

The Multi-Level Lennard-Jones Problem

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The Lennard-Jones Problem

$$V_{LJ} = \sum_{i,j} \frac{A}{\|v_i - v_j\|^{12}} - \frac{B}{\|v_i - v_j\|^6}$$



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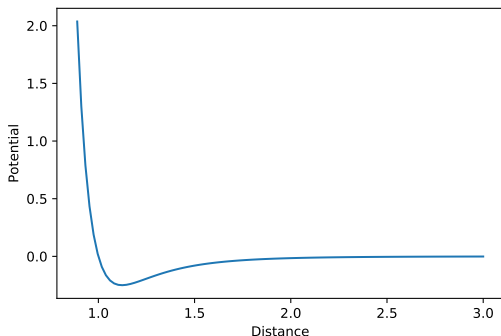


Figure: The 1-d Lennard Jones Potential



The Lennard-Jones Problem

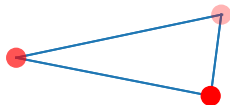


Figure: Global minima for 3 atoms

The Lennard-Jones Problem

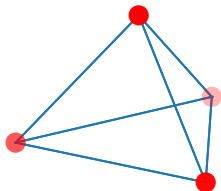


Figure: Global minima for 4 atoms

The Lennard-Jones Problem

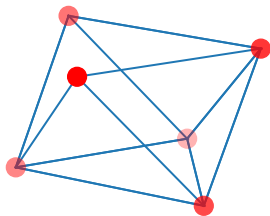


Figure: Global minima for 6 atoms

The Lennard-Jones Problem

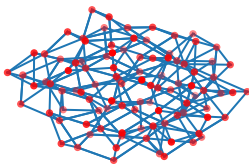
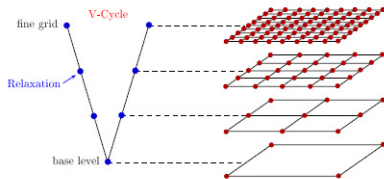


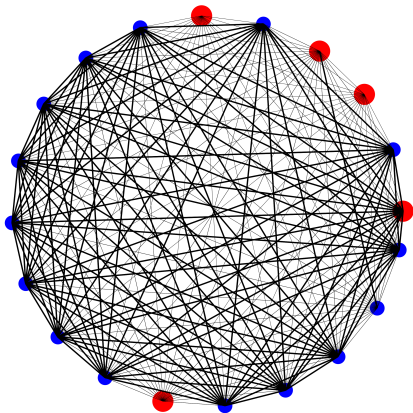
Figure: Global minima for 100 atoms

Multigrid

$$Ax = b$$



Algebraic Multigrid



Does a local minima for fewer atoms help?

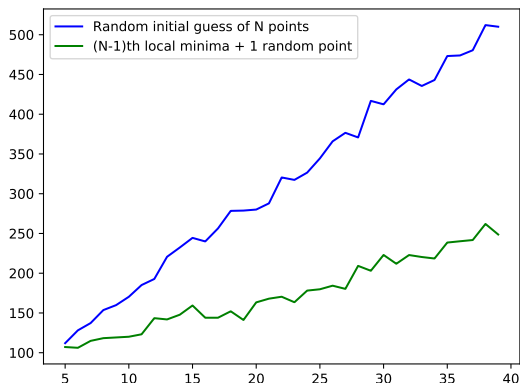


Figure: Iterations needed for a random guess versus a guess that uses the (N-1)th local minima



Delaunay triangulation

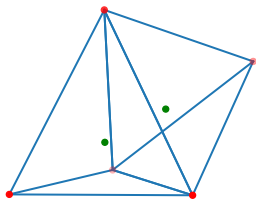


Figure: Delaunay simplices for 5 atoms



Delaunay surfaces

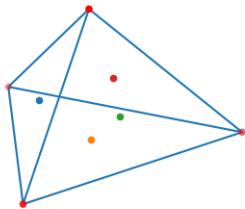


Figure: Delaunay simplices for 5 atoms

How many points should we add?

