

Consider that numAtoms is n ,

```
public static double calc(double[][] coords, int numAtoms) {
```

```
    double energySum = 0.0;
    double r0 = 1.2;
```

```
    for (int i=0; i < numAtoms-1; i++) {
```

```
        for (int j= i+1; j < numAtoms; j++) {
```

```
            double distance = Math.sqrt( (coords[i][0] - coords[j][0]) * (coords[i][0] - coords[j][0]) +
                                           (coords[i][1] - coords[j][1]) * (coords[i][1] - coords[j][1]) +
                                           (coords[i][2] - coords[j][2]) * (coords[i][2] - coords[j][2]) );
```

```
            double partialTerm1cubed= (r0/distance) * (r0/distance)*(r0/distance);
```

```
            double term2 = partialTerm1cubed * partialTerm1cubed ;
```

```
            double term1 = term2 * term2;
```

```
            energySum = energySum + (term1 - 2.0 * term2);
```

```
        }
```

```
    }
    return energySum;
```

```
}
```

This for loop starts at 'i + 1' and goes until n . This essentially leaves the same trace as the first program but divides work by half.

All assignments and operators here costs 26 ticks total.

This loop runs for ' $n-1$ ' times

Due to the reasons above, the program will run

$\frac{n^2-n}{2}$ times and cost $26 \left(\frac{n^2-n}{2} \right)$ ticks, The

numerator dividing by two makes a huge difference

Compared to the first algorithm, but in terms of big-O notation, the function is defined as $\frac{1}{2}(n^2-n)$

So thus, according to the Big-Oh rules, the function remains at a $O(n^2)$ complexity.