



A Real-Space Genetic Algorithm for Crystal Structure Determination

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March 13th, 2006

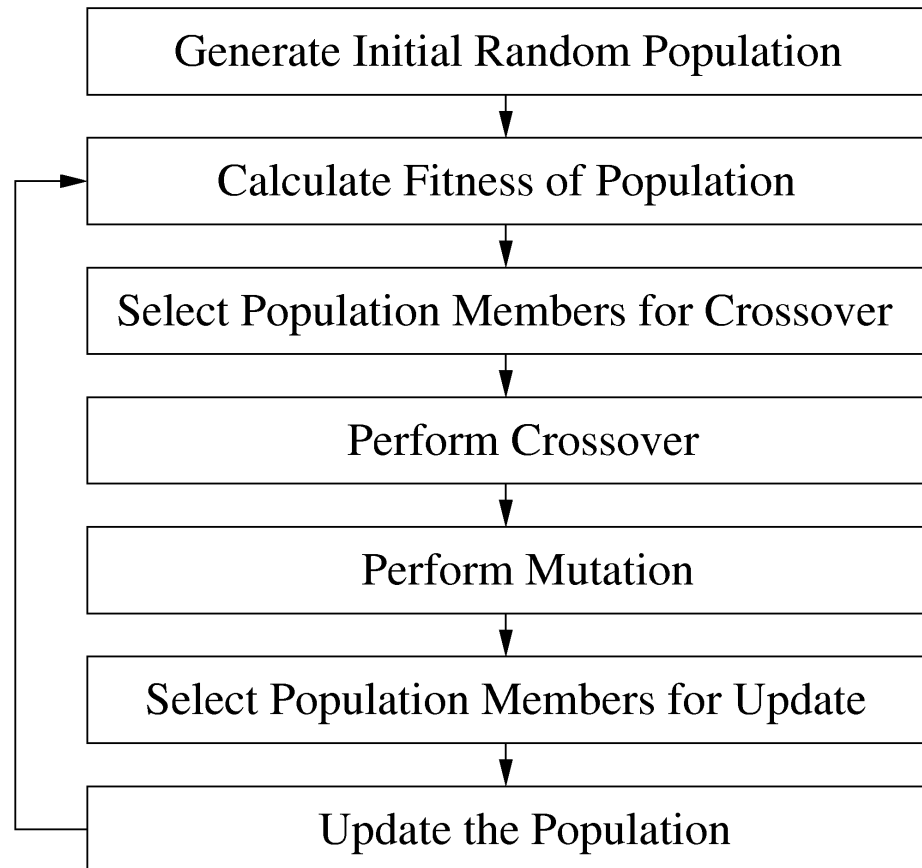
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Outline of Talk

- Genetic Algorithms applied to Real-Space systems
 - Application to Clusters
 - Application to Periodic Systems
- Results from Empirical Potentials
- Conclusions
- Future Research

Basic Outline of a GA





Genetic Algorithms applied to Real-Space systems

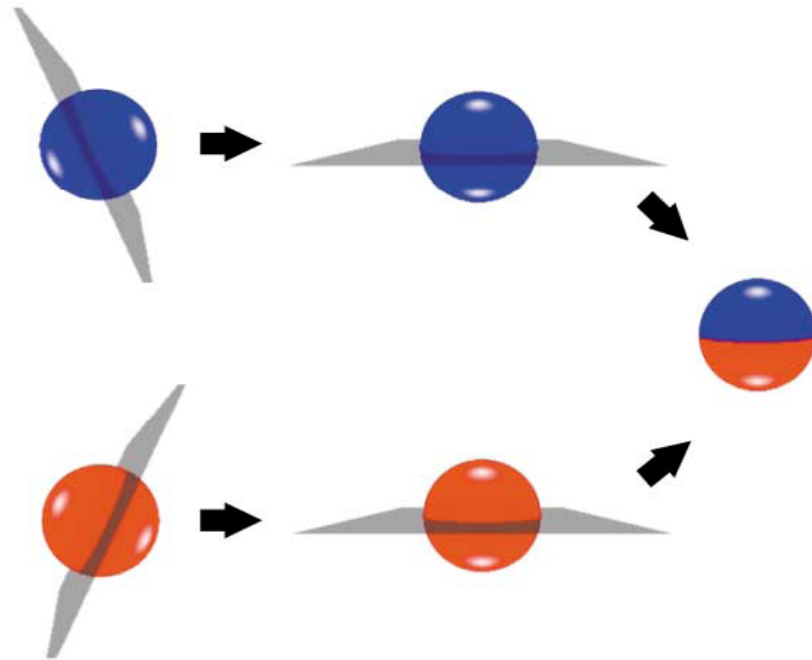
- Instead of a binary representation, GAs applied to physical systems require a real-space approach.
- Technique was first applied to clusters ¹
- This has since been applied in the study of nanowires ² and surfaces ³.