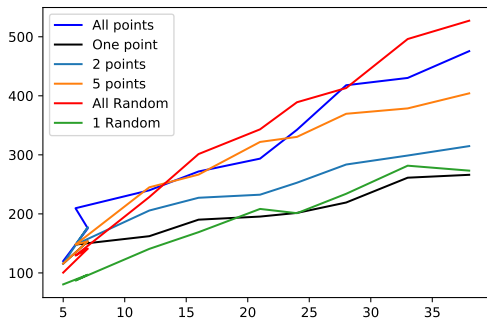


Figure: Number of iterations needed to reach a local minima for number of atoms



Heuristics fail

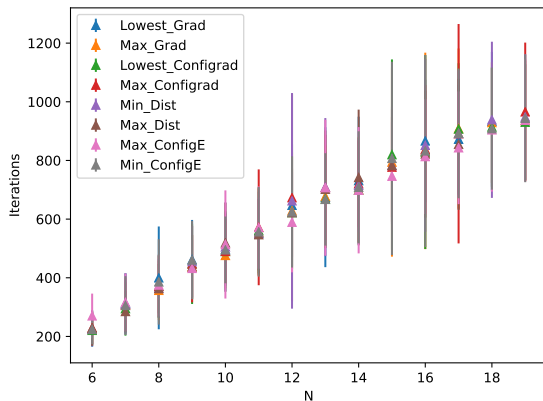
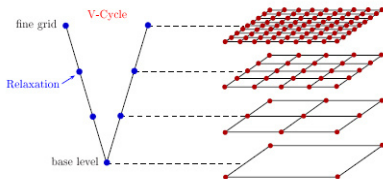


Figure: No clear heuristic for choosing a good point

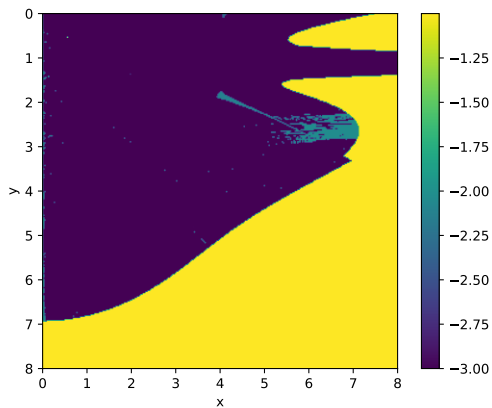


minimize $f(x_h)$

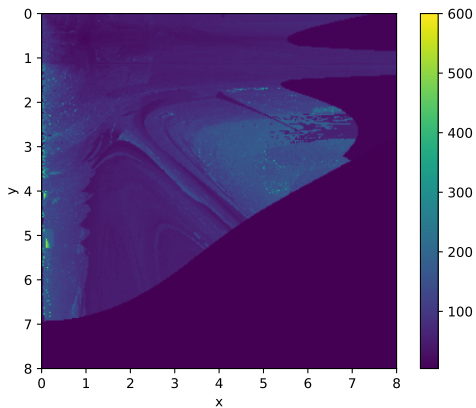


minimize $f(x_H) - V^T(x_H)$

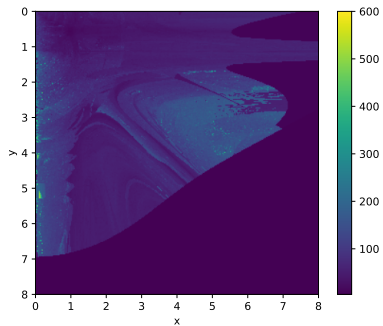
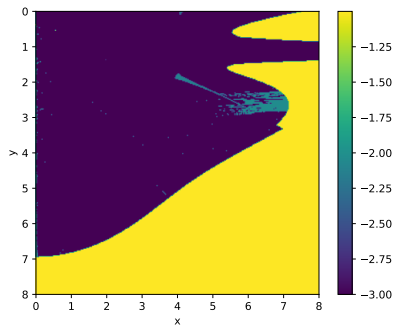
The energy landscape for 3 atoms



