

From Games and Films to Molecular Simulation and Design

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ABSTRACT

This paper describes our experience at Autodesk Research in repurposing Nucleus, a physics engine included in a computer graphics software package called Autodesk Maya to create order instead of naturally looking chaos. Since our intention is not to animate molecular interactions but to get to a state closer to simulation, our work focused on the local inter-particle interactions such as those represented by Lennard-Jones potentials from which an emergent behavior unfolds. Preliminary tests were able to qualitatively reproduce four basic segregation phases for an A_mB_n style diblock copolymer system. We believe these are promising results since 1) they help to open a wider door to repurpose computational resources invested in games and films into the advancement of science, 2) they show the ability to easily create different levels of sophistication and consequent accuracy, all this within a single platform, which points to the potential democratization of molecular simulation and design to a larger number of scientists and would-be-scientists and engineers.

Keywords: diblock copolymer, micro-phase separation, molecular dynamics simulation, Maya.

1 INTRODUCTION

Propelled by the multi-billion dollar game and film industries, computer graphics software has evolved dramatically in sophistication. Effects range from realistic explosions to the chaotic movements driven by wind and other fluids. This paper describes our experience at Autodesk Research in repurposing Nucleus, a physics engine included in Autodesk[®] Maya [1], to create order instead of naturally looking chaos. Autodesk[®] Maya (Maya for short hereafter) is a 3D computer animation software delivering an end-to-end creative workflow with comprehensive tools for modeling, animation, visual effects and 3D rendering. Nucleus is a unified dynamics framework integrated in Maya based on particles with constraints.

In this paper, we chose as a test case the self-assembly of diblock copolymers. A diblock copolymer is a chain molecule composed of two different blocks, one of which is composed of type A molecules, and the other is composed of type B molecules. Usually, type B molecules are selected so that they resist coexistence with type A molecules [2]. The immiscibility between these two types of molecules

and the topological constraints drive the mixture to be separated into regular patterns of alternating A -rich and B -rich regions around the nanometer length scale [3]. Research on diblock copolymers has increased dramatically in recent years due to their unique and interesting phase behavior. A wide variety of micro-patterns, typically including lamellae, gyroid, cylinder and sphere, have been studied [4,5,6].

A micro-phase diagram has been revealed by self-consistent field theory [6], which describes various micro-structure domains in terms of interactions between unlike molecule pairs and their compositions. This paper aims at reproducing four basic micro-structures using Nucleus within Maya, which are in agreement with experimental observations. Other micro-structures such as diamond conformations [7] are outside of our consideration.

Using and programming Maya is also beyond the scope of this paper. Readers can refer to [8] for detailed information.

2 METHODOLOGY

2.1 Lennard-Jones potential

In our simulation, we use Molecular Dynamics (MD) to study micro-phase behavior. To provide an excluded volume effect, the molecules have a repulsive hard core.

For a pair of particles i and j located at r_i and r_j in space, the Lennard-Jones potential is:

$$U_{ij} = \begin{cases} 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 + \frac{1}{4} \right] & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c \end{cases} \quad (1)$$

where ε_{ij} is the interaction parameter between particles i and j , σ_{ij} is the distance at which the inter-particle potential is zero. r_c is the cutoff radius. $r_{ij} = |r_i - r_j|$ is the distance between two particles.

Based on previous work [9], the cutoff radius r_c is chosen to be small enough so there are purely repulsive forces active, thus increasing the performance of the simulation while maintaining acceptable results.

In order to induce the phase separation in a diblock copolymer system, the Lennard-Jones parameters have to be set appropriately. We here adopt the same scheme as shown in [9]:

$$\begin{aligned}\mathcal{E}_{AA} &= \mathcal{E}_{BB} = \mathcal{E} \\ \mathcal{E}_{AB} &= (1 + \tilde{\epsilon})\mathcal{E} \\ \sigma_{AA} &= \sigma_{BB} = \sigma_{AB} = \sigma\end{aligned}$$

where $\tilde{\epsilon}$ is the interaction parameter between unlike types of molecules. The subscript implies the types of molecular interactions. This scheme introduces a larger repulsion force between unlike molecule pairs.

According to the definition of the Lennard-Jones potential, the force that particle j exerts on particle i can be formulated as:

$$F_{ij} = -\frac{24\mathcal{E}_{ij}}{\sigma^2} \left[2\left(\frac{\sigma}{r_{ij}}\right)^{14} - \left(\frac{\sigma}{r_{ij}}\right)^8 \right] \vec{r}_{ij} \quad (2)$$

where $\vec{r}_{ij} = r_i - r_j$ is the vector from r_j to r_i .

