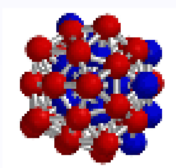
Silicon Cluster Optimization Using Extended Compact Genetic Algorithm (ECGA)

Kumara Sastry Guanghua Xiao

University of Illinois at Urbana-Champaign

{ksastry, gxiao}@uiuc.edu

December 12, 2000



MatSE 385

ATOMIC SCALE SIMULATION

Outline

- Motivation
- Overview of ECGA
- Marginal Product Models and BBs
- Silicon Potential
- Algorithm Implementation
- Results
- Conclusions

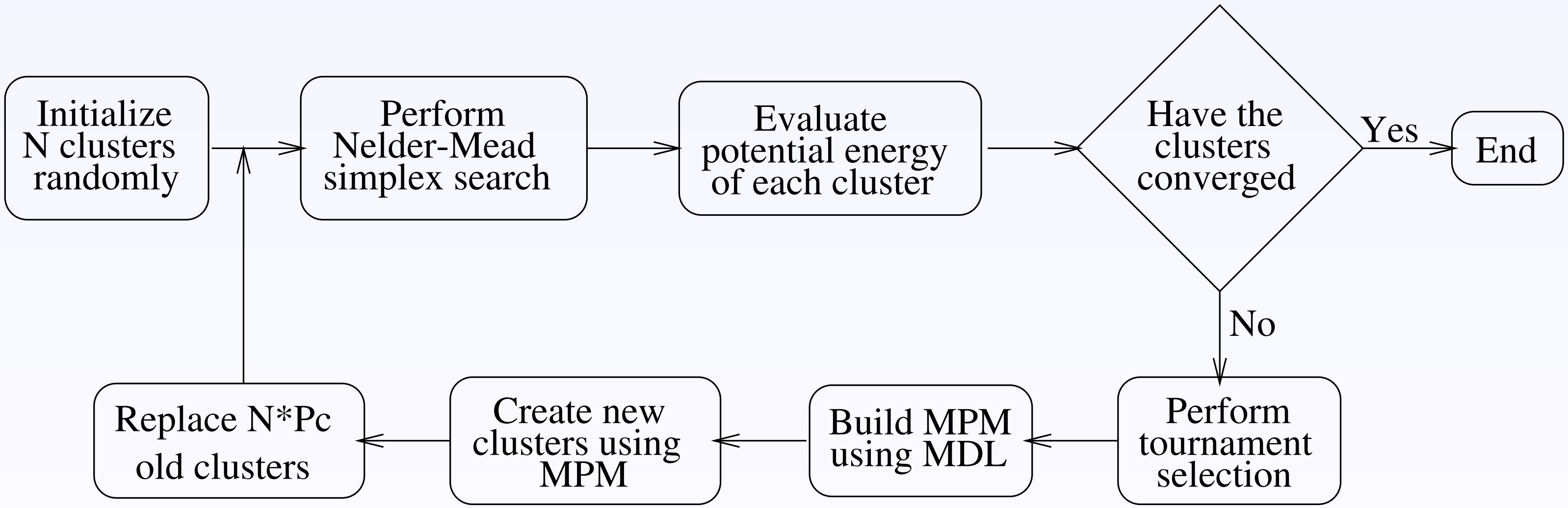
Motivation

- Existing algorithms use "not-so-good" operators
  - Proportionate selection
  - Single point crossover
- Increased interest in competent GAs
  - Solves hard problems quickly reliably and accurately
- An interesting competent GA is ECGA (Harik, 1999)
  - builds models of good data as linkage groups
- Cluster optimization is a NP-hard problem (Wille and Vennik, 1985)

