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HW7: Particle Interaction

The general strategy of the parallelization effort was to implement the ring algorithm using MPI. I used Scatter as the collective communication operation because it would distribute the particles evenly among the processors. Each of those processors calculates the van der Waals forces between its set of particles and the set of particles it just received by Receive in MPI. I used MPI_Isend instead of MPI_send to prevent race conditions from occurring. I used Gather as the collective communication operation because it would collect particles at rank 0.

63000			
	3 cores	15 cores	63 cores
Run 1	40.068374	4.550294	0.999946
Run 2	48.111465	4.495321	0.919350
Run 3	48.101092	4.494071	0.933705
Average	45.426977	4.513229	0.951000
Speedup	2.4649857	24.81081	117.7464
Efficiency	0.821662	1.654054	1.868990

As shown in the table, the speedup increases with the number of cores. The serial runtime was 111.97685 seconds which is much higher than using at least three cores.

A performance bottleneck for this program is the communication time. Using more processors means that more messages need to be sent. This can be seen in the table because the efficiency per core is reduced as more cores are used with a large N, in this case 63000.