

Parallel Genetic Algorithms for Structural Characterisations of Nanoalloys



Challenges

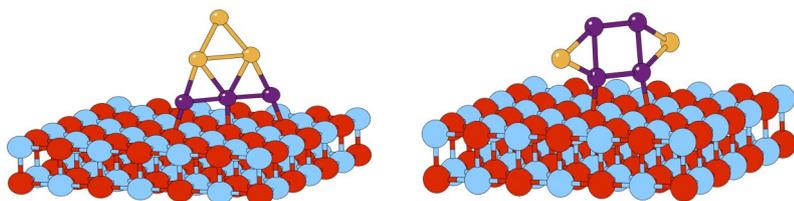
To develop and apply efficient parallel methodologies to benefit from the vast computational resources available from massively parallel high performance computers.

Background

Nanoalloys are nanoparticles composed of two or more metallic elements. The combination of metals results in properties which are not only dependent on size and shape of the nanoalloy but on the composition and chemical ordering of the elements. Nanoalloys have possible magnetic, optical and catalytic applications, however, to understand these properties their structural characterisation is essential. There are a wide variety of methods for the structural characterisation of nanoalloys, including basin-hopping, statistical mechanical methods and genetics algorithms.

Results

The Birmingham Parallel Genetic Algorithm (BPGA) is a newly developed genetic algorithm for the direct density functional theory global optimisation of nanoalloys. The use of density functional theory allows for the identification of quantum-size effects commonly seen in sub-nanometre clusters, however, this greatly increases the computational effort required for the global optimisation of a system. This limits the size of cluster it is possible to study with such methods. The BPGA utilises a pool genetic algorithm methodology which allows the program to efficiently utilise computational resources within a parallel scheme. The program has the ability to characterise the structures of both gas-phase and surface supported clusters while scaling well beyond previous cluster size restrictions. The BPGA was developed and tested on the BlueBEAR high performance computer. BEAR provided an excellent test bed for the programs development before its eventual application on to the UK's national supercomputer, ARCHER. On ARCHER users can be penalised for the use of inefficient or under-developed programs. We we're able to quickly resolve any issues arising on ARHCER using BlueBEAR. The BPGA is now being applied to wide range of mono and bimetallic systems.



Case study



Client Profile

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Product Used

VASP
Birmingham Parallel Genetic
Algorithm

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