Intelligent Water Drops with Perturbation Operators for Atomic Cluster Optimization

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Overview

The Intelligent Water Drops algorithm was modified (MIWD) and adapted to allow it to determine the most stable configurations, for the first time, of Lennard-Jones (LJ), Binary LJ (BinLJ) and Morse Clusters. The algorithm, referred as MIWD+PerturbOp, is an unbiased type of algorithm where no *a priori* cluster geometry information and construction were used during initialization. Cluster perturbation operators were applied to clusters generated by MIWD to further generate lower energies. Application of the limited-memory quasi-Newton algorithm L-BFGS was also utilized to further relax clusters to its nearby local minimum.

Basic Properties of IWD

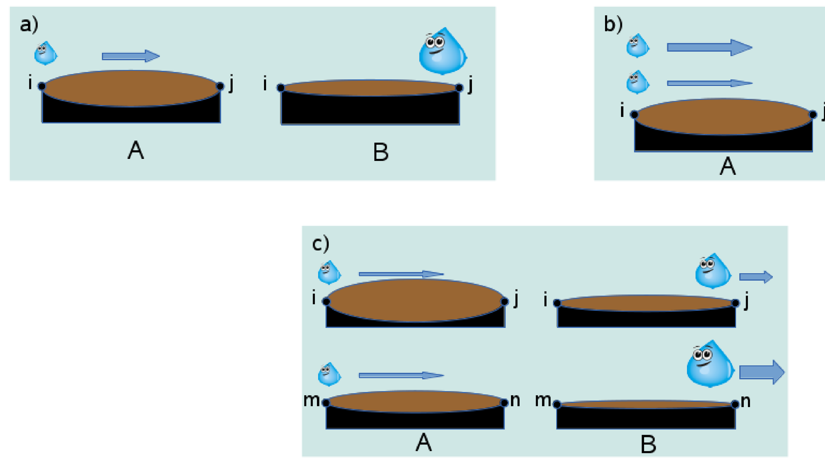

Figure 1: A path measures quality of connectivity between particles. (a) An IWD gathers soil (brown ellipse) as it flows from particle i to particle j while path(i,j) loses an amount of soil; (b) Soil gathered increases with IWD velocity; (c) An IWD travelling on a path with lesser soil, path(m,n), will gather more soil and higher velocity. The algorithm aims to generate connectivities with desirable (lesser) measures eventually generating an IWD comprising these connectivities.

Modifications to IWD

1. The probability of choosing a path depends on amount of soil and the potential energy.

$$p_{i,j}^{IWD} = \frac{f(soil(i,j))\eta(i,j)}{\sum_{k \in V_a^{IWD}} f(soil(i,j))\eta(i,j)}$$

$$\eta(i,j) = \frac{1}{2+V_{type}(r_{i,j})} \qquad V_M = e^{a(1-r_{i,j})}(e^{a(1-r_{i,j})}-2)$$

$$V_{LJ}(r_{i,j}) = 4\varepsilon_{i,j}((\frac{\sigma_{i,j}}{r_{i,j}})^{12} - (\frac{\sigma_{i,j}}{r_{i,j}})^{6})$$

2. An appropriate heuristic undesirability factor, *HUD*, is chosen to fit the LJ cluster optimization.

$$HUD_{i,j} = 2 + V_{type}(r_{i,j}) + \mu r_{i,j} + \beta(max(0, r_{i,j}^2 - D^2))^2$$

3. Worst iteration agent, *TIW*, affects the soil content as well.

$$soil_{i,j} = (1+\rho)soil_{i,j} + P_{i,j} \qquad P_{i,j} = \rho(\frac{soil^{IWD}}{N-1})$$

4. L-BFGS was used as a relaxation algorithm for IWDs.

Operators and Volume

LJ Operators : *Inversion, Power Mutation, Twinning, Grow-and-Etch*, Etch-and-Grow, Laplace Crossover, Geometric Mean, Arithmetic Mean, N-Pt Crossover and 2-Pt Crossover.
BinLJ Operators : *Cut Splice Variant*, Knead, Energy-based swap (Type 1 (2) High energy with Low energy type 2 (1)).
Morse Operators: *Grow-Etch*.
Initial Volume : Initial atom sites scattered in sphere with radius a) 5.5 units (Wales); b) variable radius (Cai); square box with lengths c) 4 units (Hodgson) and d) 3 units (Chen).

