Centre for Scientific Computing

Computer Simulation of Lipid Bilayers

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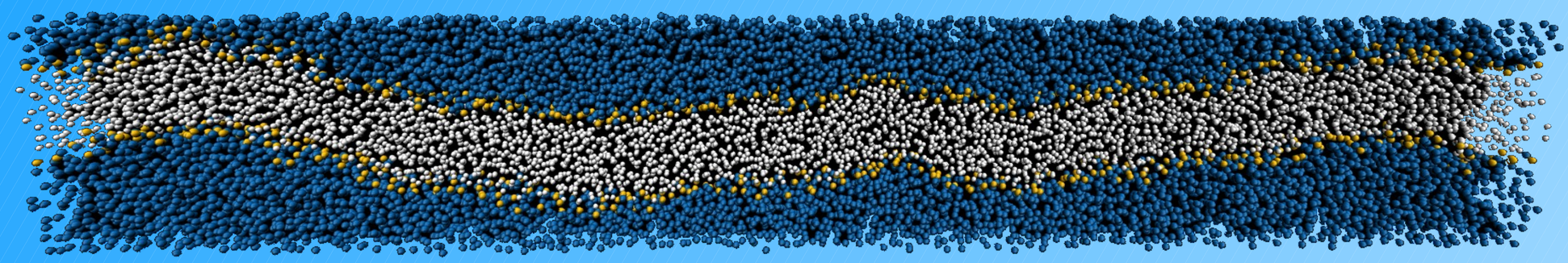


Introduction

Lipids are the main components of biological membranes. This project investigated diffusion properties of lipid bilayers (of width W, length L, height H) in water.

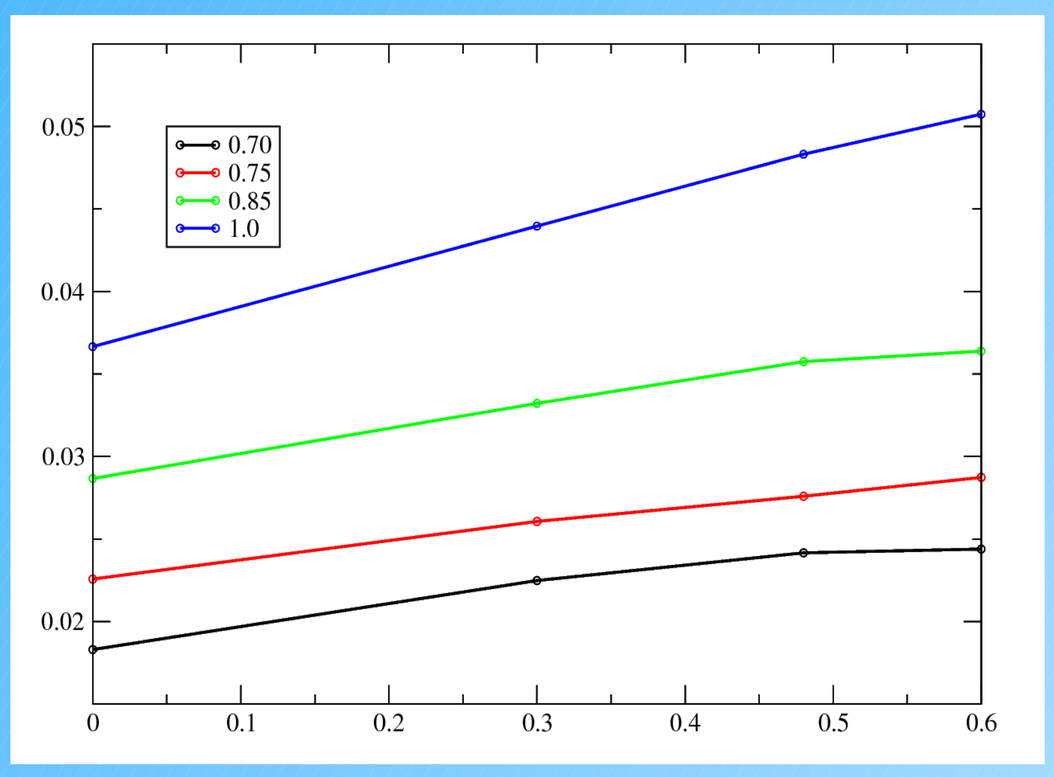
Computer Simulation

A Dissipative Particle Dynamics (DPD) simulation program was developed to include a multiple time step update scheme to improve the efficiency of the calculations.