¹Deaven and Ho, *Phys. Rev. Lett.* **75** 288 (1995)

²Wang *et al*, *Phys. Rev. Lett.* **86** 2046 (2001)

³Chuang *et al*, *Surf. Sci.* **573** L375 (2004)

Real-Space Crossover



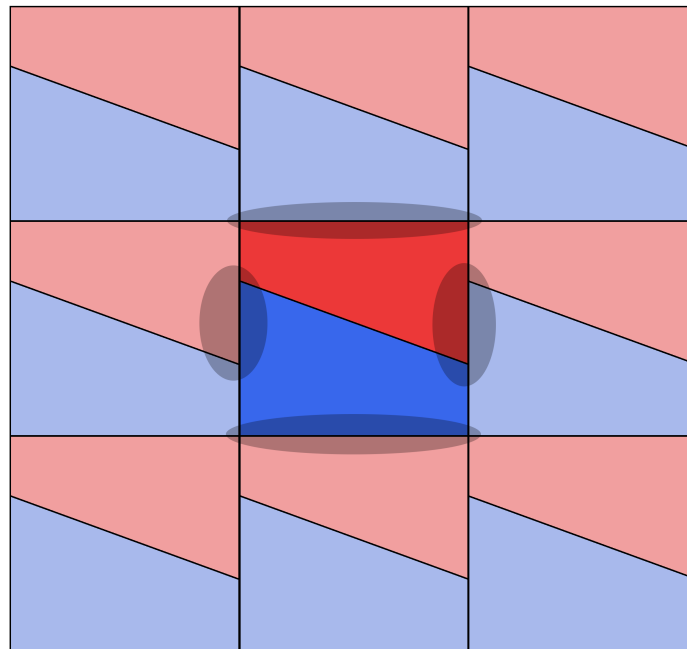
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⁴Johnston, *Dalton Trans.* **22** 4193-4207

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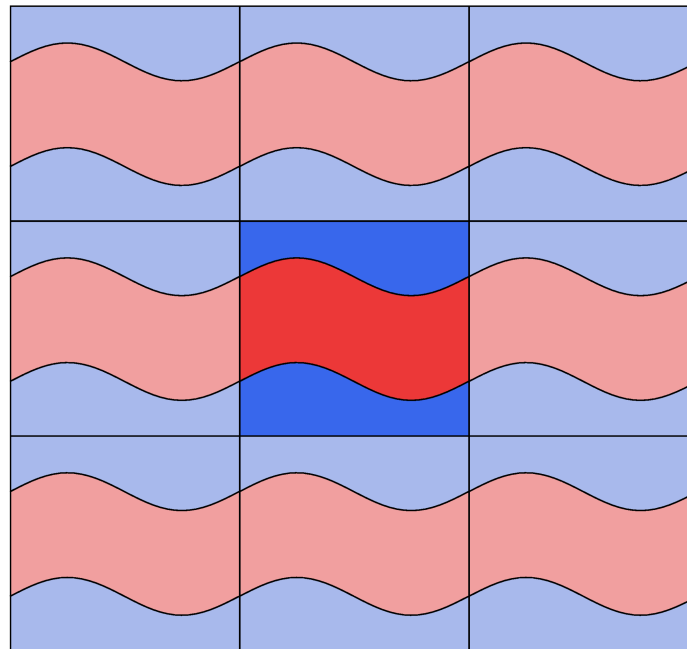
Application to Periodic Systems

- Calculations are performed in a supercell approach.
 - Crossover produces discontinuities at cell boundaries



