

## Robin Johnson HW1 - Bonus

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

```
    double energySum = 0.0; 1 tick
```

```
    double r0 = 1.2; 1 tick
```

```
    for (int i = 0; i < numAtoms-1; i++) {N+1+1
        for (int j = i + 1; j < numAtoms; j++) {N
            double distance = Math.sqrt(Math.pow(coords[i][0] - coords[j][0], 2) +9 (10+4(2))
                Math.pow(coords[i][1] - coords[j][1], 2) +(10+4(2))
                Math.pow(coords[i][2] - coords[j][2], 2));(10+4(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
```

Outer For Loop  
Inner For Loop  
Inner For Loop Body

```
    return energySum;
```

### • Inner Loop Body

•  $9 + 1 + 18 + 1 + 18 + 1 + 1 + 18 + 1 = 68$  ticks

•  $1 + (10 + 4(12)) = 59$  ticks

•  $1 + (10 + 4(6)) = 35$  ticks

•  $1 + 9 + 1 + 1 + 1 = 13$  Ticks

•  $1 + 1 + 1 + 1 + 1 + 1 = 6$  ticks

$= 181$  ticks

$181N + 1 + 1 + N + 1 + N$

$183N + 3$

Inner Loop

$$N(183N + 3) + 1 + N + 2 + N$$

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

$$183N^2 + 5N + 3$$

$$O(N^2)$$