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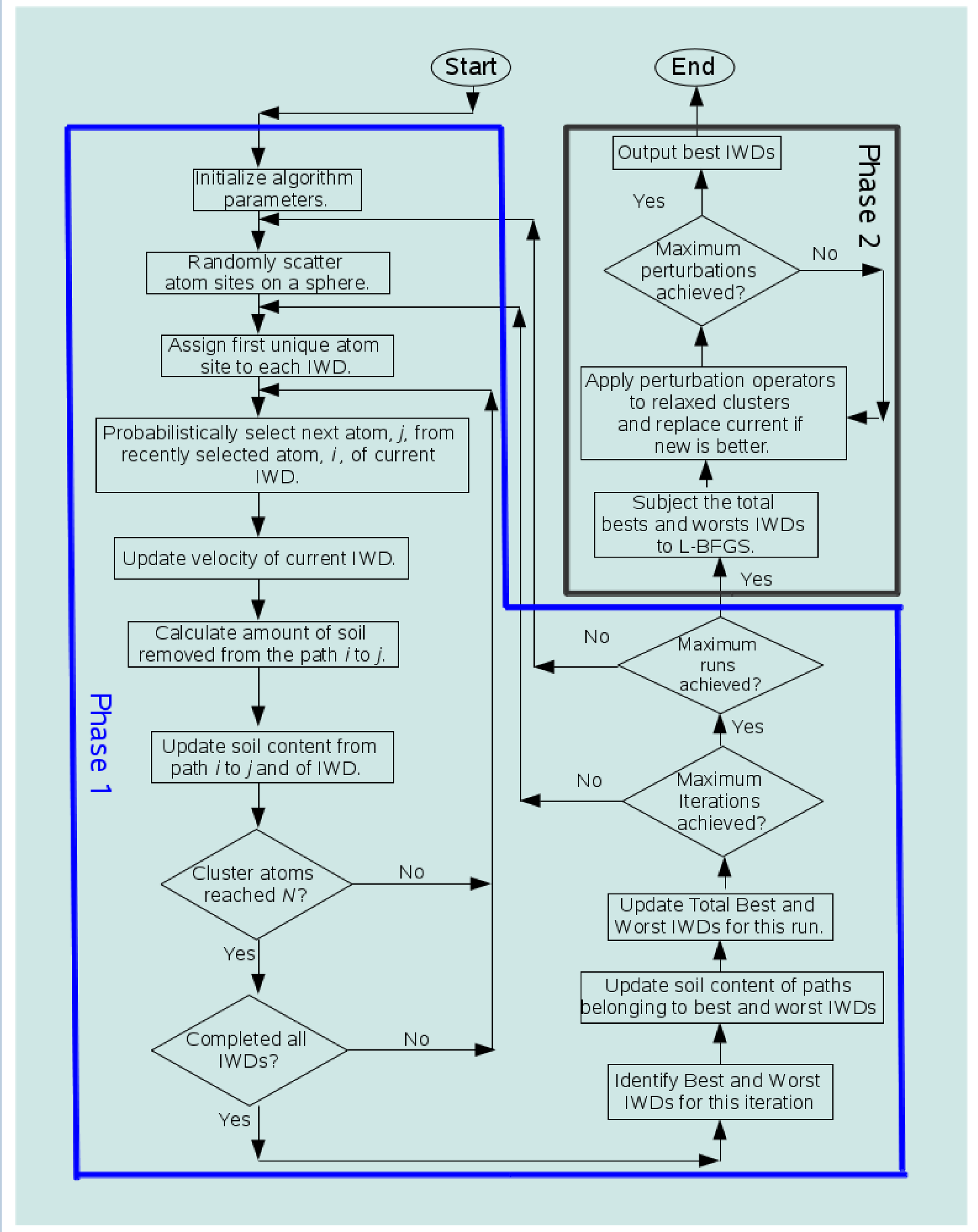
FlowChart



