# A Genetic Algorithm for Surface Reconstructions

and other Periodic Systems

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**Abstract**

Genetic Algorithms can be suitably applied to the study of atomic and molecular clusters (Deaven and Ho, 1995) and surfaces (Fu et al., 1997), but only very recently has research has been done in applying the techniques of real-space genetic algorithms to surfaces (Chuang et al., 2004). We propose a real-space represented genetic algorithm which is suitable for studying surface reconstructions, and which also incorporates a novel crossover technique. This approach uses a periodic slice through the system to reduce the discontinuities generated by the mating procedure and which can be more easily generalised for different bulk and surface systems. We will present results obtained using this algorithm, as applied to suitably chosen model systems. We will also discuss the application of this method to the study of interfaces.

## 1 Introduction

Genetic Algorithms (GA's) are becoming widely used to determine the minimum energy configurations of atomic clusters (Deaven and Ho, 1995; Johnston, 2003), and more recently surfaces (Chuang et al., 2004, 2005). These previous studies made use of a planar cut in the crossover operation, slicing each parent in two, and then swapping halves to generate offspring (see Johnston (2003) for a review on clusters). While there is no periodicity in the cluster case, there are periodic boundary conditions (PBC's) in the surface case, and a planar cut does not takes these PBC's into account.

# 2 Genetic Algorithms

- Genetic Algorithms are a stochastic minimisation technique inspired by Darwin's Theory of Evolution (Holland, 1992).
- The "population" is made up of a number of members, each of which is a viable solution to the problem being studied.
- Typically, a GA requires a number of things: representation, calculation of fitness (dependent on the problem studied), selection for crossover (reproduction) and update, and how crossover and mutation are performed.
  - originally a binary string was used to represent a member of the population
  - crossover was performed by swapping sections of two (or more) parent strings to produce offspring
  - mutation was incorporated by flipping a percentage of bits in the string