The iterations landscape for 3 atoms



Landscapes



Trilateration

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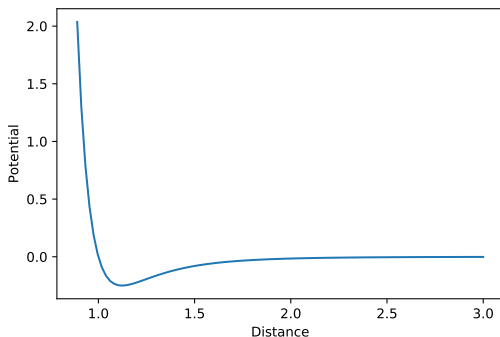
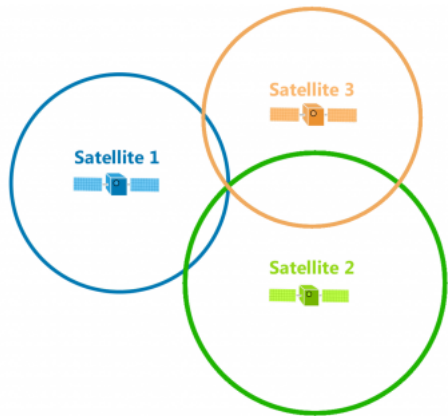
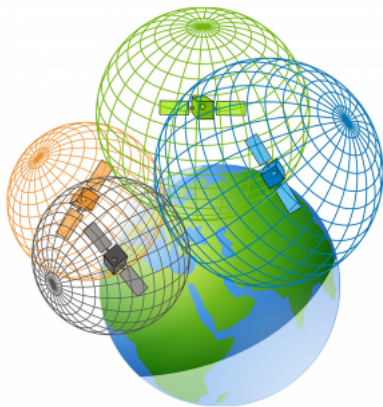


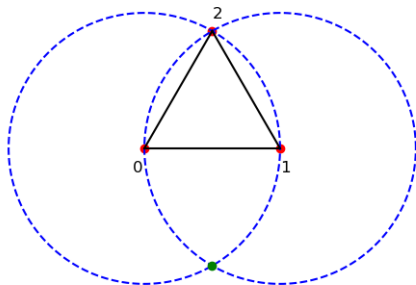
Figure: The 1-d Lennard Jones Potential



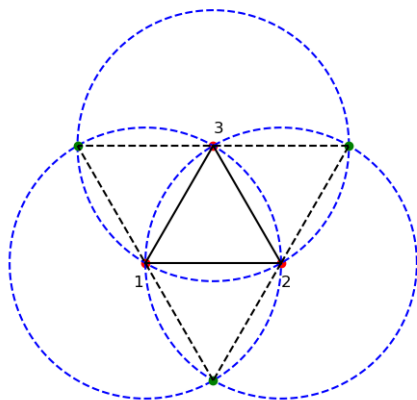
Trilateration



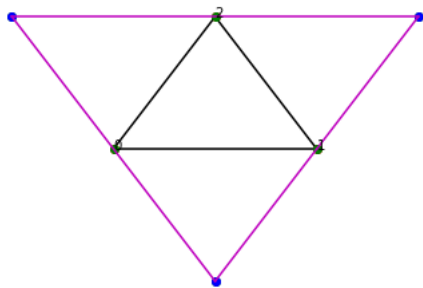
Trilateration



Trilateration



A really good initial guess



Trilateration

Starting at 5, the trilateration goes to

11, 23, 41, 47, 59, 65



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Iterations needed at each step

37, 123, 118, 142, 222, 151

Sums to 828.