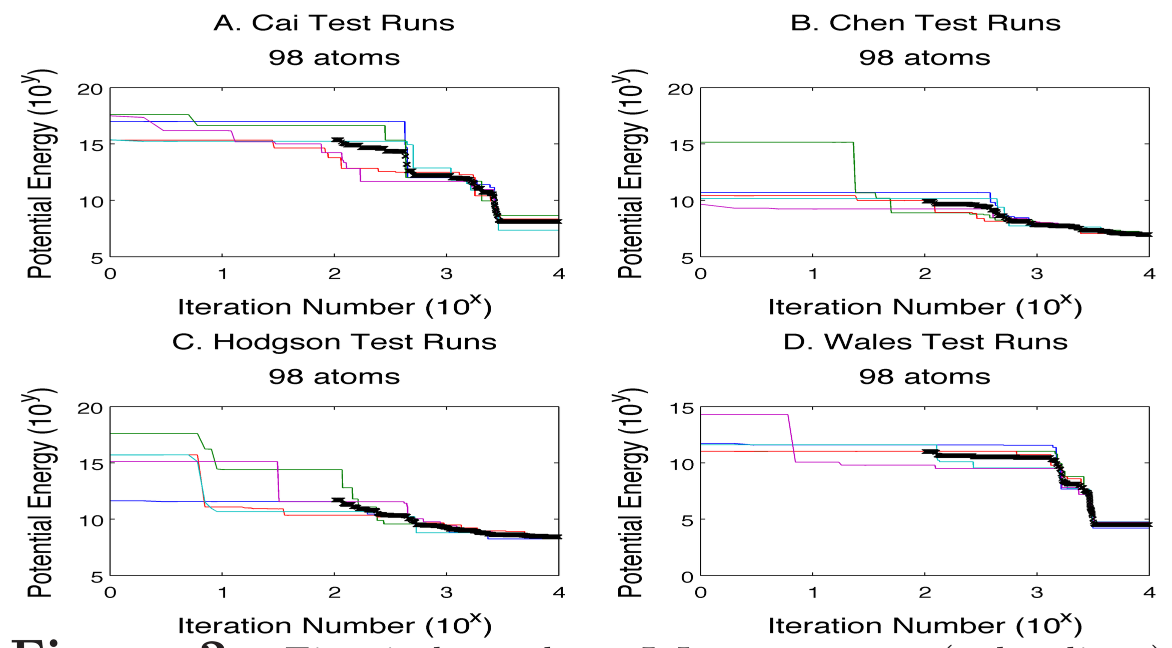


Figure 2: Five independent LJ_{98} test runs (color lines) (10,000 iterations/run) for different bounding volumes showing decline in cluster energy.

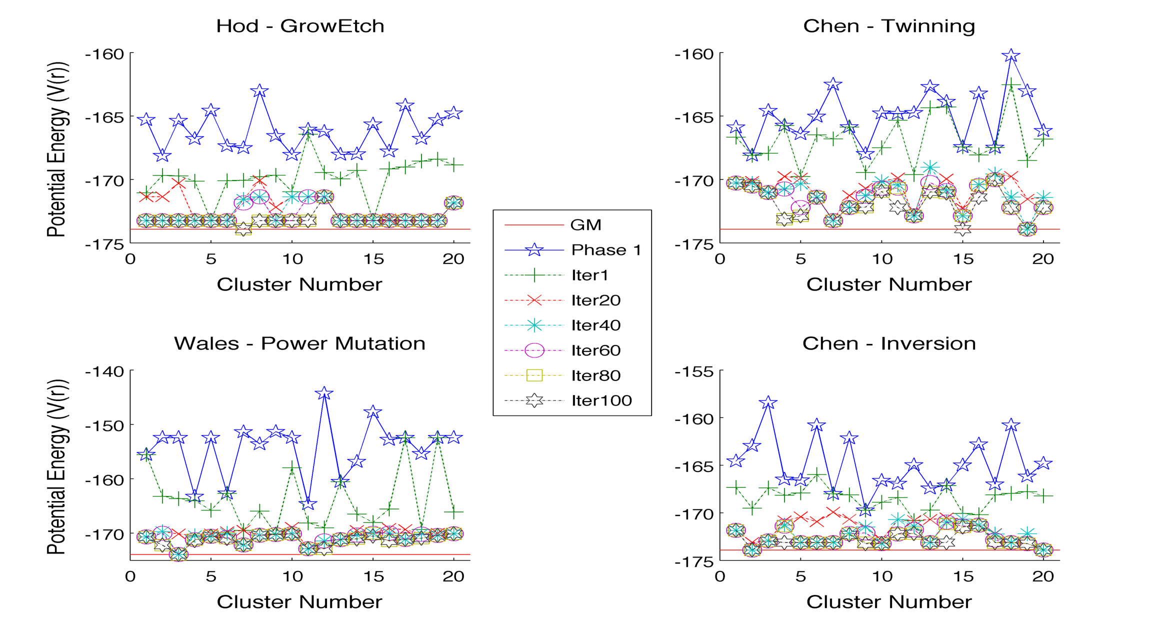


Figure 3: Best performing results of bounding volume/perturbation operator combination tested on LJ_{38}.

