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 give particles. Different numbers of molecules were tested, results in table-. The elapsed time was meatured using openMp function omp_get_wtime for both serial and parallel functions; to give a unified time reference.

The results for table- can be explained by taking into account the overhead introduced by the parallelization process. So, it is expected for N=100 and lower values, increasing the number of course will result in decrease in Speed. The serial code is the most fit for such a small N.

For N=1000 in table-, the parallel code performed better as the number of cores doubled. However, the speed up graph does not fit with Amdahl's law.

$N = 100$

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	100%
	4	0.000194034	0.62	100%
	8	0.000236925	0.51	100%
	16	0.000313766	0.38	100%

$N = 1000$

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	117.6%
	4	0.00509077	3.41	117.3%
	8	0.00318944	5.44	147.1%
	16	0.0020295	8.55	187.1%

$N = 10000$

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	100%
	4	0.318269	2.63	100%
	8	0.180262	4.64	100%
	16	0.102834	8.13	100% height