain. If the average distance between connecting particles is assumed constant, we can express $\mathbf{s}_i \cdot \mathbf{s}_j = r_o^2 \cos\theta_{ij}$, where θ_{ij} is the angle between $\mathbf{s}_i$ and $\mathbf{s}_j$ and r_o is the distance between particles. The mean-squared radius is computed over different realizations as

$$\langle R^2 \rangle = r_o^2 \left(\sum_{i}^{N} \sum_{j}^{N} \langle \cos\theta_{ij} \rangle \right). \tag{16}$$

The radius of gyration R_g is in general proportional to R, and is the second moment around the center of mass for the segments position $\mathbf{r}_{cm}$ in a polymer chain, we compute the radius of gyration as

$$R_g^2 = \frac{1}{N} \sum_{i=1}^{N} \left\langle (\mathbf{r}_i - \mathbf{r}_{cm})^2 \right\rangle = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=i}^{N} \left\langle (\mathbf{r}_i - \mathbf{r}_j)^2 \right\rangle. \tag{17}$$

where $\mathbf{r}_i$ is the position vector of the ith particle. The last parameter we use to characterize the size of a DPD chain is the *contour length* l_c, which we defined as

$$l_c = \sum^{N} |\mathbf{s}_i| \approx r_o N. \tag{18}$$

To evaluate the efficacy of the coarse grain methodology used [18] we define the ratio Q between the different preserved properties. Given a property A in its fine and coarse grained representation, we compute

$$Q = 1 - \frac{|A_{coarse} - A_{fine}|}{A_{fine}}, \tag{19}$$

where Q tends to one when A is properly preserved after the coarse graining.

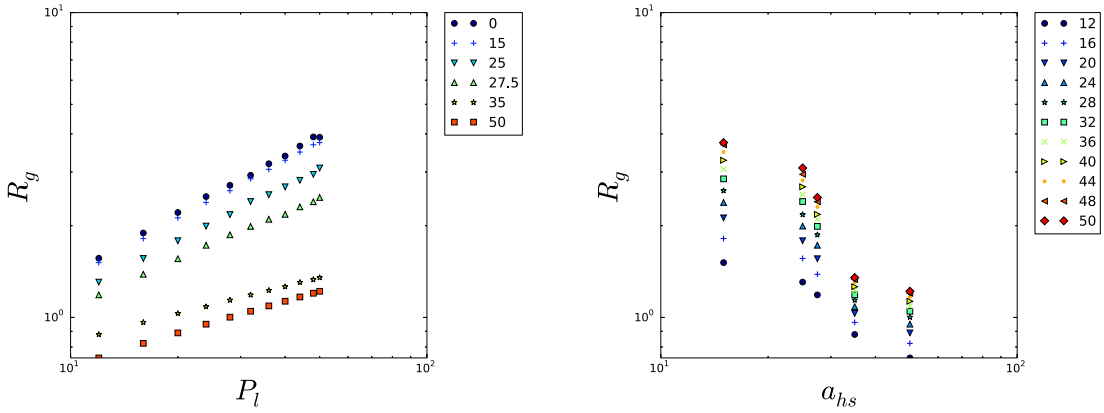
4 Results

In this section we showed why the applicability of the model reduction proposed by [18] is limited to short DPD chain model, and there is not a considerable freedom choosing the mapping from monomer to beads, when high molecular weight polymers are modelled.

Chain size variation

The dependence of the polymer size with the number of beads per chain has already been reported by different authors [25, 26, 27, 20, 23] showing that power laws underlying polymer physics [28] are captured in DPD chain models. Ilnytskyi and Holovatch [29] showed that the chain size variation with the polymer-solvent interactions, in the range of athermal to very-good solvent are in agreement with the experimental and theoretical results. Here, we extend the analysis of the variations in the characteristic size of the chain models, to demonstrate why the size of the chain is a relevant restriction in the model reduction.

In Figure 1 it is depicted the dependence of the radius of gyration with the number of beads per chain P_l and the polymer-solvent interactions a_{ps}, for systems with polymer lengths between 12 to 50 beads per chain with interactions ranging from good to poor solvent.



a) *b)*

Figure 1: Radius of gyration R_g variation with the number of beads per chain (a) and different interaction parameters a_{ps} (b). For larger chains there is a pronounced jump in R_g corresponding to the transition between theta to poor-solvent. In contrast, for short chains the transition at the theta point is weaker and the change in the chain size is negligible.