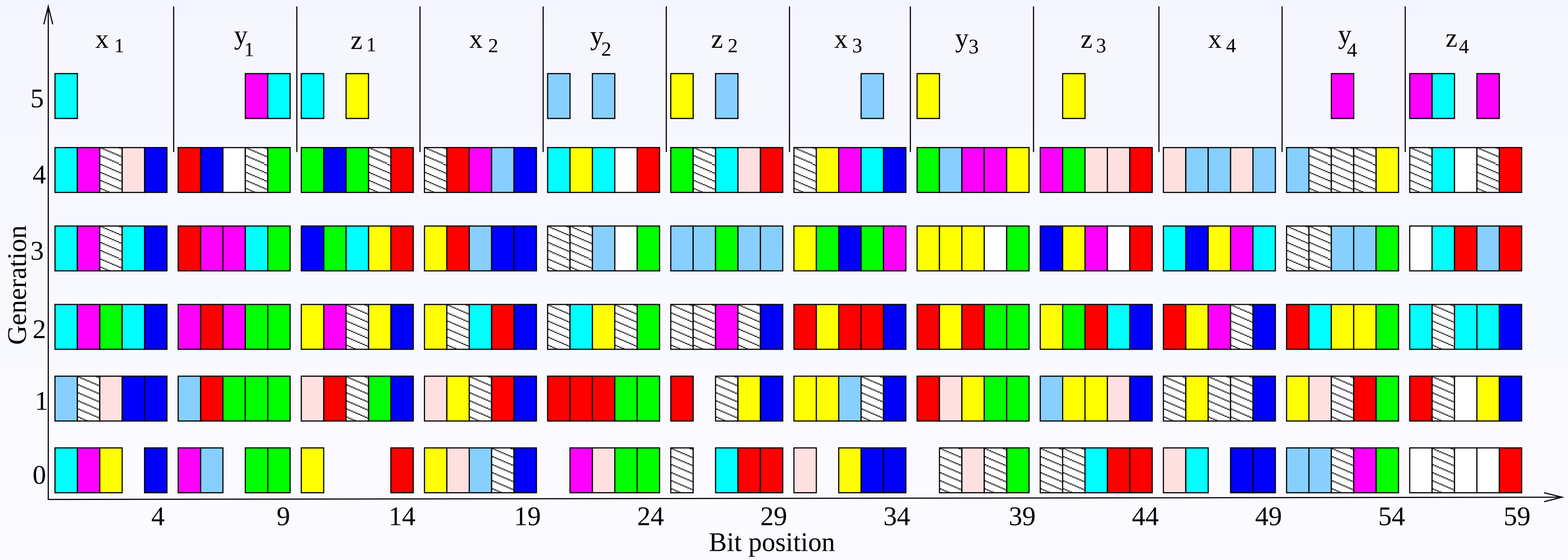
Overview of ECGA

- Key Idea: Good probability distribution ≡ *Linkage learning*
- Probability distribution: *Marginal Product Models* (MPM)
- Quantified based on *Minimum Description Length* (MDL)
- MDL Concept: Simpler distributions are better

Flowchart of Optimization Algorithm



MPM and Building Blocks



Marginal Product Models

- Product of marginal distributions on a partition of genes
- Similar to CGA (Harik et. al;1998) and PBIL(Baluja;1994)
- Represent more than one gene in a partition
- Make exposition simpler
- Gene partition maps to linkage groups

Minimum Description Length Models

- Hypothesis: Good distributions are those for which
  - Representation of the distribution is minimum (*model complexity*, C_m).
  - Representation of population compressed is minimum (*compressed population complexity*, C_p).
- Penalize complex models
- Penalize inaccurate models
- Combined complexity, $C_c = C_m + C_p$

Building MPM using MDL

Uses a steepest ascent search:

1. Assume all the genes to be independent ([1],[2],$\cdots$,[L]) and compute C_c.
2. Form all possible combinations ($N_{bb}(N_{bb}$-1)/2) of merging two subsets. eg., ([1,2],[3],$\cdots$,[L]), $\cdots$, ([1],[2],[3],$\cdots$,[L-1,L]).
3. Select the set with minimum combined complexity (C'_c).
4. If $C_c > C'_c$ go to step 6.
5. Use the set with C'_c as the current MPM and go to step 2.
6. Merging is not possible, exit with set from step 2 as MPM.