2.2 Thermal motion

Thermal motion is another force we have to take into account. Thermal motion is the temperature-driven rapid random movement of atoms or molecules, which forces them to collide with each other and with the walls of container.

Unlike the macro world, the atomic world is in a state of motion at all temperatures above absolute zero. The thermal motion of atoms or molecules rises with temperature and follows the laws of thermodynamics. The root mean square velocity of the particles is calculated by the expression of the kinetic energy of a molecule:

$$\frac{1}{2}mv^2 = \frac{3}{2}K_B T \quad (3)$$

where m is the particle mass, v is the root mean square velocity, K_B is the Boltzmann constant, and T is the absolute temperature.

We simulated the thermal motion of molecules by adding a contributing random velocity vector, following a Boltzmann distribution, to every particle in the system.

2.3 Custom nodes

Maya is designed to be an open, flexible and easy-to-extend product. External applications can be loaded in Maya as plug-ins. These plug-ins are usually represented in Maya as nodes that can be connected to other nodes, allowing the data to flow from one node to another.

Two custom nodes were created for our simulation, a Lennard-Jones node and a thermal motion node. These nodes were implemented as C++ classes derived from the Maya APIs: MPxFieldNode and MPxNode, respectively.

The Lennard-Jones node computes the Lennard-Jones forces exerted on a particle. The thermal motion node applies a random force field to a particle system, which results in the assignment of a contributing velocity vector to each particle.

The Lennard-Jones and the thermal motion nodes are connected to a copolymer system.

3 SIMULATION

3.1 Diblock copolymer model

The model we used for the diblock copolymer reflects a course-grained structure [12]. The copolymer chains are linear and mono-disperse. The chains of length N are constructed by a block of fN molecules of type A connected to a block of $(1-f)N$ molecules of type B , where f is the ratio of the length of the A -block relative to the length of the entire chain.

We used a particle system in Maya to represent the molecules. We formed a particle chain via a Nucleus constraint called *pointToPoint* constraint. Figure 1 shows the construction of a symmetric copolymer chain ($f=0.5$).

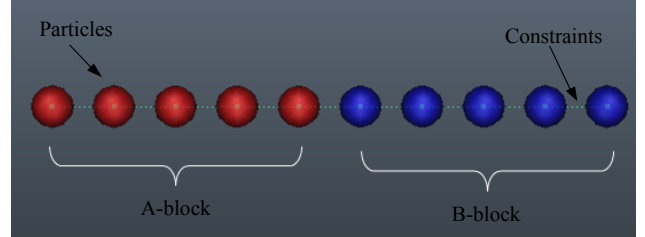


Figure 1: Model of a diblock copolymer chain

3.2 Computational considerations

Reduced units [13] were used in our simulations. The mass m is set to unity so that the time is measured in units of $\tau = \sigma(m/\omega)^{1/2}$. We also set $\sigma = \mathcal{E} = 1$.

The simulations were initially carried out within a bounding box of $21\sigma \cdot 21\sigma \cdot 21\sigma$ containing a total of 8,000 particles. As described in previous research [14], we noticed that the bounding box could be affecting some of the final conformations. Because of this, in the case of $f=0.4$ and 0.16 we used a larger bounding box of $32\sigma \cdot 32\sigma \cdot 32\sigma$ with 27,000 particles. Ideally we would have preferred to use the same bounding box size and number of particles for all the scenarios considered.

The simulations were characterized by a classical particle system with number density satisfying $\rho \approx 0.85$, and $K_B T = 1.0$. The time step was set to $\Delta t = 0.01\tau$. The

cutoff radius is $r_c = 2^{1/6} \sigma = 1.12$. The interaction parameter between unlike molecule pairs is $\tilde{\epsilon} = 5$.

We initialized the simulation by distributing the diblock copolymer chains randomly in the bounding box. A series of simulations were carried out to study the micro-phase behavior across the following f values: 0.5, 0.4, 0.3 and 0.16.

3.3 Nucleus Considerations

Nucleus is a unified particle solver, which computes the interaction dynamics for a wide variety of elements and constraints. By taking advantage of the built-in features in Nucleus, it becomes easier to do qualitative molecular dynamics simulations.

