Robin Johnson HW1 - Standard

```
public double calculateEnergy(double[][] coords, double[] eps, int numAtoms) {

    double energySum = 0.0;
    double r0 = 1.2;
    for (int i = 0; i < numAtoms-1; i++) {
        for (int j = 0; j < numAtoms; j++) {
            double distance = Math.sqrt(Math.pow(coords[i][0] - coords[j][0], 2 )
                              Math.pow(coords[i][1] - coords[j][1], 2 ) +
                              Math.pow(coords[i][2] - coords[j][2], 2 ));
            double term2 = Math.pow( (r0/distance), 12 ) ;
            double term1 = Math.pow( (r0/distance),  6) ;
            double epsilon = Math.sqrt( eps[i] * eps[i] + eps[j] * eps[j]);
            energySum = energySum + (4.0 * epsilon * (term1 - 2.0 * term2));
        }//end of inner for loop
    }//end of outer for loop
    return energySum;
```

Outer for Loop
Inner for Loop
Inner Loop Body

1 Tick
1 Tick
(4N+1) N+1
(3N+1) N+1
9
(10+4(2))
(10+4(2))
(10+4(2))
(10+4(12))
(10+4(6))
9
1 Tick

Inner Loop Body

- $9+1+(10+4(2))+1+(10+4(2))+1+1+(10+4(2))+1 = 68$ Ticks
  (18, 18)
- $1+(10+4(12)) = 59$ ticks
- $1+(10+4(6)) = 36$ ticks
- $1+9+1+1+1 = 13$ Ticks
- 6 ticks

$= 181$ ticks

- The Math

Inner Loop

$181N+1N+1+N$

$183N+2$

$N \cdot (183N+2) + 1 + N + 2 + N$

$N \cdot (183N+2) + 2N + 3$

$183N^2 + 2N + 2N + 3$

$183N^2 + 4N + 3$

$O(N^2)$