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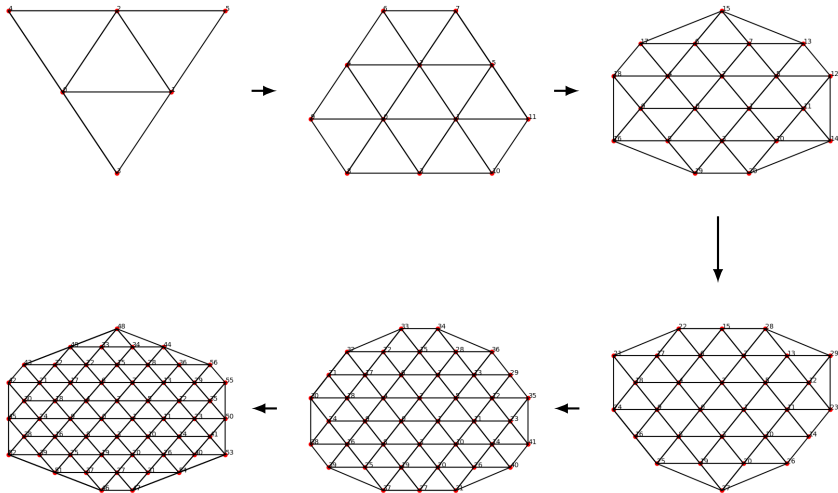
Sums to 828.