From Figure 1.a it can be noticed that the relationship between the chain size and the number of beads follows the form

$$R_g \propto N^b, \tag{20}$$

where $N = P_l - 1$ is the number of bonds per chain. The exponent b is consistent with the theoretical values [28] expected for polymers in good, athermal, theta, and poor solvents. In

Figure 1.a the identified values of b are presented for good ($\approx 3/5$), theta ($\approx 1/2$) and poor ($\approx 1/3$) solvents. The interaction parameter a_{ps} for theta solvent corresponds with the interaction intervals found by other authors [29, 30].

The existence of different correlation between beads along the polymer chains associated with the exponent b is the most important restriction in the applicability of the model reduction proposed by [18]. During the model reduction it is assumed that fine grained beads are homogeneously mixed in the volume of the coarse grained particle, however, since the fine-grained chains exhibit particular conformations it is erroneous to assume that the fine particles can be arbitrary mixed in homogeneous coarse particles. In Figure 4 it is illustrated this limitations, showing how the mixing assumptions do not preserve the geometrical properties of the original fine grained system.

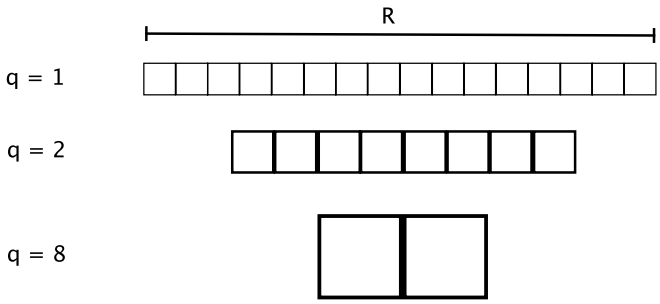


Figure 2: Sketch of successive model reduction stages assuming homogeneous mixing into coarse grained representations. In this case the mass density is effectively preserved along the model reduction however it is clear that the geometrical features of the original model are not conserved. The lack on the preservation of the characteristic size in the reduced model modifies the relative size of the species in the systems, and therefore its phase diagram.

In Figure 1.b we present the change in the radius of gyration for a given chain as the solvent affinity decrease. From this figure we can see that the variation in R_g with the interactions parameter is stronger as the number of beads per chain increases, therefore, it explains why the model reduction proposed by [18] reproduces the phase diagram of the fine systems only if the chains have a few beads ($P_l \leq 40$). Although the model reduction does not preserve the geometry of the original fine system the variation in short chains is negligible.

On the other hand it is also possible to foresee the upper limit in the level of coarse graining ($q = 5^{1/3}$), reported by [18]. This upper limit also appears when the variation in the characteristic size becomes large enough. As it is illustrated in Figure 4 when the level of coarse graining increases the size of the coarse-grained models is reduced.

Model reduction of semidilute systems

In Figure 3 we presente the ratio Q between different preserved properties of the polymeric system. Based on equation (19) we compute the efficiency of the model reduction to preserve

the pressure p, temperature T, contour length l_c, radius of gyration R_g, end-to-end distance R_f, and the radial distribution function $g(r/r_c)$. From Figure 3 it is evident that for short polymer chains with small coarse graining the variation in size of the reduced model is not significant, while for coarser systems the size deviations are larger than 50%. In both cases the contour length of the chains is equally affected due to the reduction in the interfacial area when particles are grouped.

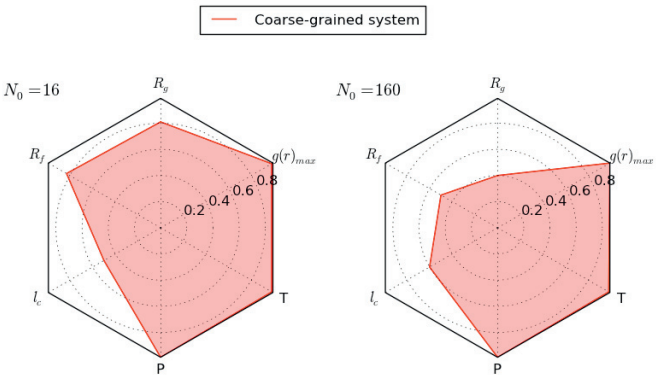


Figure 3: Preservation of DPD target variables, for original fine systems constituted by 16 and 160 beads per chain, with levels of coarse graining of 4 and 10 respectively. The deviation in the fine-grained size increases with the level of coarse graining

Due to the dramatic modification in the chain size at high levels of coarse graining, it is expected that during the polymer-solvent phase separation the size of the domains must be also affected. In Figure 4 it is depicted the final phase-separation structure for a fine-grained system and the equivalent reduced model. As it is stressed before, the model reduction considerably affects the effective polymer size, producing a decrease in the size and shape of the final aggregate.

