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Future Generation Computer Systems 10 (1994) 359–361

FGCS
FUTURE GENERATION COMPUTER SYSTEMS

Crystallization on a sphere

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Abstract

We present a parallel simulated annealing algorithm for crystallization of N-body systems. The implementation uses systolic simulated annealing with additional parallel cost function evaluation. We have a hybrid topology which consists of a systolic ring and attached to each ring processor a tree of processors. Our research topic is crystallization of particles on a spherical surface. Some results of the crystallization experiments are presented.

Key words: Parallel simulated annealing; Hybrid topology; Crystallization

We present the quasi crystallization of particles on closed two dimensional surfaces. This research is mainly motivated by the – experimentally observed – size discreteness in biological vesicles. Simulation of the involved holonomic constraints, arising from 'spherical' nucleation, is poorly understood but essential with respect to the crystallization of such structures.

Crystallization on flat 2D surfaces has been studied extensively for the influence of defects. The crystallization on curved surfaces has some important differences compared to flat surfaces since there have to be irregularities in the distribution as a consequence of the topology. It is expected that these defects have a strong influence on various properties of the system, including phase changes.

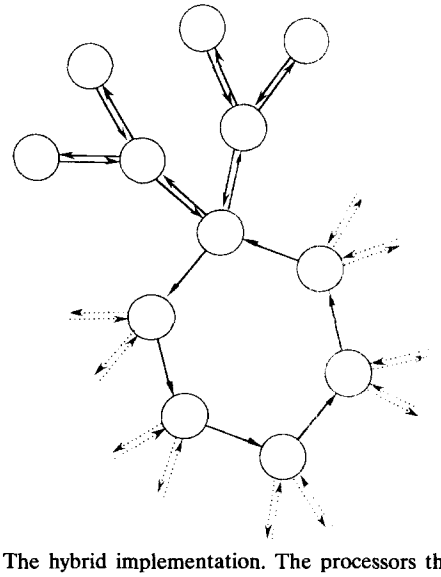

Fig. 1. The hybrid implementation. The processors that execute the systolic algorithm are connected in a ring, attached to each systolic processors is a farm of processors connected in a tree.

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SSDI 0167-739X(94)00034-C

The reason for our interest in vesicles, a spherical structure consisting of a bilayer of lipid molecules which encloses a volume, is that it has been observed that only specific sizes are stable in nature. Actually the preferred sizes fit neatly in two simple geometric series. We postulated that the inner surface of the vesicle resembles a solid state and acts as a 'backbone' to the vesicle. As a consequence this inner surface is the main component in determining the overall shape and size. Our hypothesis for this behaviour is that, given the interaction potential between the headgroups, only specific numbers of particles can be distributed in an ordered (quasi crystalline) structure.

To find the optimum distributions (i.e. minimal energy) we use simulated annealing. The algorithm can shortly be described as making a Markov chain with the Metropolis algorithm at a certain temperature, then lowering the temperature and again making a Markov chain. This continues until a certain stop criterion is met.

With a sequential implementation we can reach system sizes of $N = 500$, our goal is to do simulation of biologically relevant systems with $N = 10000$. Due to the computational intensity of such nucleation simulations we have started to investigate the possibilities of parallel execution of the simulation codes. The simulated annealing algorithms have been implemented for both parallel- and vector-computer architectures. Several methods for parallelization of these algorithms exist. One of the most obvious methods is functional decomposition (making perturbations, calculating the energy difference and updating). From our experiments however it was defferred that this type of parallelization is not sufficient to obtain the required system sizes. Other forms of parallelism are currently being examined such as systolic annealing [1]. Here the Markov chains are generated in parallel. We have extensively studied the stability and algorithmic behaviour of the systolic implementations. One of the implementations has an hybrid topology: the processors that execute the systolic algorithm are connected and attached to each systolic processor is a farm of processors that executes the calculation of the interaction energies in parallel (see Fig. 1). Currently we are exploring the merits of a geometrical decomposition where the hierarchical organisation of the crystallization patterns are mapped on a tightly coupled parallel platform.

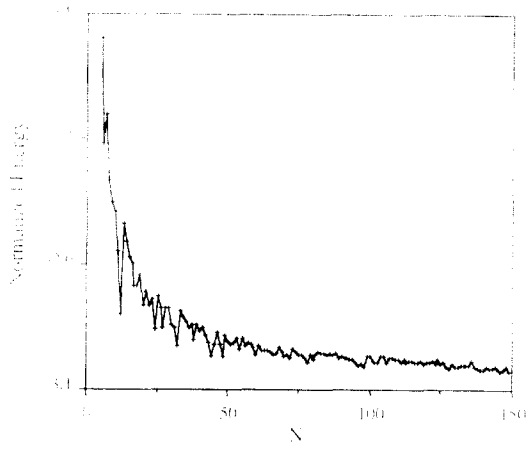

Fig. 2. The (normalized) potential energy as a function of the number of particles N.

First results of experiments with a few hundred particles [2] show that systems with a number of particles that can be distributed in a crystalline order, do have a lower energy than systems with numbers of particles that can not be located nicely (see Fig. 2). It is this local ordering that will be exploited in the new implementations.

In a crystalline solid only specific distances between the particles are found. In Fig. 3 the distance distribution in a spherical crystalline solid as found by the Simulated Annealing algorithm

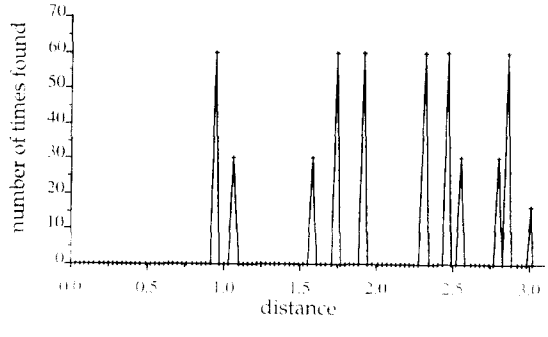

Fig. 3. The distances found in the optimal solution for $N = 32$.

for $N = 32$ particles. This can be used to construct order parameters to monitor the crystallization.

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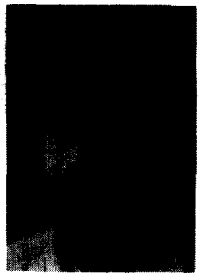
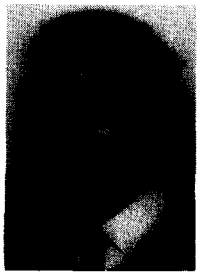
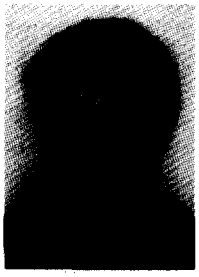


Jeroen Voogd (1966) studied computational physics at the University of Amsterdam. He started his Ph. D. research on September 1992 in the Parallel Scientific Computing Group at the Department of Mathematics and Computer Science at the University of Amsterdam.



René van Dantzig (1937) is groupleader at the National Institute of Nuclear and High Energy Physics (NIKHEF) in Amsterdam, The Netherlands, from where – with the NIKHEF-team – he participates in experiments at CERN, Geneva, Switzerland. Besides he is active in distributed computing.



Peter M.A. Sloot (1956) got his Master's degree in Chemical and Theoretical Physics at the University of Amsterdam (UoA) in 1983 and a Ph. D. in Computer Science 1988. Currently he is an Associate Professor in Parallel and Scientific Computing at the UoA. He has founded in 1990 the interdisciplinary working group Parallel Scientific Computing and Simulation.