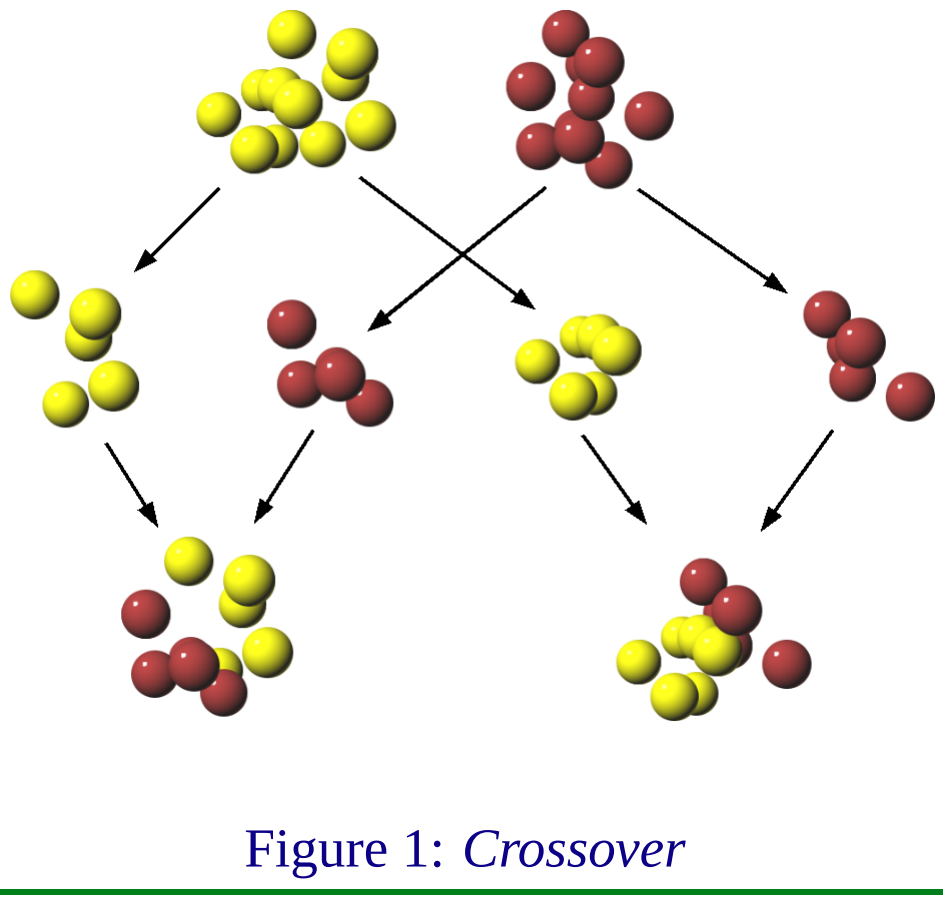

Figure 1: *Crossover*

A Genetic Algorithm

1: generate initial population
2: calculate fitness of each member of the population
3: select population members for crossover
4: perform crossover
5: mutate offspring (typically 5-15 % mutation rate)
6: calculate fitness of offspring
7: update the population
8: return to step 2

- For physical systems, binary strings are not the most efficient representation (Deaven and Ho, 1995).
  - members are represented by an array of atomic position vectors
  - crossover is done by taking a plane through the centre of mass of the two parent structures and swapping the halves (see figure 1)
  - mutation and selection can be done in a number of methods
  - after crossover/mutation a direct minimiser is applied to relax the offspring
- Fitness is calculated from energy. "Fitter" members are more likely to be selected for crossover/update.

# 3 Crossover in Periodic Systems

- Most of the previous applications of GA's to atomic configurations have focused on non-periodic clusters (Deaven and Ho, 1995; Johnston, 2003).
- Only more recently have surfaces with periodic boundary conditions been studied using these methods (Chuang et al., 2004, 2005).

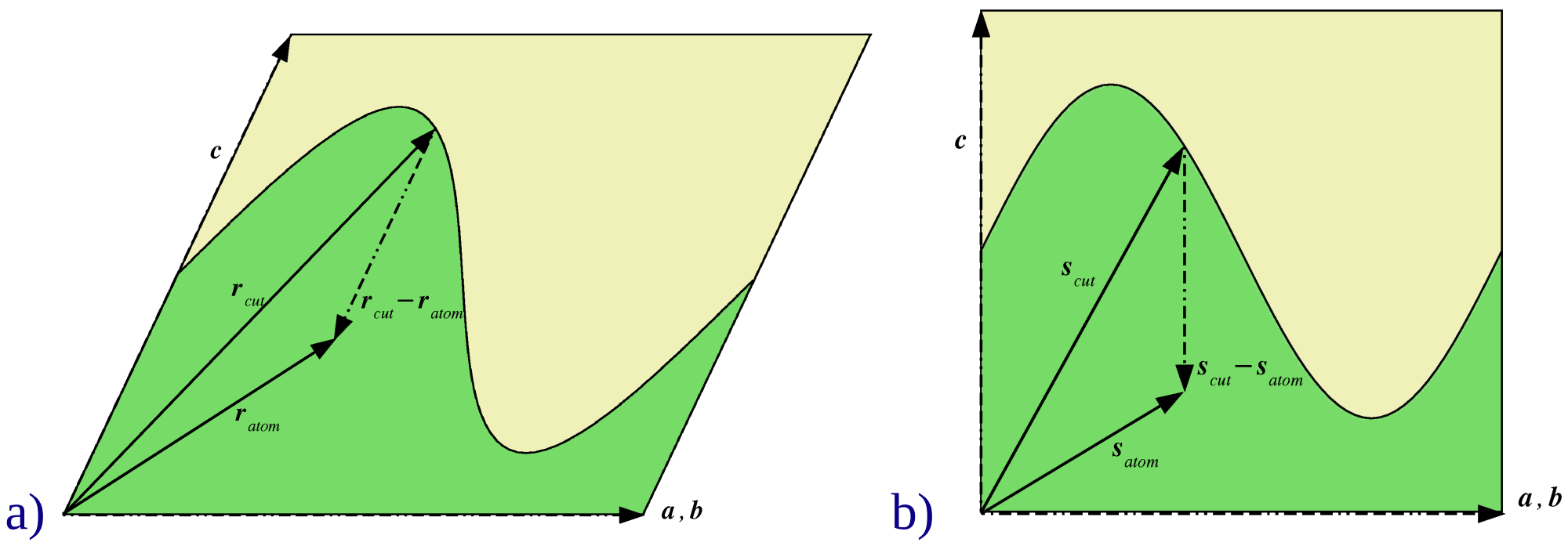


Figure 2: Diagram showing crossover in a) absolute representation and b) fractional representation