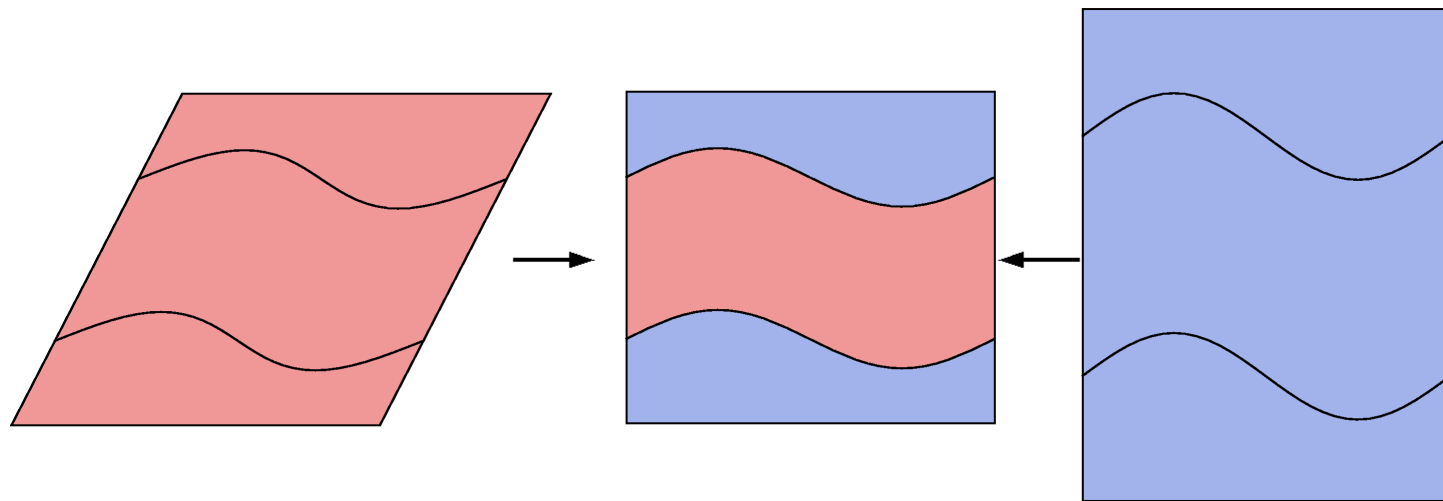
Application to Periodic Systems

- Periodic Cuts remove these discontinuities.



Application to Periodic Systems

- Performing crossover in fractional co-ordinates allows parents to have different cells.

