Macroscopic structures formed by nanoparticle interactions

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INTRODUCTION

Nanoparticles are extremely small particles, on the scale of a few nanometers, which tend to exhibit quantum mechanical behavior. Due to their size and special physical properties, they are especially useful in the development of biosensors and imaging devices [1]. Much of their usefulness depends on their ability to be placed on a surface with a specific macroscopic structure in mind [2]. These structures are a result of the interactions between nanoparticles as well as the interactions between nanoparticles and a solvent. Currently, the mechanism behind the formation of nanoparticle structures is not completely clear in all instances. The present study attempts to model and understand the formation of new nanoparticle structures.

Rabani et. al. have already created a model that simulates evaporation on a lattice with nanoparticles that attract each other [3]. As the solvent evaporates, the nanoparticles become virtually frozen at their current locations, leaving complex structures such as dots, aggregates, and clumps, depending upon the initial conditions and parameters. Further, the results of their simulations qualitatively matched the structures that had been observed in the laboratory. The present study will extend the work of Rabani et. al. To extend their efforts, we will experiment with additional types of interactions during the evaporation process.

The proposed study will be divided into four stages:

1. Reconstruction of the simulation performed by Rabani et. al. [3]. Given the conditions used in their simulations, we aim to observe the same patterns. This step will also include the development of a visualization method for analyzing
the results qualitatively.

2. Expansion of the simulation to consider other types of nanoparticle interactions, such as electric charge.

3. Execution of the simulation under a variety of conditions. This step will include a great deal of exploration, and multiple simulations will be performed near values of parameters which are deemed interesting.

4. An attempt to model and understand the patterns observed in the laboratory.

METHOD

At first, the program will create a lattice completely filled with liquid. Then, it will randomly cover the surface with nanoparticles at a given density. After this, the simulation will proceed using the Metropolis Monte Carlo algorithm [4]. It will randomly choose a cell on the lattice, and attempt to perform a move in configuration space based on that cell. A move could involve evaporating a liquid, physically moving a nanoparticle, or condensing gas into liquid. Each move will be accepted with the Metropolis probability. If the move lowers the energy of the system, it will be accepted. If not, it will be accepted with a probability based on how much it increases the energy of the system. This probability is computed as

\[ p = \exp \left( \frac{-\Delta E}{k_B T} \right). \]  

Different interactions can be modeled by changing the method for computing the total energy \( E_i \) of the system in a given state.

Periodically, as the program models the system, it will save its current state to a file, so that the simulations can be reconstructed visually at a later time. Each time the program saves the two-dimensional lattice, it will also record the number of existing liquid cells on the lattice at that point in time.

The program itself will be developed in the Fortran 90 programming language. Fortran 90 is a high-level language particularly suited to this type of numerical computing. After the program is developed and debugged on a Dell Pentium 4 workstation, it will be executed on a 16-node Beowulf cluster (Altix Model 350) at Duquesne University. This setup will allow multiple simulations to be performed simultaneously, each with different parameters. We
plan to vary the size of the nanoparticles, strength of attraction between nanoparticles, initial density of nanoparticles, and temperature. Further, we plan to experiment with various amounts of charge on the nanoparticles, and we plan to model evaporation conditions that are not homogeneous in space and time. Other nanoparticle interactions will be considered as time allows.

RESULTS

The output of the computer program will be visualized as a two dimensional grid, where liquid, gas, and nanoparticles are each represented by a different color. This will likely be done using an existing software package such as Open Data Explorer, which will allow animations to be created which represent the evolution of each simulation in time.

We plan to categorize each simulation based on its qualitative structure as it evolves. For instance, we expect to see clumps and textured aggregates, and we hope to observe ring-like structures as well as spiral patterns. Further, we hope to find critical points in the parameters where the qualitative nature of the system changes abruptly.

The present study will help us understand the complex structures that nanoparticles form when placed on a surface. This improved understanding will directly aid in the development of biomedical sensors and imaging devices. In order to control assemblies of nanoparticles, we must first be able to simulate and understand them. This study will also provide a bridge between interactions at the nano scale and qualitative structures that are larger in dimension.


