Simulations of Lipid Bilayers with the MDPD-Martini Force-Field

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Introduction

Molecular dynamics (MD) is a key research tool in physics and biophysics, powered by accessible software like LAMMPS and GROMACS. Force-fields, such as the MARTINI coarse-grained model, simplify simulations by reducing computational demands while enabling studies of diverse systems like proteins and polymers. Martini's modular design and community-driven development make it highly versatile and efficient. Many-body dissipative particle dynamics (MDPD) offers an alternative for simulating large, multi-phase systems at lower costs, combining Martini's strengths with enhanced scalability, opening new avenues for research in soft matter and fluid physics.

Methodology

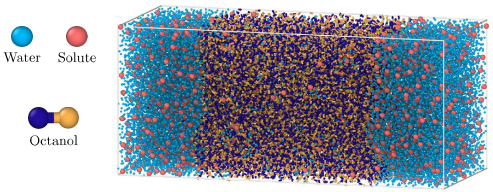


Figure: Octanol—water partition coefficient simulation.

We categorize our beads and parametrize their interactions through measurements of the octanol—water partition coefficient:

$$\log P_{o/w} = \log \frac{[S]_o}{[S]_w}$$

Results

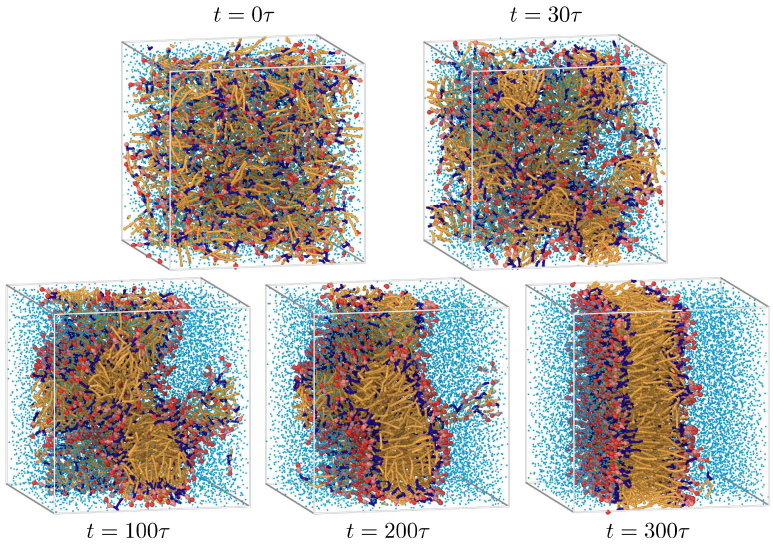


Figure: DPPC lipid self assembly into a bilayer membrane. MDPD simulations done with 512 lipid molecules.

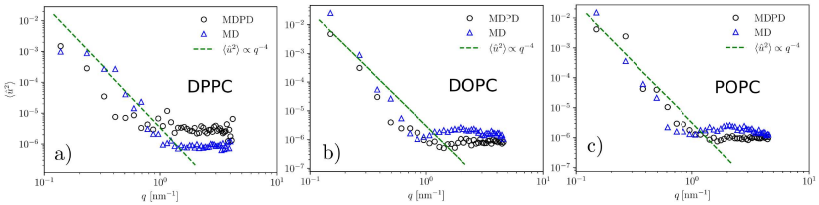


Figure: Undulation power spectrum comparison between MDPD and MD simulations. Both exhibit the same expected behavior at long wavelengths with bending modulus value comparable to experimental results (dashed line).

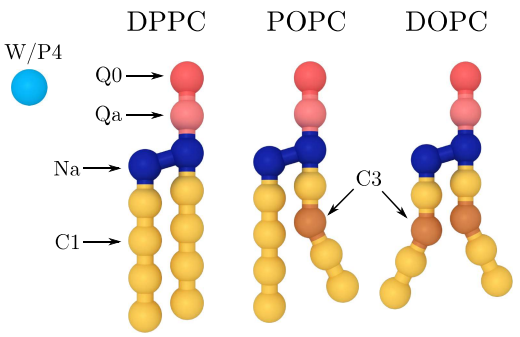


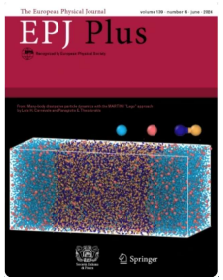
Figure: MD Martini 2.0 and MDPD coarse-grained lipid models

Conclusions

- MDPD and MD Martini both accurately simulate lipid bilayer properties, matching experimental data.
- MDPD enables faster, efficient simulations for large-scale systems using soft, short-range interactions.
- The adaptable MDPD-Martini approach extends to diverse and complex molecular systems.

1) L. H. Carnevale, P. E. Theodorakis. Eur. Phys. J. Plus 139, 539 (2024) (Journal Cover)

2) Kramarz, N., Carnevale, L.H., Theodorakis, P.E. arxiv.org/abs/2501.01225 (Under Review)



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