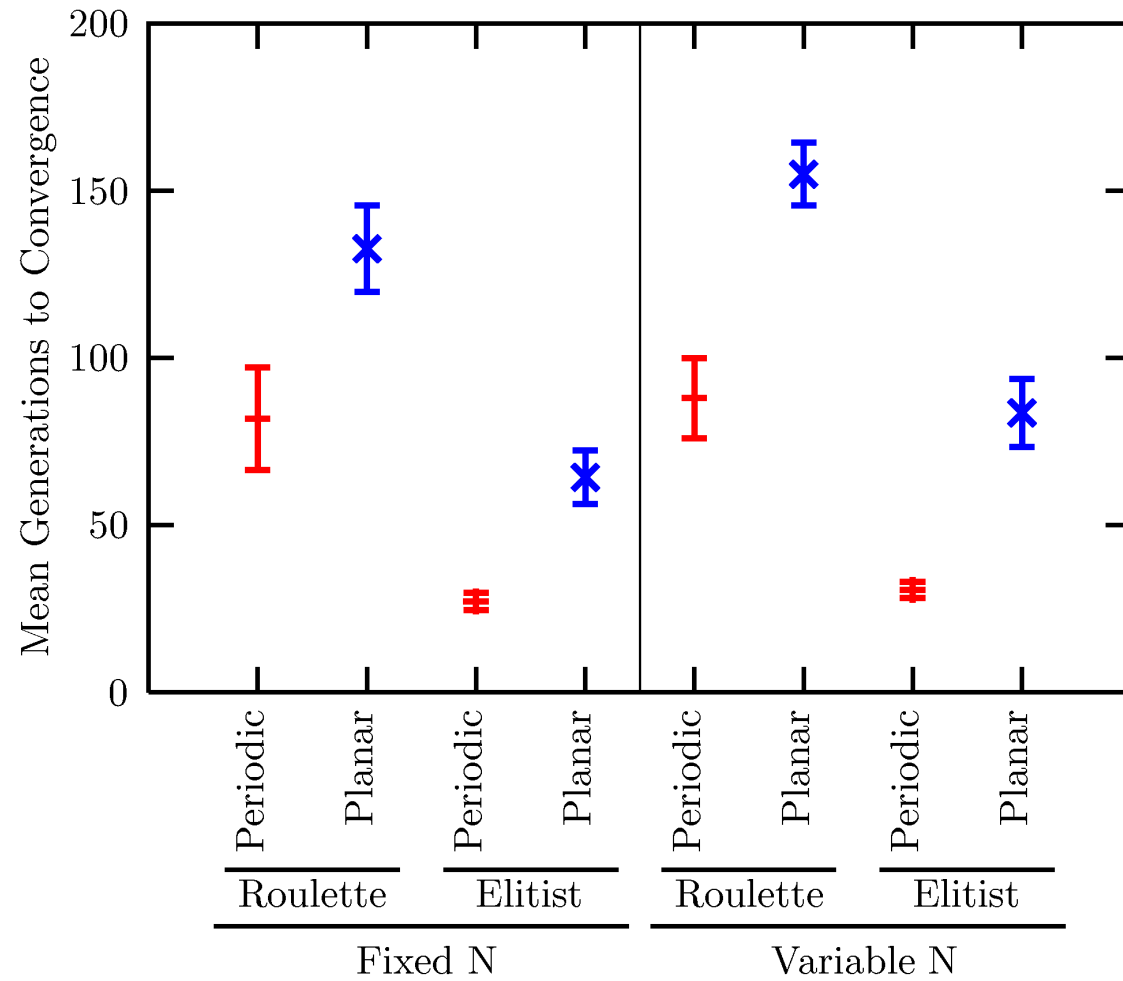




Results from Empirical Potentials

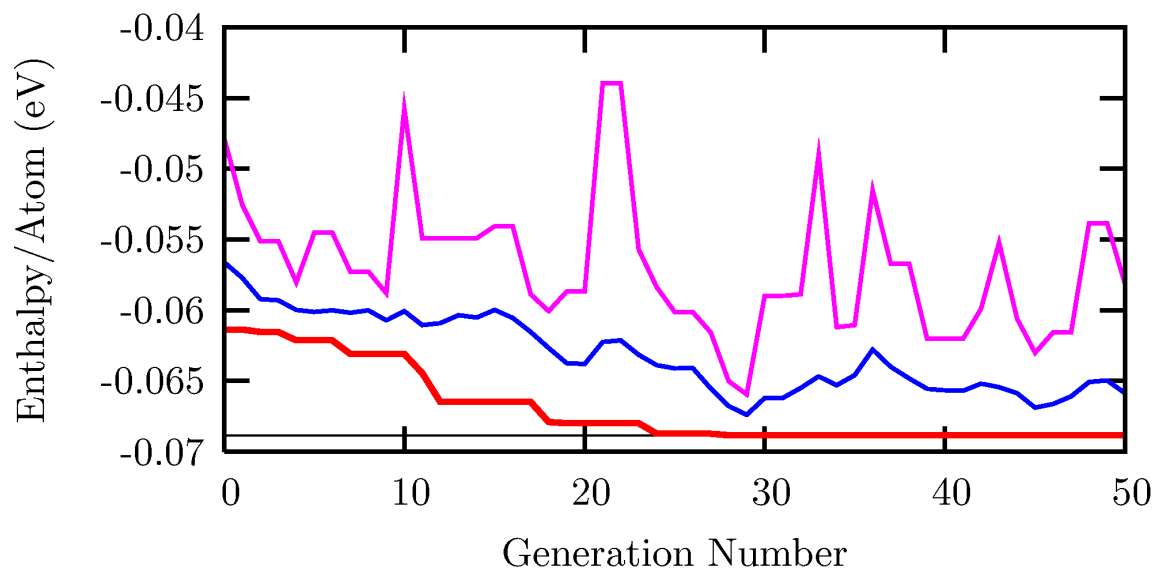
- Calculations performed on 150-atom Lennard-Jones bulk.
 - Supercell commensurate with HCP or FCC
- Crossover:
 - Periodic or Planar
- Update:
 - Use *Roulette Wheel* or *Elitist* selection
- The number of atoms can be kept fixed or be allowed to vary after crossover.