- We have developed a general method for crossover which can be used to study surface, interface and bulk systems.
  - crossover is performed in fractional coordinates (see figure 2)
  - the cut is defined by any function with the same periodicity as the supercell, $\mathbf{s}_{cut} = f\left(\mathbf{s}_{atom}^{\mathbf{a},\mathbf{b}}\right)$, ($\mathbf{s}_{atom}^{\mathbf{a},\mathbf{b}}$ is the position vector for each atom in the $\mathbf{a}$ and $\mathbf{b}$ directions)
  - the metric tensor $\underline{\underline{g}} = \underline{\underline{h}}^{\mathrm{T}}\underline{\underline{h}}$ (where $\underline{\underline{h}} = [\mathbf{a}, \mathbf{b}, \mathbf{c}]$) is used to calculate the product $\alpha_{cut}$ (see equation 1)
  - $\alpha_{cut}$ is then used to generate halves to create offspring (see equation 2)

$$\alpha_{cut} = \left(\mathbf{s}_{cut} - \mathbf{s}_{atom}\right)^{\mathrm{T}} \underline{\underline{g}}\, \mathbf{c} \tag{1}$$

$$\alpha_{cut} \begin{cases} > 0 & \text{the atom is } \textit{“above”} \text{ (outside) the cut} \\ \leq 0 & \text{the atom is } \textit{“below”} \text{ (inside) the cut} \end{cases} \tag{2}$$

# 4 Applications

## 4.1 Surfaces and Interfaces

- Figure 3 shows the crossover operation for surfaces and interfaces (in a surface case species A would be vacuum).
- The amplitude of the cut can be altered to change the degree of mixing of the two species (see figure 4).

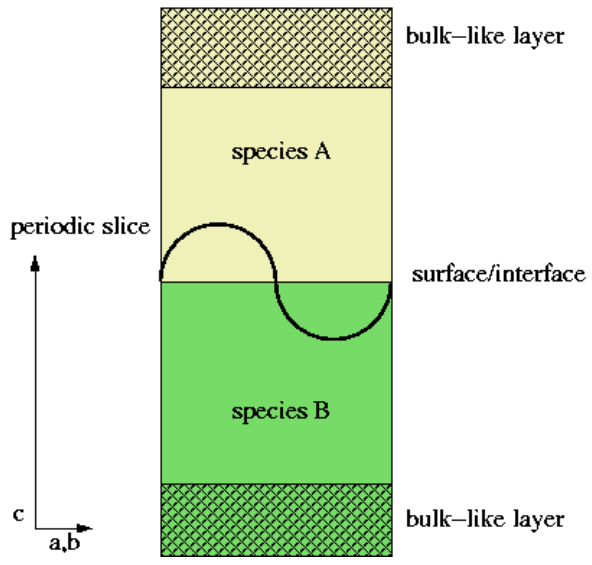


Figure 3: Crossover operation for surfaces/interfaces before crossover

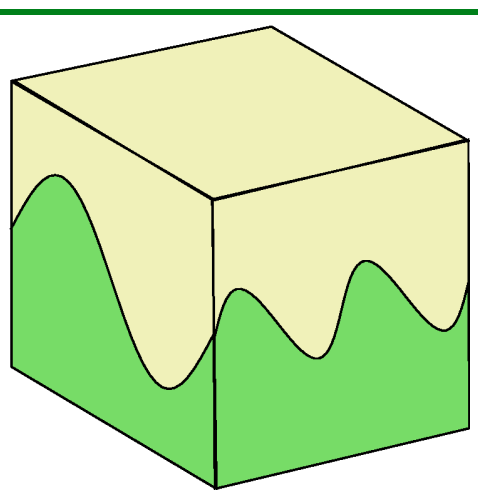

Figure 4: Different wavelengths and amplitudes for the crossover operation can be used along different cell vectors

- The crossover operation allows varying surface heights to make step edges and adatoms appear on the surface (see figure 5).

## 4.2 Bulk

- In this case two cuts are required to prevent a mismatch along the periodic boundary in the **a b**-plane where $\left|\mathbf{s}^{\mathbf{c}}_{atom}\right| \equiv 0 \equiv 1$ (see figure 6).