Generation of New Population

- Transfer N_p*(1-P_c) best individuals to the next generation
- The rest N_p*P_c individuals are generated as follows:
  - Take each of the subset of MPM from one of the individuals.
  - Similar to multiple point crossover.
  - Number of crossover points = N_{bb}.
  - Instead of two parents we have N_{bb} parents.

Silicon Potential

Gong Potential

- Gong, X.G. *Phys. Rev. B* **47**, 2329 (1993)
- Empirical three body potential
- Based on Stillinger Weber potential
- Reflects both tetrahedral ($\sim 109^\circ$) and preferred bond angles ($\sim 60^\circ$)
- Accurate for predicting structural properties

Gong Potential: Equations

$$U_{\text{tot}} = \sum_{i<j}^{n} v_2(i,j) + \sum_{i<j<k}^{n} v_3(i,j,k)$$

$$v_2(i,j) = A\left(Br_{ij}^{-p} - r_{ij}^{-q}\right)\exp\left[(r_{ij}-a)^{-1}\right], \quad |r_{ij}| < a$$

$$v_3(i,j,k) = h\left(r_{ji}, r_{ki}\right) + h\left(r_{kj}, r_{ij}\right) + h\left(r_{ik}, r_{jk}\right)$$

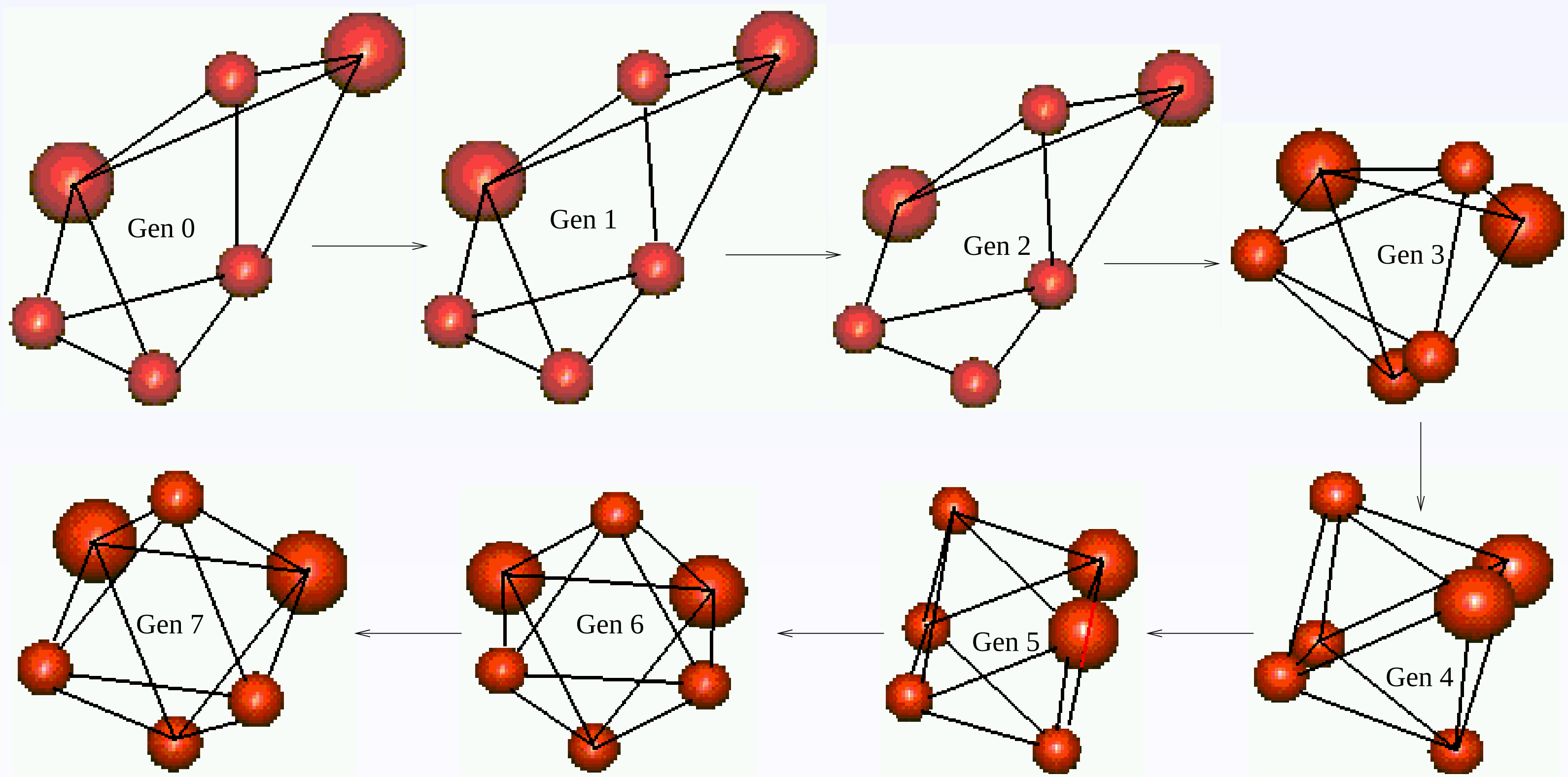
$$h\left(r_{ji}, r_{ki}\right) = \begin{array}{ll} \lambda \exp\left[\gamma\left((r_{ij}-a)^{-1} + (r_{ki}-a)^{-1}\right)\right] & |r_{ij}| < a \\ \left(\cos\theta_{jik} + \frac{1}{3}\right)^2 \left[(\cos\theta_{jik} + c_0)^2 + c_1\right], & |r_{ki}| < a \end{array}$$