On LJ Clusters

1. Phase 1 was tested on difficult LJ clusters : LJ_{38} and LJ_{98}. MIWD takes around 100 iterations to shape "soil" but searches progressively lower energy clusters thereafter (Fig. 2).
2. LJ_{13} best performing operators and bounding volume: Inversion, Power Mutation, Twinning and Grow-Etch (best operator). Chen, Hodgson and Wales performed equally well while Cai performed worse. LJ_{38} tests (Fig. 3) show Grow-Etch produced generally better results.
3. Final runs of the algorithm utilized the Hodgson – Grow Etch combination. MIWd+GrowEtch agrees with high-accuracy to (Cambridge Cluster Database) CCD results of up to 104 atoms. Compactness measures (Fig. 4) of this study versus CCD results show high-accuracy. Rotation and translation reveal that chiral clusters were generated (Fig. 5). MIWD+GrowEtch achieved relatively high-success rates for difficult clusters compared to, by far the most reliable algorithm to search for lowest-energy structure of atomic clusters which is based on Monte Carlo Minimization, Basin-Hopping with Occasional Jumping (BHOJ)(Table 1).

N	MIWD+GrowEt	BHOJ	Energy
38	100%	96%	-173.928426591
75	50%	5%	-397.492330983
76	20%	10%	-402.894866009
77	10%	5%	-409.083517124
98	75%	10%	-543.665360771
102	35%	16%	-569.363652496
103	40%	13%	-575.766130870
104	15%	12%	-582.086642068

Table 1: Good success rates with all "difficult" LJ clusters.

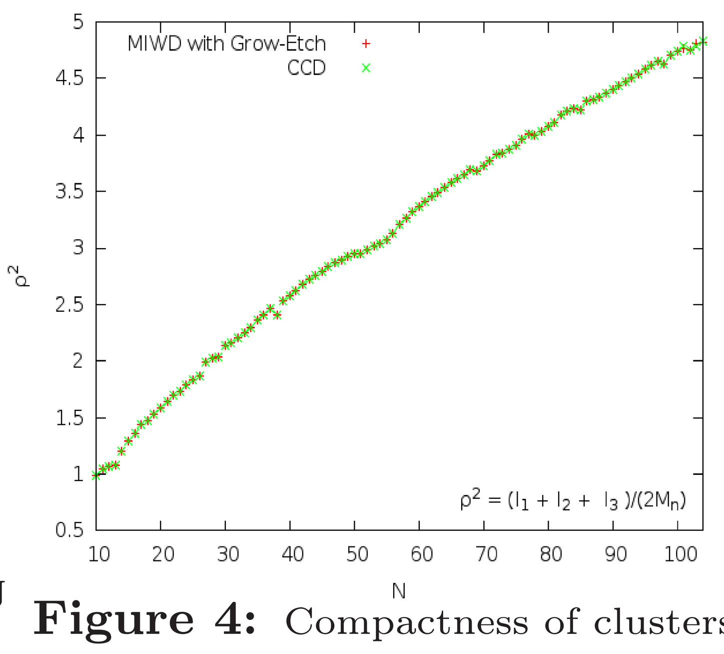


Figure 4: Compactness of clusters.

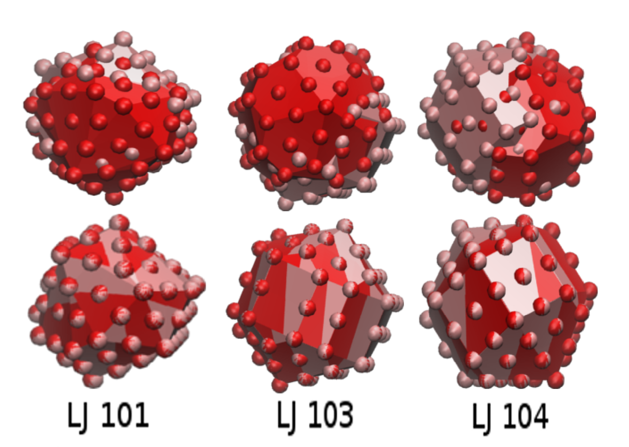


Figure 5: Row 1 : Overlayed clusters showing unmatched positions. Row 2 : Rotated and translated clusters showing matching configurations.