Our molecular model uses Nucleus constraints to configure molecular chains instead of defining another potential, as it would be done under a more conventional MD method [9].

Another advantage of using Nucleus is that we do not need to necessarily implement any integration algorithms such as the calculation of the particles' velocities using a Verlet algorithm. Being a physics engine, Nucleus resolves those calculations automatically wherever possible.

Although Nucleus is fine tuned for some specific physical phenomena, it is still an approximation of the real physics. One has to be careful in setting the parameters for the Nucleus solver and for the Nucleus particles, *i.e.*, the particles that the solver evaluates and transforms. We show below the list of parameters we used:

Nucleus Solver

```
setAttr "nucleus1.gravity" 0;
setAttr "nucleus1.subSteps" 1;
setAttr "nucleus1.maxCollisionIterations" 1;
setAttr "nucleus1.timeScale" 10;
```

Nucleus Particles

```
setAttr "nParticleShape1.bounce" 1;
setAttr "nParticleShape1.stickiness" 0;
setAttr "nParticleShape1.friction" 0;
```

We also explored a more rigorous method where we measured the total energy at every time step, and adjusted the particles' velocities accordingly to maintain the total energy perfectly constant. Since the simulation became considerably slower, we decided to stay with the fine-tuned Nucleus parameters scenario, which gave a reasonable first set of results. As the underlying Nucleus code is further optimized we expect to reconsider more rigorous simulations that predict quantitative data obtained experimentally.

4 RESULTS AND DISCUSSION

We present the results of our simulation of the self-assembly of the $A_m B_n$ diblock copolymer system. We started the simulation with $f = 0.5$. We observed that the $A_5 B_5$ system converged to a lamellar phase. Figure 2 shows the typical formation process of a lamellar micro-structure [14]. The copolymers initially aggregate into local spherical and cylindrical micro-structures (see Fig. 2a). These micro-structures aggregate further and construct a gyroid-like morphology (see Fig. 2b). Next, the gyroid structures start to stretch and construct an irregular lamellar morphology in which some micro-domains between two adjacent layers are connected (see Fig. 2c). This is consistent with previous work [15], which reported similar perforated irregular lamellar morphologies in their experiments. Finally, the connections between alternating layers are broken and the complete lamellar conformation appears (see Fig. 2d).

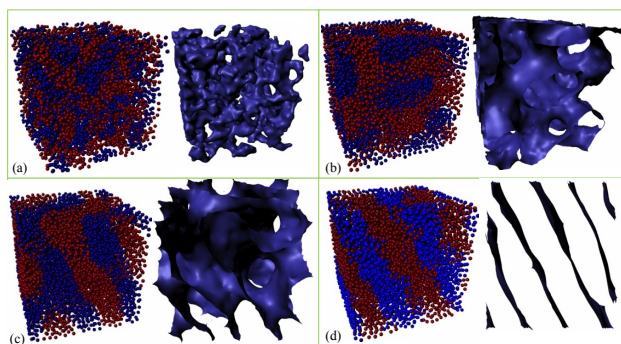


Figure 2: Formation of a lamellar morphology. Molecular and interfacial representations are collocated.

When f decreases from 0.5 to 0.4, the gyroid micro-structure is observed (see Fig. 3). Once the gyroid is observed, it remains stable.

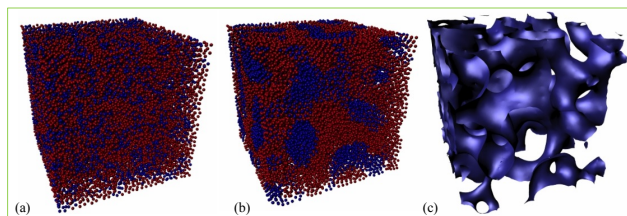


Figure 3: Formation of a gyroid morphology.

As f continues to decrease to 0.3, the hexagonal packed cylinder morphology is observed. Figure 4 shows the transition to the cylindrical conformation of the $A_3 B_7$ copolymer system.

As f decreases even further to 0.16, the copolymer system displays a spherical morphology (see Fig. 5). The spheres are slightly different from the spherical morphology observed in previous work [6,16]. Our morphology is not

exactly cubic symmetric. As explored previously by others [12], this may be explained by the short length of the diblock copolymers ($N=10$) and the limited size of the bounding box.