Diffusion

Diffusion coefficients along the bilayer were calculated at four temperatures and four widths of bilayer. The results are in agreement with theory:

$$D \propto log(W)$$



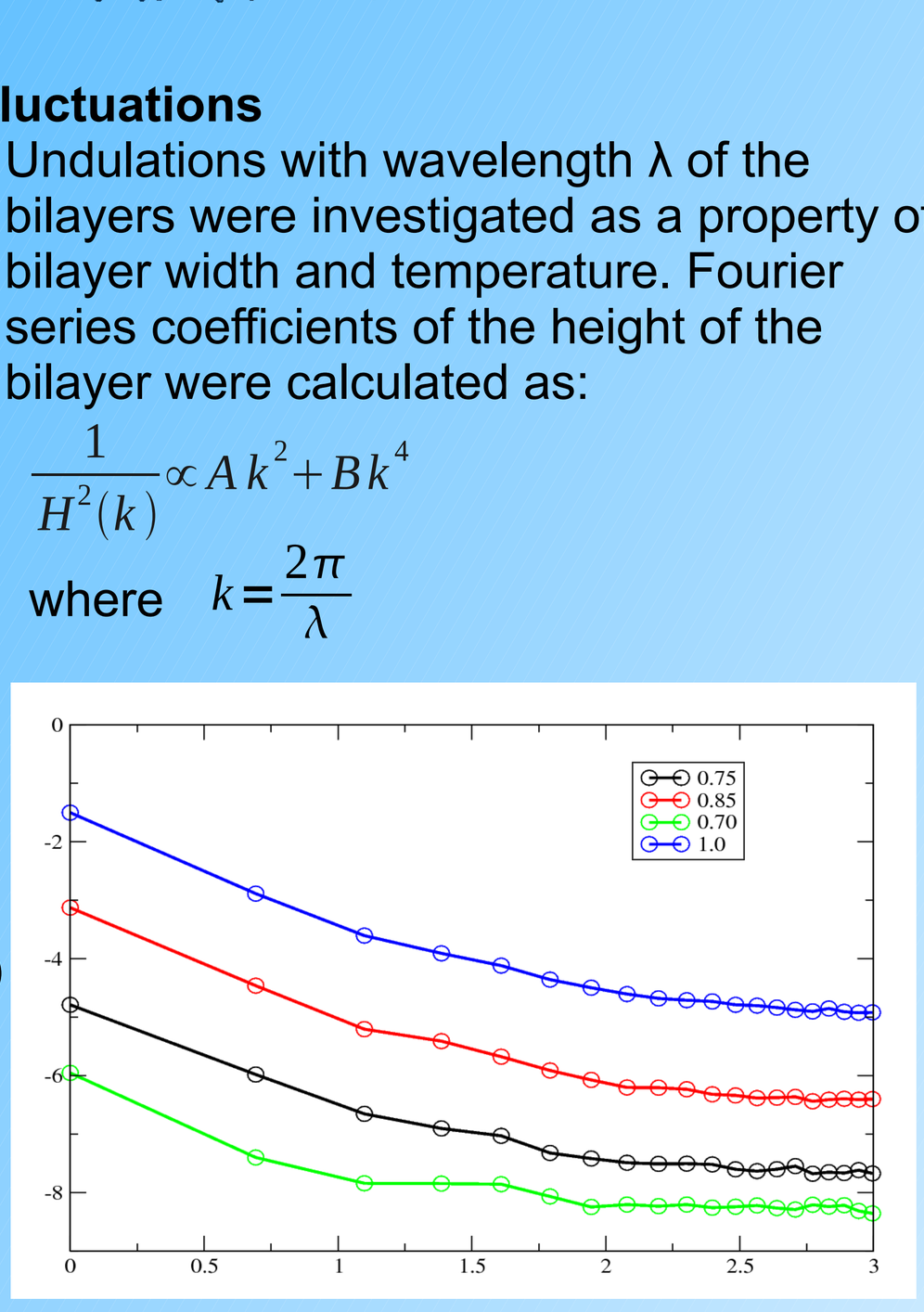
Plot of the diffusion coefficient against the logarithm of the bilayer width at different temperatures

Fluctuations

Undulations with wavelength λ of the bilayers were investigated as a property of bilayer width and temperature. Fourier series coefficients of the height of the bilayer were calculated as:

$$\frac{1}{H^2(k)} \propto A k^2 + B k^4$$

where $k = \frac{2\pi}{\lambda}$



Logarithmic plot of the inverse of the Fourier coefficient against k

- **Outlook**
  To improve the results, a wider range of bilayer widths and temperatures could be investigated. A larger number of time steps could be used in the DPD simulation.

References

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