On Binary LJ and Morse Clusters

MIWD+PerturbOp was also tested on more complicated, not well-studied, clusters such as Morse and Binary LJ clusters. This algorithm was able to locate known GM more often for the test clusters without having to provide *a priori* geometry information.
BINARY LJ : Tested for up to 50 atoms on 6 instances of $\sigma_{BB} = 1.05 - 1.30$. MIWD+Knead rediscovered the GM for most of the clusters except for N = 41,43, 45 -49 for $\sigma_{BB} = 1.05$ and N = 47 for $\sigma_{BB} = 1.10$. MIWD+CutSpliceVar rediscovered most of the GM except for N = 30-32 for $\sigma_{BB} = 1.30$, N = 35 for $\sigma_{BB} = 1.05, 1.15$, N = 36, 39-50 for BB = 1.05 and N = 47, 49-50 for $\sigma_{BB} = 1.10$. Comparison for distribution of atoms for some of the MIWD+CutSpliceVar non-optimal clusters with CCD results to compare geometries. Misplacement of a few atoms in some shells necessitates for a combination of perturbation operators (CombiOp) in Phase 2 (CutSplice+Knead, CutSplice+H1L2, CutSplice+H2L1, Knead+H1L2 and Knead+H2L1). Tested on N = 30-32 for $\sigma_{BB} = 1.30$, N = 35, 40, 45 for $\sigma_{BB} = 1.05$ and N = 35 for $\sigma_{BB} = 1.15$. Combinations were able to arrive at the GM except for N = 45 for $\sigma_{BB} = 1.05$ (Fig. 6).
MORSE : Tested for up to 60 atoms on 2 values of interparticle force range ($a = 6, 14$). MIWD+GrowEtch located the GM for most of the clusters except for N = 47, 55, 57, 58, 60 for $a = 14$.

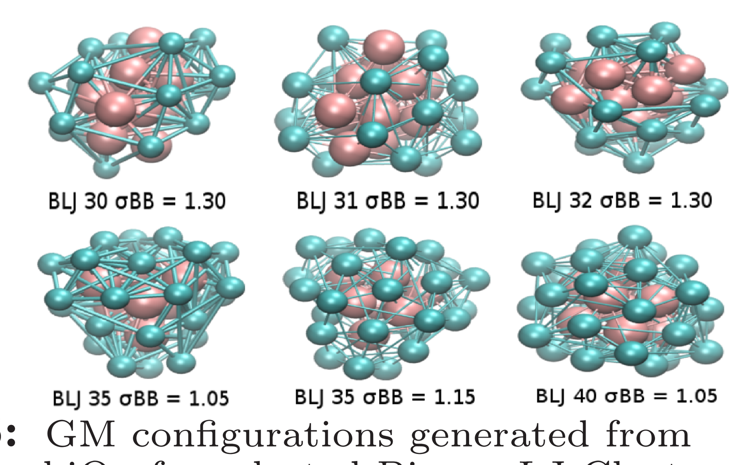


Figure 6: GM configurations generated from MIWD+CombiOp for selected Binary LJ Clusters.

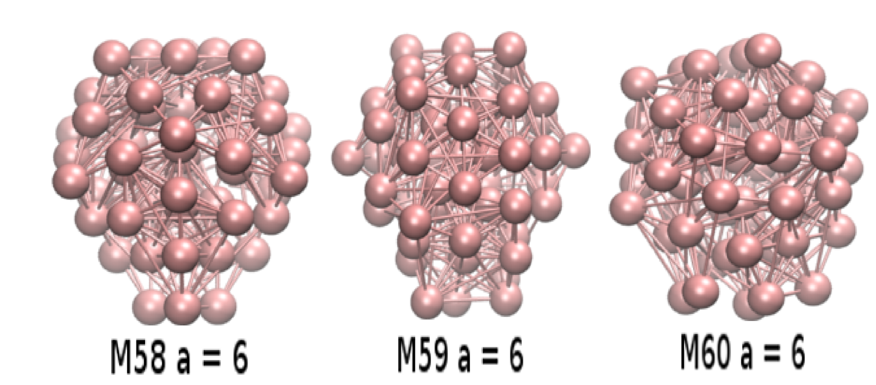


Figure 7: GM configurations from MIWD+GrowEtch for selected Morse Clusters.