- A = 7.0496, B = 0.6022, a = 1.8, p = 4, q = 0.
- λ = 25, γ = 1.2, c_0 = -0.5, c_1 = 0.45

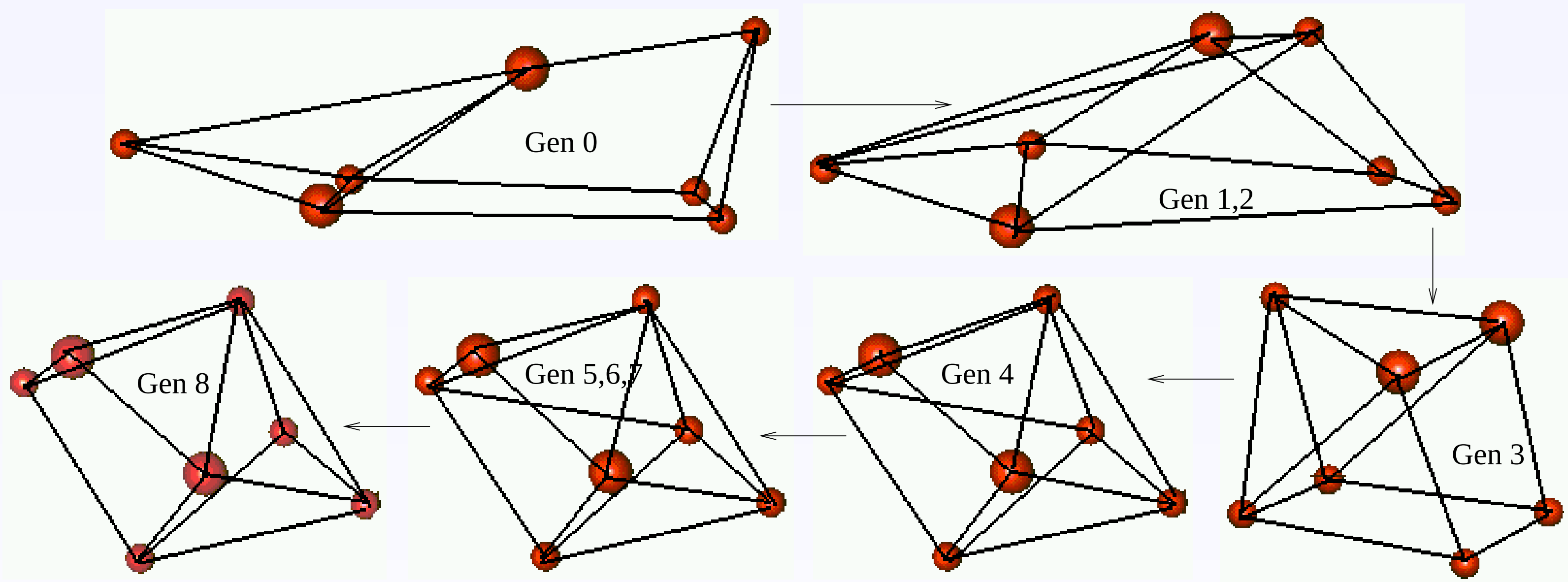
Algorithm Implementation

- Variables are fixed-space Cartesian coordinates
- Each coordinate is encoded by 5-bit binary
- 25 independent runs, $p_c = 0.8$, 4-11 atoms
- Nelder-Mead simplex: Press et al
- Termination criteria:
  - Fitness variance ≤ 0.1
  - Population variance ≤ 0.1
- At most one failure allowed

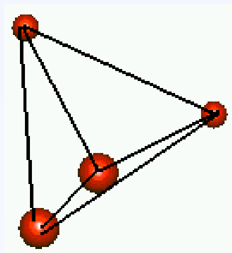
Results: Single GA Run



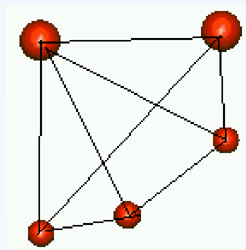
Results: Single GA Run



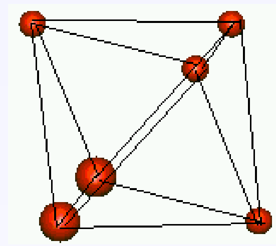
Results: Optimal Structures



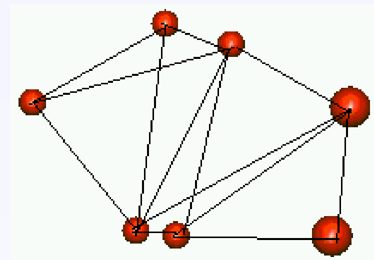
Tetrahedron
U = -4.0016



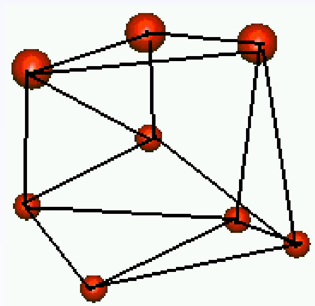
Compressed trigonal bipyramid, U = -5.7518



