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Optimizing Atomic Structures through Geno-Mathematical Programming

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Abstract. In this paper, we describe our initiative to utilize a modern well-tested numerical platform in the field of material physics: the Genetic Hybrid Algorithm (GHA). Our aim is to develop a powerful special-purpose tool for finding ground state structures. Our task is to find the diamond bulk atomic structure of a silicon supercell through optimization. We are using the semi-empirical Tersoff potential. We focus on a 2x2x1 supercell of cubic silicon unit cells; of the 32 atoms present, we have fixed 12 atoms at their correct positions, leaving 20 atoms for optimization. We have been able to find the known global minimum of the system in different 19-, 43- and 60-parameter cases. We compare the results obtained with our algorithm to traditional methods of steepest descent, simulated annealing and basin hopping. The difficulties of the optimization task arise from the local minimum dense energy landscape of materials and a large amount of parameters. We need to navigate our way efficiently through these minima without being stuck in some unfavorable area of the parameter space. We employ different techniques and optimization algorithms to do this.

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1 Introduction

Our interest in especially semiconductor-oxide interface and surface structures is due to their prevalence in modern electronics and devices; these structures heavily affect the

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performance of the different components present in the devices. On the interface there are two different interconnected crystal structures often leading to structures hard to predict. This is what makes them a difficult research object. Finding these structures by hand, i.e. designing the interfaces by trial and error needs special knowledge and takes a lot of time, which is why a flexible, powerful optimizing tool would be beneficial for many research problems across the field. Measuring the interface structures experimentally is also difficult as they are buried in the material. That is why simulations and calculations conducted on many different interface models are indispensable in understanding the nature and behavior of these structures. The scale of these structures is often measured in Ångström's (Å) which is short for 10^{-10}m.

We started a collaboration between the School of Business and Economics at Åbo Akademi University and University of Turku's Materials Research Laboratory in order to develop a tool for optimizing atomic structures, with the algorithm especially tuned for interface structures. In geno-mathematical programming artificial intelligence is connected to mathematical programming methodology on parallel supercomputers. The approach provides a powerful basis for coping with difficult irregular optimization problems and solving them concurrently. We were also interested in the performance of our special-purpose algorithm in the physics based problem of optimizing atomic structures of materials, designed using a modern numerical platform as a base. The optimization is done by minimizing the potential energy, measured in electronvolts (eV), of the structure. The difficulty does not lie in finding a nearby local minimum from a given starting structure, as this can usually be achieved through the steepest descent method in a small amount of steps, but in navigating past all these minima to the global minimum. The energy landscape is filled with these local traps that do not reveal much if any indication on where the true global minimum lies.

Exploring the whole landscape is only doable in very small cases. This is because along with the increasing parameter count the number of local minima of the task rises exponentially with the number of atoms: for example with Lennard-Jones clusters it was shown that the number of minima multiplies by around 2-3 per atom added [23]. This makes almost any interesting interface or surface system hard to study. In this article, we show that even our small silicon case can be problematic if not treated properly.

In theory, good molecular dynamics (MD) simulation should be able to find the global minimum given enough time and proper annealing. In practice, the required time is often very large and might require a lot of parameter fine-tuning while still leaving defects at the end of the simulation. Of course, even then we can never be sure that the result is the true global minimum, unless we know the answer beforehand. Large scale computing is a crucial part of bigger MD simulations and advances in that field continue to be made even today, for example speeding up node and core communication [7, 26], reducing memory usage [7], improving threading [14] and creating faster algorithms for force computations [8]. In our work presented in this paper, all the cores work fairly independently, but in the future the algorithm could be expanded to include more communication between the cores. We did a series of MD simulations of our silicon test case