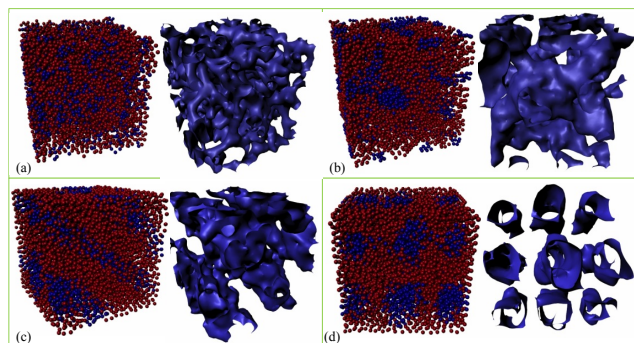


Figure 4: Formation of a cylindrical morphology.

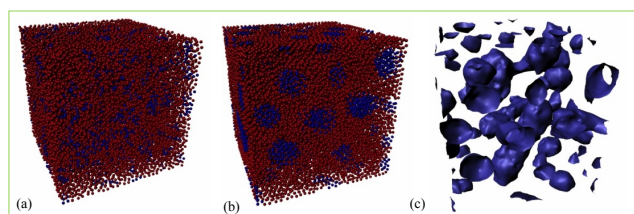


Figure 5: Formation of a spherical morphology.

5 CONCLUSIONS

We built a molecular dynamics simulation in Autodesk[®] Maya using Nucleus, a unified dynamics framework normally used in the creation of highly realistic effects in games and films. “The heart of the framework treats the interaction of all elements as a system of particles that collide and exert forces on each other. The complex behaviors of dynamic elements like cloth, hair and water emerge from these simple rules.” [18].

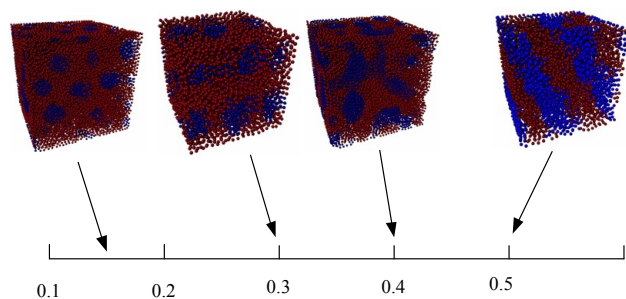


Figure 6: Simulated morphologies vs. f fractions

In our simulation, we reproduced the four basic segregation phases for an A_mB_n style diblock copolymer system (see Fig. 6), *i.e.* lamellae, gyroid, cylindrical, and spherical, which is qualitatively consistent with previous work [2, 14, 17].

The ability to easily create different levels of sophistication and consequent accuracy, all this within a single platform, points to the potential democratization of molecular simulation and design to a larger number of scientists and would-be-scientists and engineers.

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REFERENCES

- [1] Autodesk[®] Maya. <<http://usa.autodesk.com/maya/>>.
- [2] B. Fraser, *etc.*, J. Poly Sci. 43, 8, 2005.
- [3] Ching-I Huang and Yu-Chieh Hsu, Phy. Rev. 74, 051802, 2006.
- [4] F. S. Bates, Phys. Today, 52:32, 1999.
- [5] I.W. Hamley, The Friction and Lubrication of Solids. Oxford University Press, London, 1999.
- [6] M.W. Matsen, F.S. Bates, Macro-molecules, 29:1091, 1996.
- [7] M.W. Matsen. J. Phys: Condens Matter, 2002
- [8] Autodesk[®] Maya Training. <<http://usa.autodesk.com/maya/training/>>
- [9] S. Gary, D. Martin, K. Kurt and M. Anshu, J.Chem.Phys., 105(23), 1996.
- [10] <http://www.chemistry-dictionary.com/definition/thermal+motion.php>
- [11] http://en.wikipedia.org/wiki/Kinetic_theory
- [12] R.D. Groot and T.J. Madden, J. Chem. Phys. 108, 8713, 1998.
- [13] D. C. Rapaport, The art of molecular dynamics simulation, Cambridge University Press, 1997.
- [14] X. Li *etc.* J. Chem. Phys. 130, 074908, 2009.
- [15] S. Mani, *etc.* Eur. Polym. J. 36,215, 2000.
- [16] L. Zhang, A. Eisenberg, Science, 268(5218):1728, 1995.
- [17] M.A. Horsch, *etc.*, J. Chem. Phys, 121, 22, 2004.
- [18] Interview with Jos Stam. CGSociety Feature Article. <http://features.cgsociety.org/story_custom.php?story_id=4026>.