The formation of the aggregate depicted Figure 4 is originated by a poor-solvent condition ($a_{ps} = 35$). Under these circumstances a single polymer chain must follow a conformation given by an exponent $b = 1/3$, which correspond to close packing of beads, which is the closest conformation to the assumption of homogeneous mixing. However this assumption is no longer valid for semidilute systems in poor solvents. For semidilute regimes is expected the existence two phases [28], the solvent rich phase and the polymer rich phase. In the polymer-rich phase the chains are completely overlapped and the polymer nearly resembles the pure melt condition, moreover the exponent governing the chain conformation changes to $b \approx 1/2$; hence the homogeneous mixing assumption breaks down.

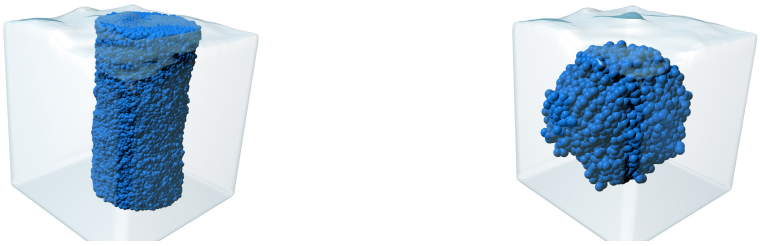


Figure 4: Final aggregate structure for fine-grained (left) system and its reduced-grained (right) counterpart. The effective change in the polymer size after coarse graining affects significantly the reachable coarse graining.

5 Conclusions

The coarse graining procedure used along this paper showed to decrease the degrees of freedom in DPD simulations preserving the pressure and the temperature of the system; however the existence of an upper limit in the applicability of the coarse graining is a significant limitation to overcome the computational cost associated with high molecular weight polymer simulation. In this paper we show how this upper limit arises from the homogeneous mixing assumption on the coarse graining, and it is reflected in the change in size of the chain model.

6 Future Work

Due to the limitations in the current coarse graining methodology, improved model reduction methodologies where the relevant size of the polymer is preserved are going to be presented in further publications.

Acknowledgements

- Texas Advanced Computing Center TACC at the University of Texas at Austin for providing HPC resources.

References

[1] Robert Rudd and Jeremy Broughton. Coarse-grained molecular dynamics and the atomic limit of finite elements. *Physical Review B*, 58(10):R5893–R5896, September 1998.

[2] P. J. Hoogerbrugge and J. M. V. A. Koelman. Simulating Microscopic Hydrodynamic Phenomena with Dissipative Particle Dynamics . *Europhysics Letters (EPL)*, 19(3):155–160, 1992.

[3] Mikio Yamanoi, Oliver Pozo, and Joao M Maia. Linear and non-linear dynamics of entangled linear polymer melts by modified tunable coarse-grained level dissipative particle dynamics. *The Journal of chemical physics*, 135(4):044904, July 2011.

[4] I. Pagonabarraga and D. Frenkel. Dissipative particle dynamics for interacting systems. *The Journal of Chemical Physics*, 115(11):5015, 2001.

[5] Robert D. Groot and Timothy J. Madden. Dynamic simulation of diblock copolymer microphase separation. *The Journal of Chemical Physics*, 108(20):8713, 1998.

[6] Maddalena Venturoli, Maria Maddalena, and Marieke Kranenburg. Mesoscopic models of biological membranes. *Physics Reports*, 437:1–54, 2006.

[7] Pep Español. Handbook of computational materials. In *Polymer*, chapter 8.6 dissip, pages 2503–2512. 2005.

[8] Julian C Shillcock. Spontaneous vesicle self-assembly: a mesoscopic view of membrane dynamics. *Langmuir : the ACS journal of surfaces and colloids*, 28(1):541–7, January 2012.

[9] Mark a Horsch, Zhenli Zhang, Christopher R Iacovella, and Sharon C Glotzer. Hydrodynamics and microphase ordering in block copolymers: are hydrodynamics required for ordered phases with periodicity in more than one dimension? *The Journal of chemical physics*, 121(22):11455–62, December 2004.

