Group 2 Project Proposal

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1. Introduction

Group 2 proposes to study the convergence properties of minimization algorithms towards finding optimal solutions for surface reconstruction mapped onto the well-known "Traveling Salesman Problem." Code will be tested to find convergence rate, wall-clock time, and for solution space exploration. Fig. 1 shows an illustration of the type of problem being considered.

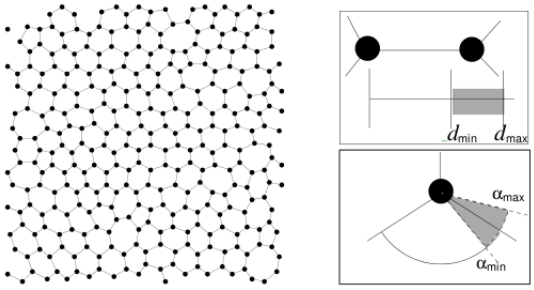

Figure 1: An example of an amorphous solid under simulation. A maximum vertex number of 3 is defined, along with minimum and maximum angles and bond lengths; taken from: Ref. 3

2. Simulated Annealing

Simulated annealing is a stochastic approach towards minimizing an energy function.

3. Genetic Algorithms

Unlike simulated annealing, genetic algorithms rely on a population approach to

4. Ant-Colony Approaches

Ant Colony Optimization [2] draws inspiration from the behavior of ants as they develop a path from their nest to a food source. As ants travel, they deposit pheromones. These pheromones can be detected by other ants and the ants are more likely to follow a path with higher pheromone concentration. In addition to the ants depositing pheromones, these pheromones will evaporate over time. This means that shorter paths will allow larger pheromone concentrations to buildup as ants will be depositing pheromones quicker than they evaporate. Eventually, the system will converge on a minimum solution. A global minimum is pursued by starting out with a large number of ants and by tuning the weight at which pheromones influence decisions.

5. Go with the Winner Approaches

Simulated annealing probabilistically convergences to the optimal solution at the rate of $O(\frac{1}{n})$ where n is the number of independent runs. Using heuristic schemes such as the "Go with the Winner" [1], hereby referred to as GWW, one can improve this convergence rate to $O(log\frac{1}{n})$ and have recently found their way into molecular modeling applications [3]. In general terms, the GWW algorithm mirrors that of simulated annealing; however, each independent run is periodically reassessed to determine if one is converging upon a losing solution. Runs with no chance for success are immediately discarded while runs with the best chance of finding an optimal solution are replicated; thus, GWW generates an ensemble of independent runs filled with "winners".

6. Analysis

To test the scientific performance of these optimization schemes, we will minimize the energy of depositing particles on a surface. Given that the deposition pattern of particles is not unique, all of the optimization schemes will need to generate an ensemble of models representing local minima on the potential energy surface. To quantify the phase space coverage of these optimization schemes, we will initially start from known particle configurations, such as a square and hexagonal lattices, and generate multiple deposition models. We will analyze the number and size of the clusters produced by each method to determine their overall optimization performance.

Additionally, we will test the computational effort involved in each optimization scheme, focusing on the wall-clock time and number of alogrithm iterations/replicates are needed to sufficent converge to a reasonable answer. If time permits, we will also test the ease of formulating these schemes into a parallel computing framework to improve their calculation efficiency.

References

[1] Aldous D. and Vazirani U. Go with the winners algorithms. *Proceedings of the 35th IEEE Symposium on Foundations of Computer Science*, pages 492–501, 1994.

[2] Marco Dorigo, Vittorio Maniezzo, and Alberto Colorni. The ant system: Optimization by a colony

of cooperating agents. *IEEE TRANSACTIONS ON SYSTEMS, MAN, AND CYBERNETICS-PART B*, 26(1):29–41, 1996.

[3] Marcus Peinado and Thomas Lengauer. 'go with the winners' generators with applications to molecular modeling. *RANDOM*, pages 135–149, 1997.