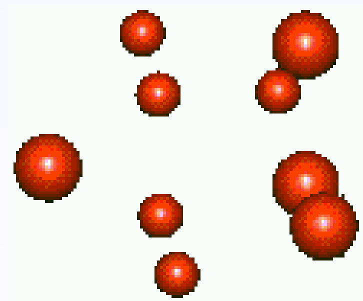
Octahedron
U = -7.6696



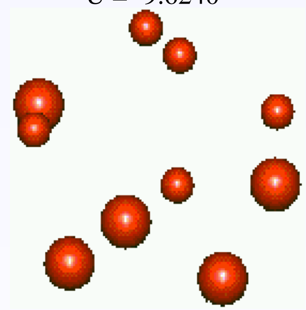
Pentagonal bipyramid
U = -9.6240



Unicapped distorted pentagonal bipyramid
U = -11.5346



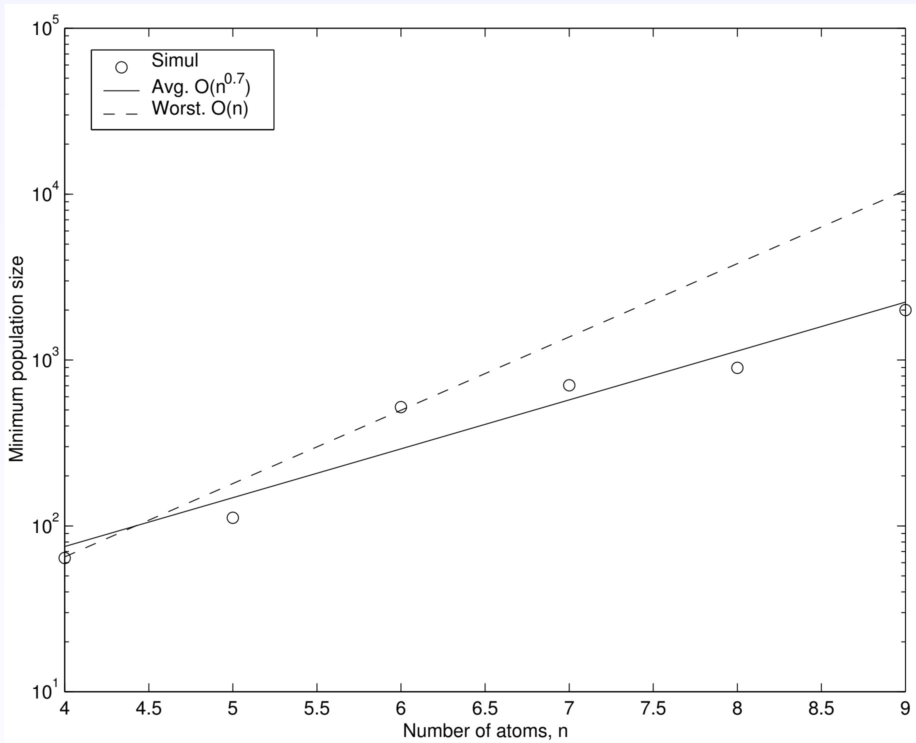
