**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] | C2070 | | | | | | | | |
| (PME) | [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] | C2070 | | | | | | | | |
| (Reaction | [1] | 2 | 10 | 25.9 | (6.67) | - | - | - | - |
| Field) | [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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