

# **Genetic Algorithms for Surfaces and Bulk**

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# I. **SUMMARY**

- What is a Genetic Algorithm?
- Choice of Mating Operator
- Solution to Problem
- Applications
- Conclusions

## II. GENETIC ALGORITHMS

- Minimisation technique for systems with a complicated potential energy surface (PES)

*(i) generate initial population*

*(ii) calculate fitness of each member of the population*

*(iii) select population members for crossover*

*(iv) perform crossover*

*(v) mutate offspring*

*(vi) determine fitness of offspring*

*(vii) update the population*

*(viii) return to step (ii)*

### III. GENETIC OPERATOR

- We wish to perform genetic operations on a variety of systems
  - bulk
  - surfaces
  - interfaces
  
- Previous studies have used a planar slice to perform the mating operation.
  - This is suitable for small isolated systems such as clusters
  - What about larger systems simulated using periodic boundary conditions?

#### IV. PERIODICITY

- *SOLUTION*: Use a periodic slice.
  - flexible - can be used in study of all required systems
  - maintains periodicity of the boundary conditions
  - does not introduce extra dislocations

## v. APPLICATIONS

- Initially trying on Lennard-Jones (still awaiting results)
- Then move on to interface of two different Lennard-Jones systems
- Also have other pair-potentials to try
- Final aim - surfaces of Ice

## VI. CONCLUSIONS

- We have developed a new mating operation for use in real-space encoded Genetic Algorithms
- It makes use of the periodicity of the boundary conditions
- It can be used in interfaces, bulk and surface systems