Tricapped trigonal prism, U = -13.5999



Bicapped tetragonal antiprism, U = - 15.6487

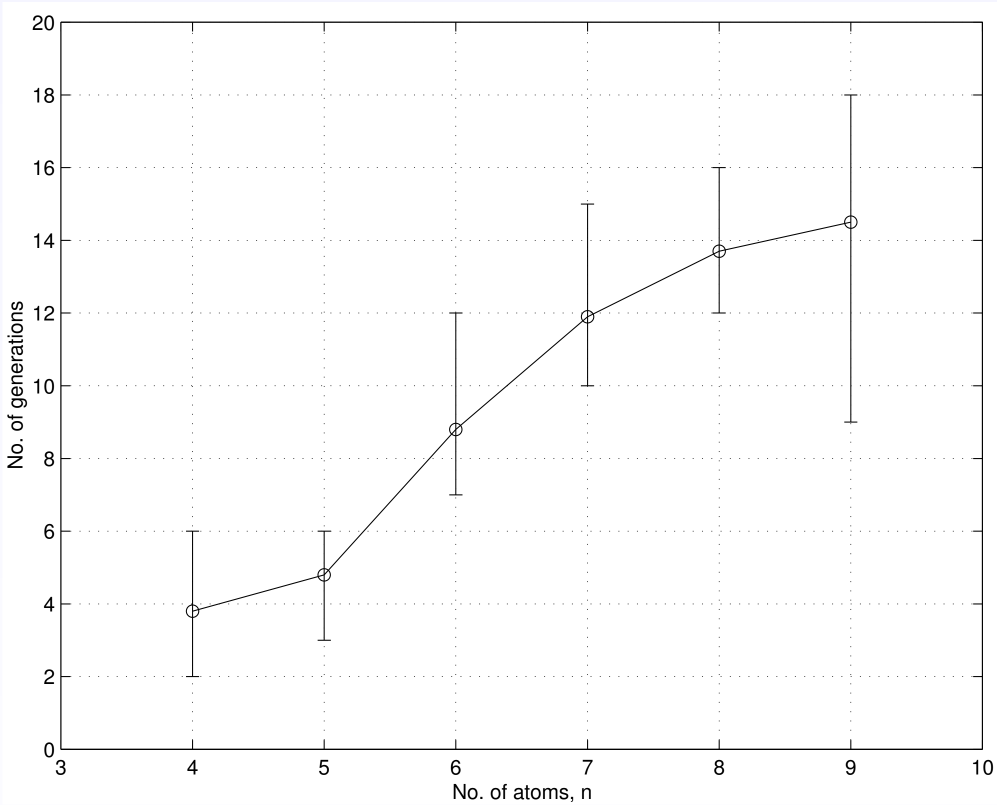
Illinois Genetic Algorithms Laboratory
Department of General Engineering
University of Illinois at Urbana-Champaign
Urbana, IL 61801. USA.

