Hybrid Simulations Using Spherical Boundaries

1. Aims

I. View morphology changes in block copolymer constrained by spherical boundary using computational methods.

II. Expect increase in boundary condition to force polymer to go from perpendicular to parallel to the walls.

III. Find future material for use in battery technology, fire resistance, nanotechnology and medicine. [1]

2. Background / application

- Cubic boundaries in prior research suggest external fields (electric fields) induce morphology change. [2]
- "Hybrid simulations" balance speed and accuracy, ideal for large-scale simulation
- Applications in drug-delivery and energy storage. [3]

3. Method

I. Computational method – Cell Dynamics Simulation (CDS).

II. Simulate spherical boundary (**see Eq. 2**).

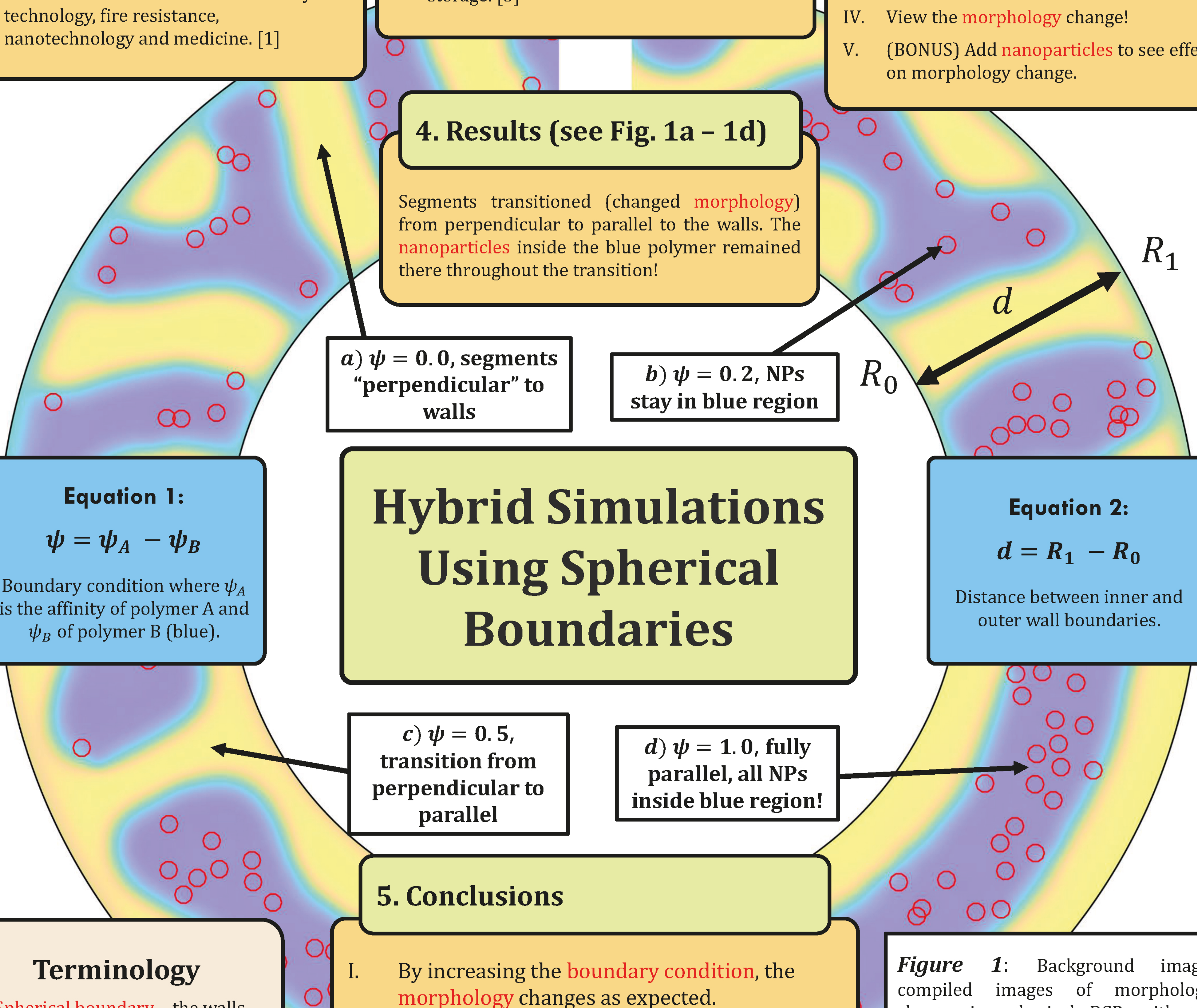
III. Increase boundary condition (change "affinity" of polymer wall, so it becomes more/less attracted to blue/yellow polymer regions) (**see Eq. 1**).

IV. View the morphology change!

V. (BONUS) Add nanoparticles to see effect on morphology change.

4. Results (see Fig. 1a – 1d)

Segments transitioned (changed morphology) from perpendicular to parallel to the walls. The nanoparticles inside the blue polymer remained there throughout the transition!



Equation 1:

$$\psi = \psi_A - \psi_B$$

Boundary condition where ψ_A is the affinity of polymer A and ψ_B of polymer B (blue).

Equation 2:

$$d = R_1 - R_0$$

Distance between inner and outer wall boundaries.

5. Conclusions

I. By increasing the boundary condition, the morphology changes as expected.

II. Location of NPs incredibly useful for drug delivery.

III. Consistent results with experimental research.

Figure 1: Background image, compiled images of morphology change in spherical BCP, with set distance, $d = 40$ between walls, and varying boundary condition, ψ, *a)* $\psi = 0.0$ (perpendicular to the walls), *b)* $\psi = 0.2$, *c)* $\psi = 0.5$ and *d)* $\psi = 1.0$ (parallel to the walls).

Terminology

- Spherical boundary – the walls of a sphere.
- Boundary condition – attraction of walls to yellow/blue polymer.
- Morphology – shape of molecule.
- Nanoparticles (NP) – particles on scale of 10^{-9} m.
- Block copolymer (BCP) – linked polymers in block, toothpaste-like fluid when heated.

References

[1] A.-C. Shi and B. Li, "Self-assembly of diblock copolymers under confinement," Soft Matter, vol. 9, no. 5, pp. 1398–1413, 2013.
[2] M. Pinna, J. Diaz, C. Denison, "Lamellar Block Copolymers Under Shear Flow," 2022.
[3] M. Pinna, S. Hiltl, X. Guo, A. Boker, and A. V. Zvelindovsky, "Block Copolymer Nanocontainers," ACS nano, vol. 4, no. 5, pp. 2845-2855, 2010.

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