Step 7: Experiments

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All parameters were tested on the same node in Hamilton queue par6; the number of processors for the node was 32. The values reflect a single time step value for computing molecular dynamics for the given number of particles. Different numbers of molecules were tested, results in table-1 to table-3. The elapsed time was meatured using openMp function omp_get_wtime for both serial and parallel functions; to give a unified time reference; this could lead to minor errors when estimating the elapsed time.

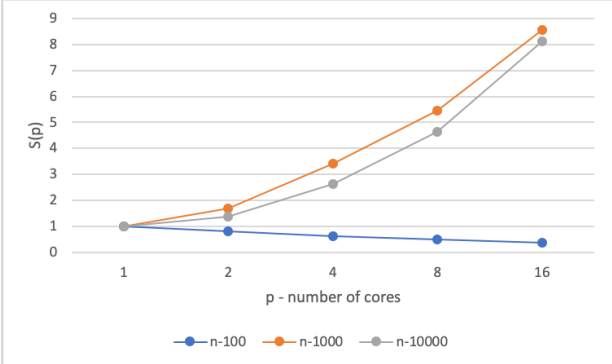

Figure 1: Speed up as number of cores increase

None of the plots follow Amdahl's law. The results for N=100, table-1, can be explained by taking into account the overhead introduced by the parallelization process. So, it is expected for N<=100, increasing the number of cores will result in a decrease in Speed. The serial code is the most fit for this setup. For N=1000 case, table-2, the parallel code performed better as the number of cores doubled.

Version	Number of Processors	Time Elapsed (seconds)	Speed Up	Efficiency
Serial	1	0.000110134	1.0	100%
Parallel	1	0.000120038	1.0	100%
	2	0.000150815	0.80	40%
	4	0.000194034	0.62	15.5%
	8	0.000236925	0.51	6.4%
	16	0.000313766	0.38	2.4%

Table 1: Results for running a single time step for 100 particles

Version	Number of Processors	Time Elapsed (seconds)	Speed Up	Efficiency
Serial	1	0.0199244	1.0	100%
Parallel	1	0.0173634	1.0	100%
	2	0.0102346	1.70	85%
	4	0.00509077	3.41	85.25%
	8	0.00318944	5.44	68%
	16	0.0020295	8.55	53.43%

Table 2: Results for running a single time step for 1000 particles

Version	Number of Processors	Time Elapsed (seconds)	Speed Up	Efficiency
Serial	1	0.895323	1.0	100%
Parallel	1	0.836319	1.0	100%
	2	0.598624	1.38	69%
	4	0.318269	2.63	65.75%
	8	0.180262	4.64	58%
	16	0.102834	8.13	50.81%

Table 3: Results for running a single time step for 10000 particles