Results: Population Size

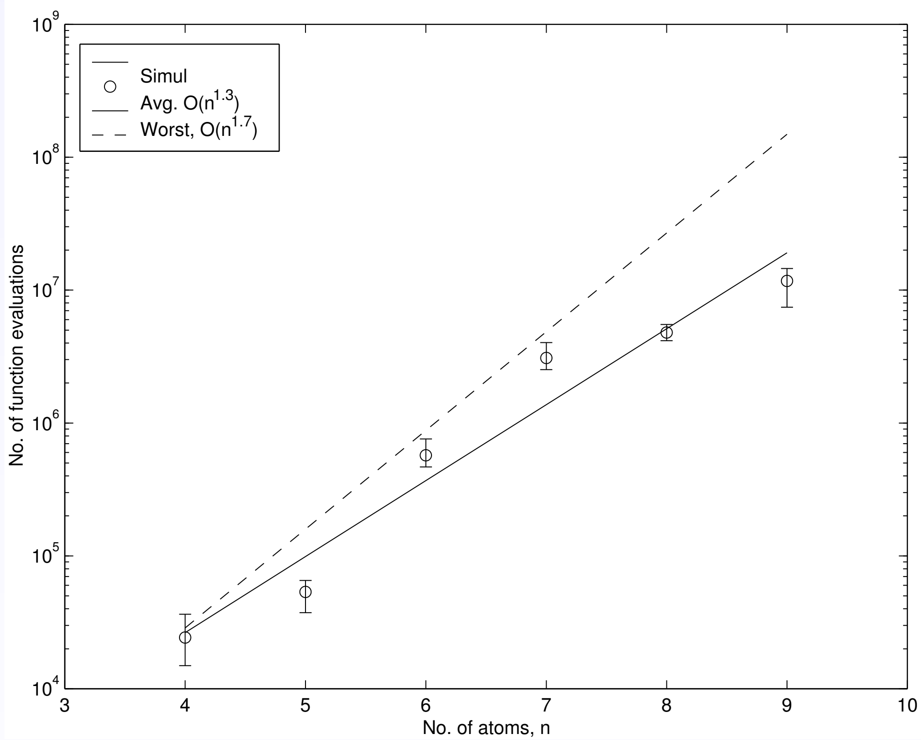


Average Case: $O(n^{0.7})$, Worst Case: $O(n)$.

Results: Convergence Time



Results: Function Evaluation



Average Case: $\mathrm{O}\left(n^{1.3}\right)$, Worst Case: $\mathrm{O}\left(n^{1.7}\right)$.

Conclusions

- Optimal structures of small Si clusters found
- Results agree with literature (Iwamtsu, M. *J. Chem. Phy.* **112** (2000))
- Convergence is very fast ($\leq$ 25 generations).
- Population size increases linearly with cluster size
- Polynomial increase of function evaluation
- Results to be confirmed with bigger clusters