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CRYSTALIZATION ON A SPHERE: PARALLEL SIMULATION ON A TRANSPUTER NETWORK

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First results are presented of a continuous optimization approach to find equilibrium configurations of $N\,(< 10^4)$ particles with Lennard-Jones interaction, moving on a sphere with variable radius. The results may help to understand the structure of spherical biomembrane vesicles showing "quantum" jumps in their size distribution.

1. Introduction

Experiments by Bont et al. have shown that sizes of *in-vitro* assembled spherical biomembrane vesicles tend to peak at values with ratio of adjacent terms $\sqrt{2}$.[1] Two such interwoven geometric series were found. We present first calculations simulating a structural organization of particles on a sphere relevant for the size quantization phenomenon.

2. Vesicle Formation

When biomembrane material (lipid and protein) after fragmentation reconstitutes a bilayer, spherical vesicles are formed. We restrict ourselves to the lipid arrangement.

Thermodynamically, lipid molecules immersed in a water medium decrease the local entropy while the mean free energy is increased. A bilayer sheet forms spontaneously driven by co-operative molecular forces while minimizing the free energy. The lipids are densely packed and consequently ordered. Bilayer fragments tend to curve to decrease edge energy. Ultimately it closes forming a vesicle.

3. 2D Simulation model for vesicle structure

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The above thermodynamic problem involves highly inelastic non-linear phenomena in three dimensions (3D). There is no realistic way to solve such a problem in closed form. The crux of our approach is the assumption that the densely packed glycerol headgroups of the inner lipidsublayer form a (quasi)crystalline shell, acting as 'backbone' determining the vesicle size.[2] The simulation of the formation (energy minimization) of the backbone is a spherical 2D problem for particles with a short range attraction and inner repulsive core (Lennard Jones (LJ) interaction). The problem resembles spreading N points homogeneously over a spherical surface.

4. Computational Model

In optimization, when dealing with many local minima, a well established approximation technique is the Simulated Annealing (SA) method. We investigated both algorithmic and functional decomposition strategies. We implemented a systolic parallel Fast SA on a ring of Transputers.[3] Further speed-up was achieved by decomposing the energy function calculation. A SA-step consists of perturbing the system and calculating the resulting energy difference (ΔE), this takes $2N$ calculations. A master processor generates Markov chains and assigns ΔE-calculation jobs to processors in a slave farm. We arrive at a hybrid topology consisting of processors connected in a ring with farms of slaves attached to them.

5. Results

We performed a large number of SA experiments. Typical results are shown below. Energy minima are observed related to the symmetry of the spherical arrangements.

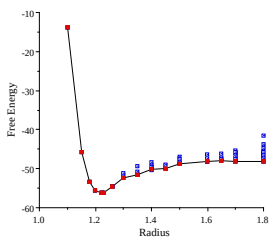

Fig. 1. Example of energy behavior as a function of radius for 20 LJ particles

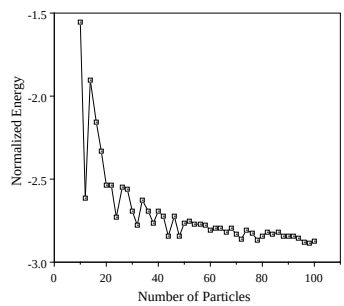

Fig. 2. Simulation of (truncated) LJ SA reveals energetic preferences

Extension to configurations with $N > 10^3$ and analysis of the crystallization patterns and their symmetries are planned for the near future.

References

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