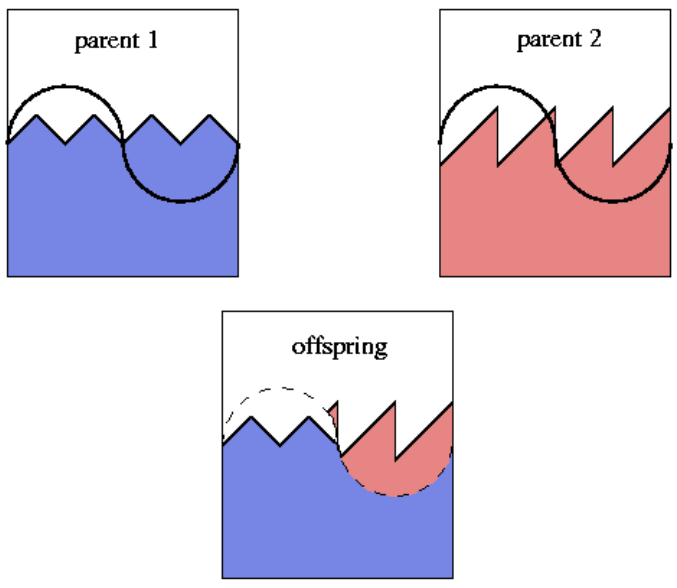


Figure 5: Crossover showing parents and offspring

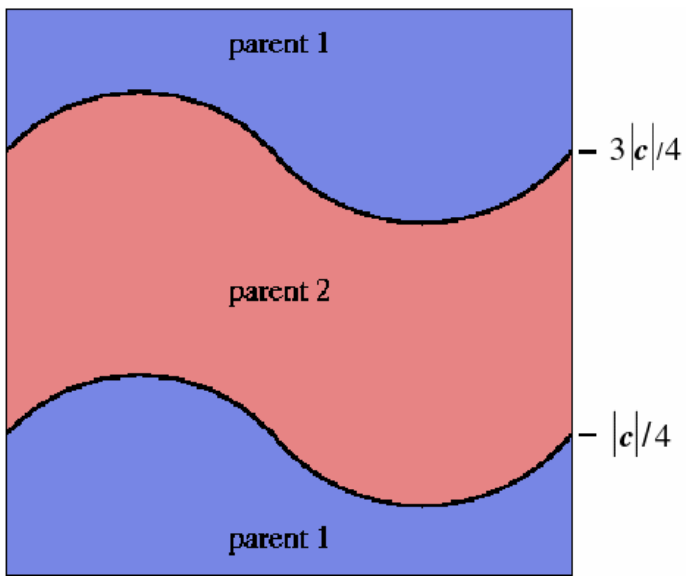


Figure 6: Crossover operation for bulk after crossover

# 5 Results

- For the results shown here, the Polak-Ribière Conjugate Gradient Method (Polak, 1971) was used as the local minimiser.
- Fitness is determined by the relative energies of the population members, and each population member was chosen for crossover based on its fitness using roulette wheel selection (Johnston, 2003).
- In the update procedure, the fittest population member was allowed to proceed, with roulette wheel selection being used for the remaining members.
- Another method for updating is to only allow the $M$ fittest population members to proceed to the next generation, from a super-population of $2M$ parents and offspring.

## 5.1 Lennard-Jones Potential

This method has been applied to atoms acting under the empirical Lennard-Jones potential (Lennard-Jones and Ingham, 1925)

$$V_{LJ}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{3}$$

- This has a HCP ground state structure (Pollack, 1964) which is almost degenerate with the FCC structure (energy difference from HCP is $+0.1\%$ (Kane and Goeppert-Mayer, 1940)).