Iterations for each size if you took a random initial guess

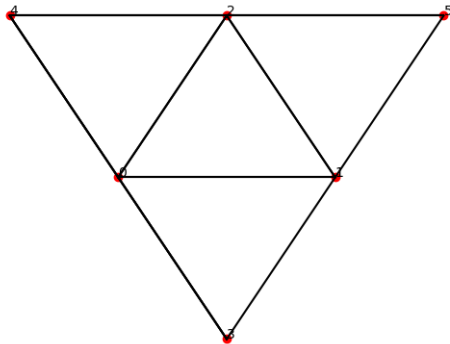
246, 498, 839, 916, 1104, 1130



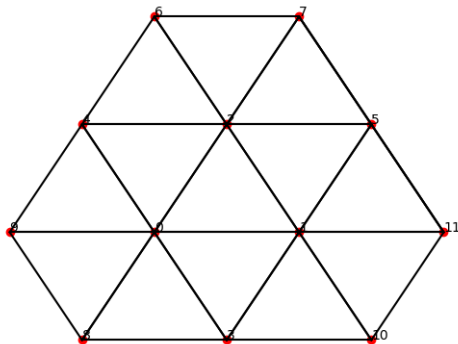
The 2d problems



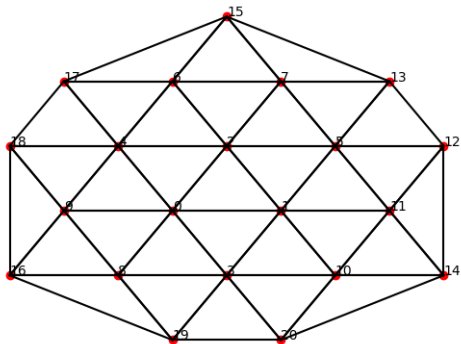
Trilateration



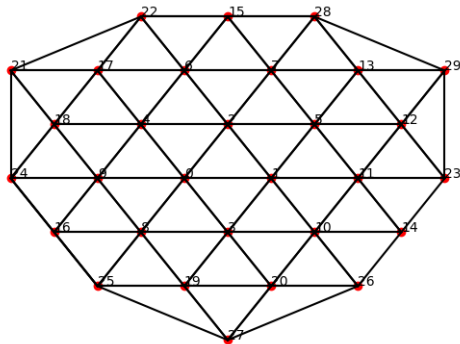
Trilateration



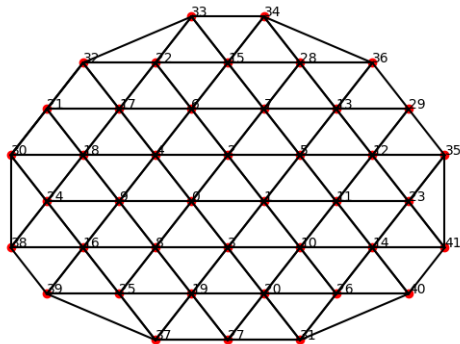
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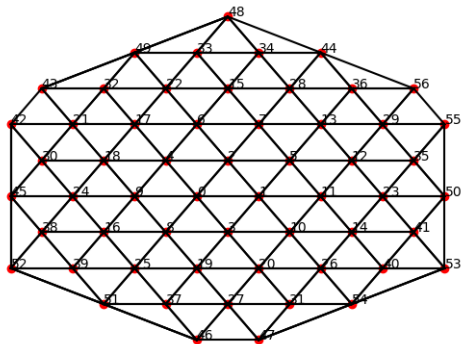
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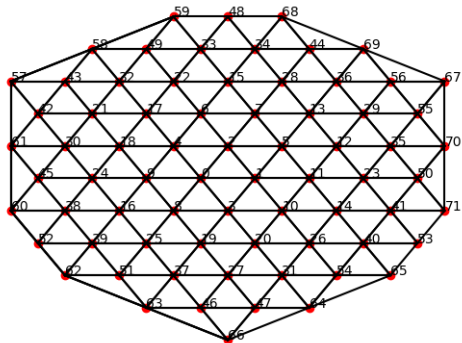
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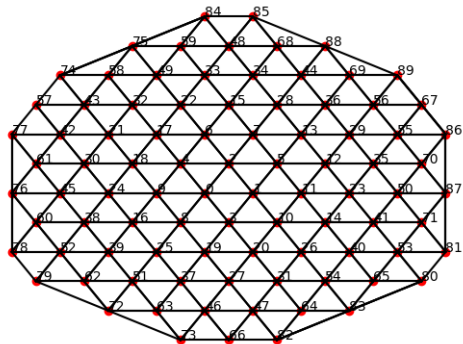
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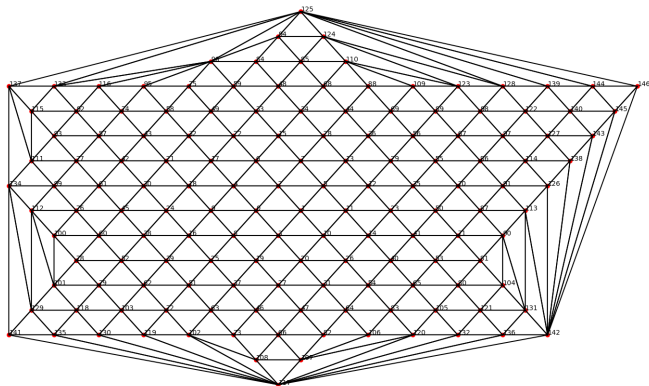
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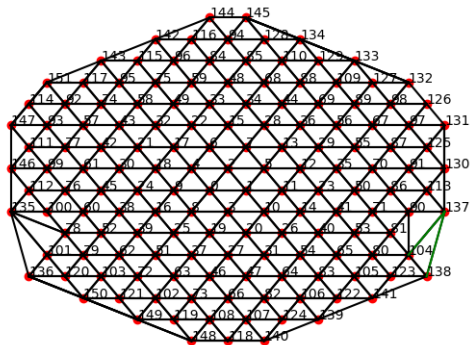
Trilateration