[10] Debora Salomon Marques, Ulla Vainio, Nicolas Moreno Chaparro, Victor Manuel Calo, Ali Reza Bezahd, Jed W. Pitera, Klaus-Viktor Peinemann, and Suzana P. Nunes. Self-assembly in casting solutions of block copolymer membranes. *Soft Matter*, 9(23):5557, May 2013.

[11] Dmitry a Fedosov, George Em Karniadakis, and Bruce Caswell. Dissipative particle dynamics simulation of depletion layer and polymer migration in micro- and nanochannels for dilute polymer solutions. *The Journal of chemical physics*, 128(14):144903, April 2008.

[12] Wenxiao Pan, Dmitry A Fedosov, Bruce Caswell, and George Em Karniadakis. Predicting dynamics and rheology of blood flow: A comparative study of multiscale and low-dimensional models of red blood cells. *Microvascular Research*, 82(2):163–170, 2011.

[13] R D Groot and K L Rabone. Mesoscopic simulation of cell membrane damage, morphology change and rupture by nonionic surfactants. *Biophysical journal*, 81(2):725–36, August 2001.

[14] Sergey Yuryevich Tromov. *Thermodynamic consistency in dissipative particle dynamics simulations of strongly nonideal liquids and liquid mixtures*. Ph.d., Technische Universiteit Eindhoven, 2003.

[15] Robert D Groot and Patrick B Warren. Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation. *Journal Chem. Phys.*, 107(11):4423–4435, 1997.

[16] J. a. Backer, C. P. Lowe, H. C. J. Hoefsloot, and P. D. Iedema. Combined length scales in dissipative particle dynamics. *The Journal of Chemical Physics*, 123(11):114905, 2005.

[17] Rudolf M Füchslin, Harold Fellermann, Anders Eriksson, and Hans-Joachim Ziock. Coarse graining and scaling in dissipative particle dynamics. *The Journal of chemical physics*, 130(21):214102, June 2009.

[18] Justin R Spaeth, Todd Dale, Ioannis G Kevrekidis, and Athanassios Z Panagiotopoulos. Coarse-Graining of Chain Models in Dissipative Particle Dynamics Simulations . *Society*, pages 69–77, 2011.

[19] Pep Español and Patrick B Warren. Statistical Mechanics of Dissipative Particle Dynamics . *Europhysics Letters (EPL)*, 30(4):191–196, 1995.

[20] Vasileios Symeonidis, George Em Karniadakis, and Bruce Caswell. Dissipative Particle Dynamics Simulations of Polymer Chains: Scaling Laws and Shearing Response Compared to DNA Experiments. *Physical Review Letters*, 95(7):076001, August 2005.

[21] C A Marsh. Static and dynamic properties of dissipative particle dynamics. *Physical Review E*, 56(2):1676–1691, 1997.

[22] Steve Plimpton. Fast Parallel Algorithms for Short-Range Molecular Dynamics. *Journal of Computational Physics*, 117(1):1–19, March 1995.

[23] Nicolas Moreno, Suzana P. Nunes, and Victor M. Calo. Geometrically-Consistent Model Reduction of Polymer Chains in Solution. Aplication to Dissipative Particle Dynamics Simulations: Model Description. In prepara, 2014.

[24] CW Schlijper, AG and Hoogerbrugge, PJ and Manke. with the dissipative particle dynamics method. *Polymer*, 39(3):567–579, 1995.

[25] CW. Schlijper, AG and Hoogerbrugge, PJ and Manke. Computer simulation of dilute polymer

solutions with the dissipative particle dynamics method. *Journal of Rheology*, 39(3):567, May 1995.

[26] Y. Kong, C. W. Manke, W. G. Madden, and A. G. Schlijper. Effect of solvent quality on the conformation and relaxation of polymers via dissipative particle dynamics. *The Journal of Chemical Physics*, 107(2):592, July 1997.

[27] N. A Spenley. Scaling laws for polymers in dissipative particle dynamics. *Europhysics Letters (EPL)*, 49(4):534–540, February 2000.

[28] Michael Rubinstein and Ralph H. Colby. *Polymer Physics*. Oxford University Press, 1st edition, 2003.

[29] J. M. Ilnytskyi and Yu. Holovatch. How does the scaling for the polymer chain in the dissipative particle dynamics hold? December 2007.

[30] Kan Yang, Aleksey Vishnyakov, and Alexander V Neimark. Polymer translocation through a nanopore: DPD study. *The journal of physical chemistry. B*, 117(13):3648–58, April 2013.