- Initial calculations were performed with the super-cell and atom number commensurate with bulk FCC:
  - HCP solution was not expected to be found
  - FCC structure was found within 5 generations
    - population size of 32 members, using a super-cell containing 108 atoms
    - starting from a *random configuration of atomic positions* (see figure 7)

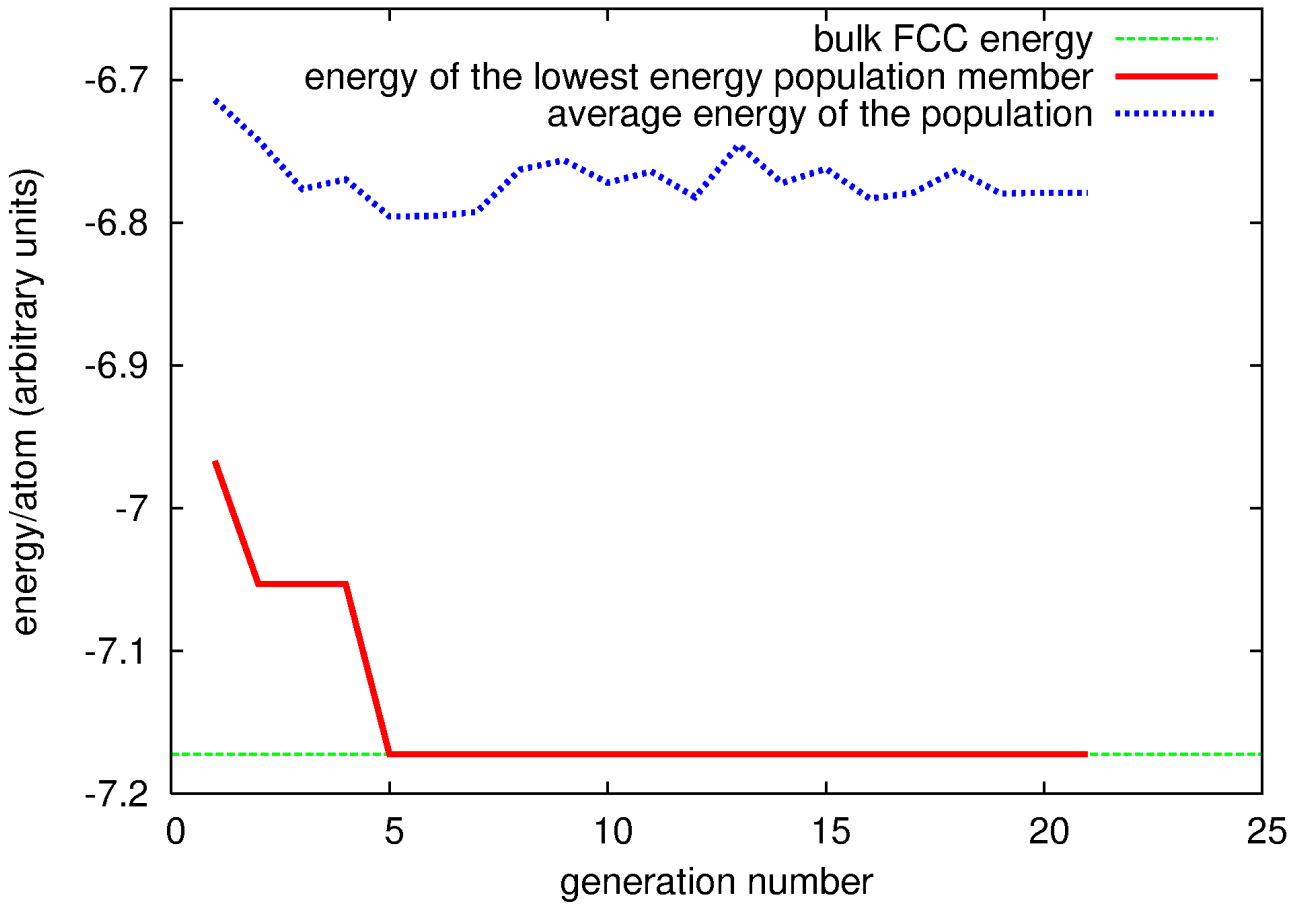


Figure 7: Results from bulk 108 atom (fixed atom number), 32 population member calculation starting from random initial configuration. Due to the selection method used for updating the population, it is possible for the average energy of the population to rise between generations.

# 6 Conclusions

By performing all crossovers in fractional coordinates each population member may be allowed to have a different unit cell, and if the local minimiser also optimises the cell vectors then the optimisation process will not be biased either by initial atom number or unit cell.

We have demonstrated a general method for optimising bulk, interface and surface structures using a genetic algorithm, which makes use of the inherent periodicity in the system in the calculation of crossover between parent members of the population. Future work will include allowing different population members to have different cells, optimised as described above, and will also include *ab initio* calculations.

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