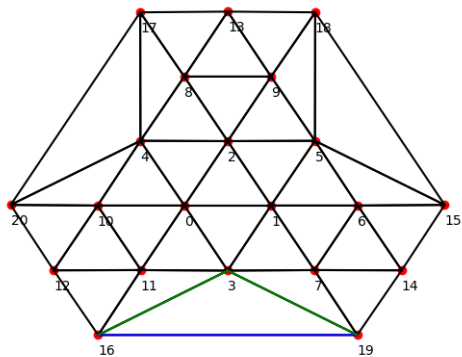
Problems arise



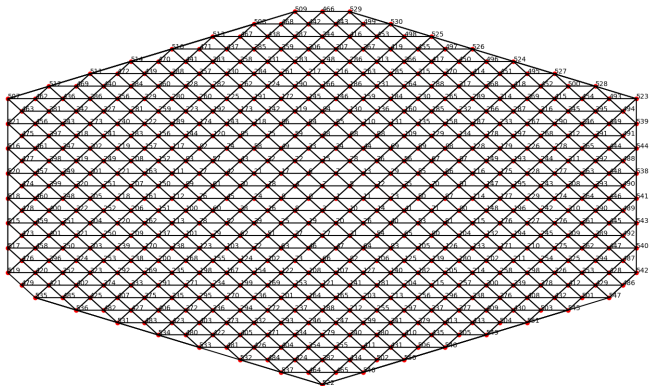
Bugs



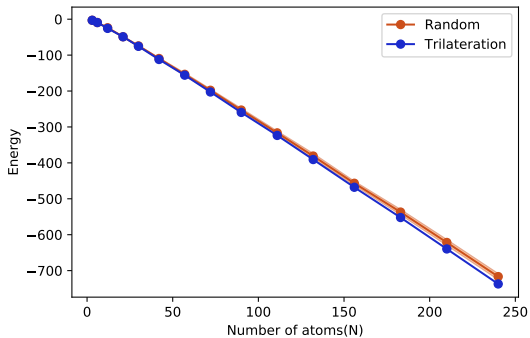
Dealing with bugs



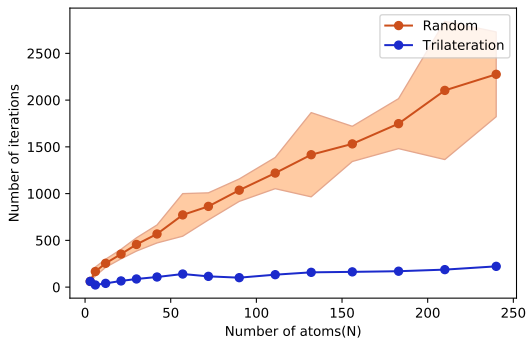
Light at the end of the tunnel



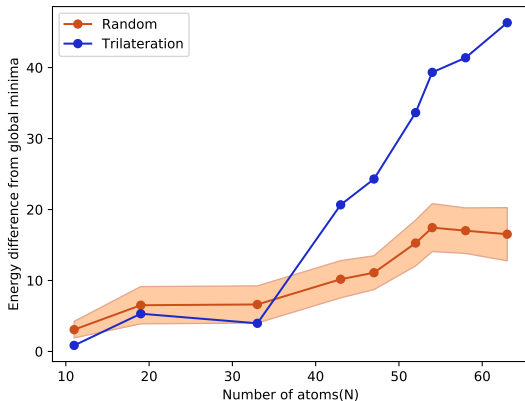
Trilateration in 2d



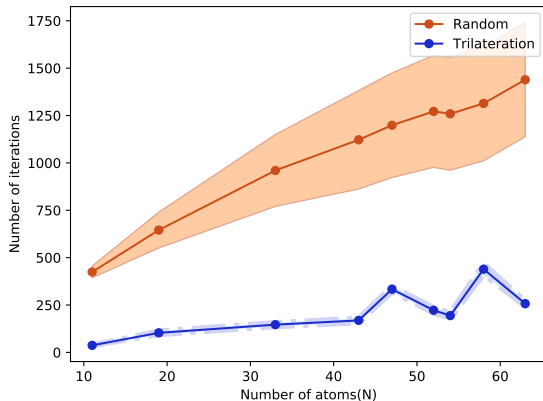
Trilateration in 2d



Trilateration in 3d



Trilateration in 3d



Thank you

