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Supplementary Material

Molecular Dynamics Simulations Accelerated by GPU for Biological Macromolecules with a Non-Ewald Scheme for Electrostatic Interactions

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Table S1: GPU-accelerated performances of Psygene-G with several other programs on three benchmark proteins (DHFR, ApoA1, and STMV)

Program	GPUs and Conditions			Throuput Timings (ns/day and ms/step)					
	GPUs [number of cores]	Time Step (fs/step)	Cutoff length (Å)	DHFR ^{a)} (23,558 atoms)		ApoA1 ^{b)} (92,224 atoms)		STMV ^{b)} (1,066,624 atoms)	
				ns/day ^{c)}	ms/step ^{d)}	ns/day ^{c)}	ms/step ^{d)}	ns/day ^{c)}	ms/step ^{d)}
Psygene-G	M2090								
	[1]	2	12	3.27	52.85	1.01	170.45	0.073	2365.83
	[8]	2	12	22.52	7.67	8.81	19.61	0.71	243.51
	[27]	2	12	-	-	-	-	1.65	104.76
	[64]	2	12	-	-	-	-	2.91	59.34
AMBER ^{e)}	M2090								
	[1]	2	8	46.20	(3.74)	-	-	-	-
NAMD ^{f)}	GTX280								
	[4]	1	12	-	-	(0.99)	87	(0.09)	960
	[8]	1	12	-	-	(1.8)	48	(0.18)	483
	[16]	1	12	-	-	(3.2)	27	(0/33)	261
	[32]	1	12	-	-	(4.8)	18	(0.56)	154
	[64]	1	12	-	-	(6.65)	13	(1.02)	85
OpenMM ^{g)} (PME)	C2070								
	[1]	2	8	16.5	(10.47)	-	-	-	-
	[2]	2	8	27.1	(6.38)	-	-	-	-
	[3]	2	8	30.1	(5.74)	-	-	-	-
	[4]	2	8	29.8	(5.80)	-	-	-	-
OpenMM ^{g)} (Reaction Field)	C2070								
	[1]	2	10	25.9	(6.67)	-	-	-	-
	[2]	2	10	40.2	(4.30)	-	-	-	-
	[3]	2	10	48.5	(3.56)	-	-	-	-
	[4]	2	10	52.3	(3.30)	-	-	-	-
GROMACS ^{h)}	Intel Core2 3 GHz [20]	1	9.6	(12.34)	7	-	-	-	-

^{a)}JAC (DHFR) benchmark, <http://ambermd.org/amber8.bench2.html>

^{b)}ApoA1 and STMV benchmarks, <http://www.ks.uiuc.edu/Research/namd/utilities/>

^{c)}The numbers in parentheses are calculated from values shown in ms/step.

^{d)}The numbers in parentheses are calculated from values shown in ns/day.

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