Real-Space GA's and expansion using Periodic Boundary Conditions

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I. RECAP OF GA'S

This is an extension to the talk that I gave last year on genetic algorithms. I will give a brief recap on the salient points. A good starting point is Holland [3].

These notes are not supposed to be a full set - they are just to state the main points and references. Please see the white-board for more information.

II. BIT-STRING REPRESENTATION

In Hollands' original work the population members were represented by bit strings. The ideas of crossover and mutation are very easily shown in table I.

	parents	children
crossover	1011|1001	1011|0011
	0110|0011	0110|1001
mutation	11100100	01100101
	↑ ↑	↑ ↑

TABLE I: bit-string crossover and mutation

To determine the fitness of each population member the information stored in the strings must be "decoded" or the fitness must be able to be calculated from the strings directly. One of the main advantages to the bit string approach is that the crossover and mutation steps are very fast.

III. REAL-SPACE REPRESENTATION

When applied to clusters (or other molecular problems) this bit-string approach is not the best to apply. The fitness function is calculated from the energy of the cluster, which requires the atomic positions, so the bit-strings would have to be translated back to positions every time the fitness needs to be calculated (at least twice in every generation), also the encoding of the strings usually requires some sort of discretisation of space, which may bias the preferred solutions in a particular direction.

A. Fitness

This is calculated from the energy of the cluster, and as such requires a real-space description of the atomic positions.

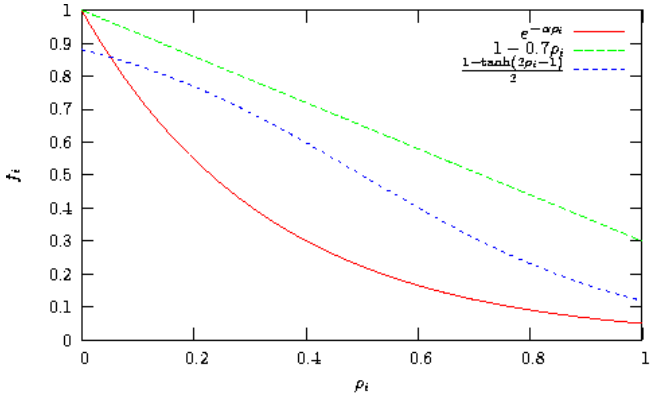

FIG. 1: Comparison of the three different fitness schemes mentioned

Since the true global minimum is not known a normalised energy is used. All positive energies are set to zero (the use of a direct minimiser prevents this in any case). See equation 1.

$$\rho_i = \frac{V_i - V_{min}}{V_{max} - V_{min}} \tag{1}$$

From this value, $\rho_i \in [0,1]$, the fitness is can then be scaled using a number of different methods (Johnston [4]):

$$\textbf{Exponential:}\quad f_i = \exp(-\alpha\rho_i) \tag{2a}$$
$$\textbf{Linear:}\quad f_i = 1 - 0.7\rho_i \tag{2b}$$
$$\textbf{Hyperbolic Tangent:}\quad f_i = \frac{[1-\tanh(2\rho_i - 1)]}{2}. \tag{2c}$$

This just places different emphasis on how the clusters are selected (see figure 1). In equation 2a α is typically set to 3.

B. Selection for Reproduction

One simple selection method is roulette selection: selection is proportional to fitness. The probability of an individual *i* being selected from its fitness f_i is

$$P_i = f_i / \sum_{j=1}^{N} f_j \tag{3}$$

A uniform random number, p, would then be generated ($p \in [0,1]$). If this number is between the cumulative probabilities

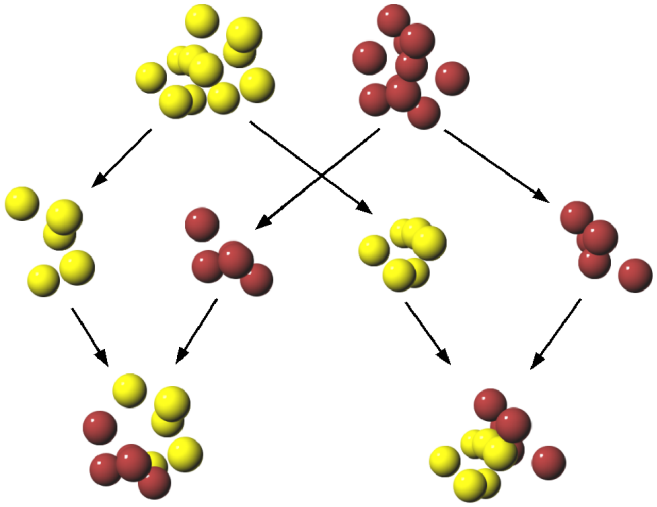

FIG. 2: Crossover

of the i^{th} and $(i+1)^{th}$ individuals, then the i^{th} individual is selected.

There are more complicated methods (known as tournament selection), but I have found that the roulette wheel method is adequate, and the added complication and time required to perform tournament selection may not give any significant advantages.

C. Crossover

This action, in the real-space representation, is completely different from bit-string crossover, however, it does have all the benefits. The clusters themselves are sliced in half and it is these halves which are crossed over, as can be seen in figure 2. This technique was first used by Deaven and Ho [1].

D. Mutation

The form of mutation in this representation is just as simple as in the bit-string representation - a random change of the position of one or more atoms, which can be done any way you like. After the combined crossover/mutation step the cluster needs to be minimised so that it's at the bottom of it's local basin of attraction.

IV. PERIODIC BOUNDARY CONDITIONS

The use of genetic algorithms to study clusters is done by a number of groups, however, their use in surface reconstruction is not. There was one study done which simulated Lennard-Jones sputtering (Miyazaki and Inoue [5]), which used a lattice based approach, and encoded the bit-strings from the lattice positions. The real-space description has not been applied, and may lead to some interesting results, especially in the case of the oscillatory Z1 (Doye et al. [2]) potential.

A. Crossover

This is the tricky part in the process - how exactly to perform the crossover. Although you are effectively dealing with a continuum of atoms, you still need to ensure that you keep the same number of atoms in the offspring's cell as in the parent's cell, but theoretically the freedom in how crossover is performed could be increased due to the PBC's.

For crossover the cell could in effect be treated like an independent cluster which is only wrapped back into the surface/bulk after crossover has occurred, and so long as the number of atoms is conserved, anything can go. The amount freedom allowed in crossover may also have some effect on the efficiency.

Any suggestions or ideas would be greatly appreciated!

[1] D. M. Deaven and K. M. Ho. Molecular-geometry optimization with a genetic algorithm. *Phys. Rev. Lett.*, 75:288–291, 1995.

[2] J. P. K. Doye, D. J. Wales, F. H. M. Zetterling, and M. Dzugutov. The favored cluster structures of model glass formers. *J. Chem. Phys.*, 118:2792–2799, 2003.

[3] John H. Holland. *Adaption in Natural and Artificial Systems*. MIT Press/Bradford Books Edition, 1992. ISBN 0-262-58111-6.

[4] R. L. Johnston. Evolving better nanoparticles: Genetic algorithms for optimising cluster geometries. *Dalton Trans.*, pages 4193–4207, 2003.

[5] Koji Miyazaki and Takayoshi Inoue. Genetic algorithm simulation for the deposited structure of atoms. *Surf. Sci.*, 501:93–101, 2002.