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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  $\sqrt{2}$ .<sup>1</sup> 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.<sup>2</sup> 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.<sup>3</sup> 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 ( $\Delta E$ ), this takes  $2N$  calculations. A master processor generates Markov chains and assigns  $\Delta E$ -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.

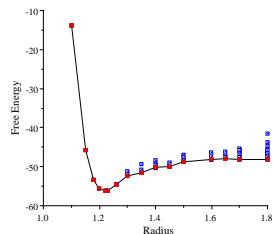


Fig. 1. Example of energy behavior as a function of radius for 20 LJ particles

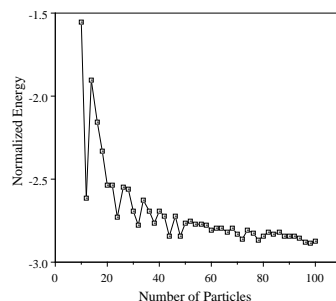


Fig. 2. Simulation of (truncated) LJ SA reveals energetic preferences

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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