Results from Empirical Potentials



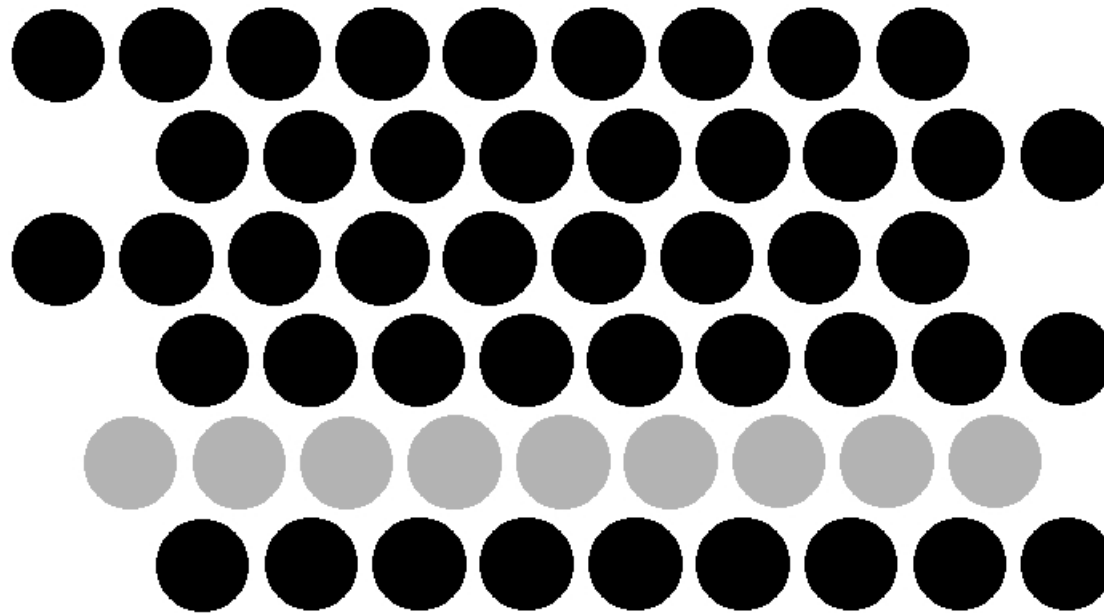
Results from Empirical Potentials

N = 150 VARIABLE, Population Size = 16, Mutation Rate = 10%,
Mutation Amp = 2.5Å, Update Scheme = ROULETTE, BULK PERIODIC SLICE



HCP Enthalpy	—	Average Enthalpy	—
Minimum Enthalpy	—	Maximum Enthalpy	—

Results from Empirical Potentials





Conclusions


- Genetic algorithms are a powerful technique that can be easily applied to bulk systems with a periodic supercell.
- For periodic systems a periodic form of crossover greatly improves convergence times.



Future Work

- This GA has been incorporated into the *ab initio* planewave DFT code CASTEP⁵
- The following research is currently ongoing using this technique
 - Polymorph searches.
 - Multi-species calculations.
 - Silicon phase transition studies.
 - Surface reconstructions.

⁵Segall *et al*, *J. Phys.: Cond. Matt.*, **14** 2717 (2002)

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- <http://www-users.york.ac.uk/~nla101/>
 - A Periodic Genetic Algorithm with Real-Space Representation for Crystal Structure and Polymorph Prediction, N.L. Abraham and M.I.J. Probert, *Phys. Rev. B.* (2006) (submitted)
 - I would like to thank the following organisations for financial support
 - EPSRC
 - Department of Physics, University of York
 - C R Barber Trust Fund
 - IoP CMMP Division
 - IoP Computational Physics Group
 - I would also like to thank Rex Godby and the rest of the CMT group for useful discussions.