Supplementary Materials

Development of massive multi-level molecular dynamics simulation program,

Platypus (PLATform for dYnamic Protein Unified Simulation),

for the elucidation of protein functions

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Table S1. Speedups and parallelization ratios for the computation of eigenvalue problems by LAPACK (dsyevd).

Number of CPUs	Number of threads	Number of cores	Elapsed time [sec]	Speedup[a]	Serial fraction [%][b]	Parallelization ratio [%][c]
1	1	1	12.448	1.000	—	—
1	8	8	4.175	2.981	25.047	75.953

[a] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with a single core processor was used as T_1.

[b] Serial fraction was evaluated by using eq. 5.

[c] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with a single core processor was used as T_1.

Table S2. Speedups and parallelization ratios for energy calculations of DIMER at the HF/cc-pVDZ level of theory.

Number of CPUs	Number of threads	Number of cores	Elapsed time[sec]		Speedup [a]		Serial fraction[%] [b]		Parallelization ratio[%] [c]	
			Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation
1	1	1	19295.980	18261.522	1.000	1.000	—	—	—	—
1	8	8	2420.357	2283.530	7.972	7.997	0.0495	0.0053	99.9505	99.9947
2	8	16	1217.018	1142.758	15.855	15.980	0.0609	0.0083	99.9391	99.9917
4	8	32	615.492	572.010	31.351	31.925	0.0668	0.0076	99.9332	99.9924
8	8	64	316.704	285.195	60.927	64.032	0.0800	-0.0008	99.9200	100.0008
16	8	128	167.661	144.157	115.089	126.678	0.0883	0.0082	99.9117	99.9918
32	8	256	90.798	73.735	212.517	247.663	0.0802	0.0132	99.9198	99.9868
64	8	512	53.444	37.804	361.053	483.052	0.0818	0.0117	99.9182	99.9883
128	8	1024	33.719	19.239	572.265	949.170	0.0772	0.0077	99.9228	99.9923
256	8	2048	23.971	10.297	804.971	1773.527	0.0754	0.0076	99.9246	99.9924
512	8	4096	19.893	5.836	969.964	3129.348	0.0787	0.0075	99.9213	99.9925
1024	8	8192	19.538	4.063	987.629	4495.108	0.0891	0.0100	99.9109	99.9900
2048	8	16384	16.314	2.922	1182.783	6249.603	0.0784	0.0099	99.9216	99.9901

[a] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with a single core processor was used as T_1.

[b] Serial fraction was evaluated by using eq. 5.

[c] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with a single core processor was used as T_1.

Table S3. Comparison of speedups and parallelization ratios for energy calculations of DIMER between 64 (64 CPUs x 1 thread) and 512 (64 CPUs x 8 threads) core processors at the HF/cc-pVDZ level of theory.

			Elapsed time[sec]		Speedup[a,b]		Serial fraction[%][a,c]		Parallelization ratio[%][a,d]	
Number of CPUs	Number of threads	Number of cores	Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation
64	1	64	373.727	300.942	1.000	1.000	—	—	—	—
64	8	512	53.444	37.804	6.993	7.960	0.0328	0.0011	99.9672	99.9989

[a] Speedup, serial fraction, and parallelization ratio were evaluated on the basis of the elapsed time measured with 64 core processors.

[b] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with 64 core processors was used as T_1.

[c] Serial fraction was evaluated by using eq. 5.

[d] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with 64 core processors was used as T_1.

Table S4. Speedups and parallelization ratios for energy calculations of DIMER at the B3LYP/cc-pVDZ level of theory.

			Elapsed time[sec]		Speedup[a]		Serial fraction[%][b]		Parallelization ratio[%][c]	
Number of CPUs	Number of threads	Number of cores	Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation
1	1	1	11657.211	10618.977	1.000	1.000	—	—	—	—
1	8	8	1470.312	1335.344	7.928	7.952	0.1290	0.0858	99.8710	99.9142
2	8	16	740.755	667.288	15.737	15.914	0.1114	0.0362	99.8886	99.9638
4	8	32	377.119	334.818	30.911	31.716	0.1136	0.0289	99.8864	99.9711
8	8	64	194.683	166.871	59.878	63.636	0.1093	0.0091	99.8907	99.9909
16	8	128	105.012	84.276	111.009	126.002	0.1205	0.0125	99.8795	99.9875
32	8	256	59.014	43.065	197.532	246.582	0.1161	0.0150	99.8839	99.9850
64	8	512	36.094	22.083	322.972	480.860	0.1145	0.0127	99.8855	99.9873
128	8	1024	24.425	11.271	477.267	942.127	0.1120	0.0085	99.8880	99.9915
256	8	2048	21.548	6.400	540.980	1659.103	0.1361	0.0115	99.8639	99.9885
512	8	4096	16.207	3.532	719.258	3006.898	0.1146	0.0088	99.8854	99.9912
1024	8	8192	15.062	2.312	773.948	4592.288	0.1170	0.0096	99.8830	99.9904
2048	8	16384	13.841	1.798	842.204	5905.298	0.1126	0.0108	99.8874	99.9892

[a] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with a single core processor was used as T_1.

[b] Serial fraction was evaluated by using eq. 5.

[c] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with a single core processor was used as T_1.

Table S5. Comparison of speedups and parallelization ratios for energy calculations of DIMER between 64 (64 CPUs x 1 thread) and 512 (64 CPUs x 8 threads) core processors at the B3LYP/cc-pVDZ level of theory.

			Elapsed time[sec]		Speedup[a,b]		Serial fraction[%][a,c]		Parallelization ratio[%][a,d]	
Number of CPUs	Number of threads	Number of cores	Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation	Total	Fock matrix generation
64	1	64	247.253	176.085	1.000	1.000	—	—	—	—
64	8	512	36.094	22.083	6.850	7.974	0.0384	0.0007	99.9616	99.9993

[a] Speedup, serial fraction, and parallelization ratio were evaluated on the basis of the elapsed time measured with 64 core processors.

[b] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with 64 core processors was used as T_1.

[c] Serial fraction was evaluated by using eq. 5.

[d] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with 64 core processors was used as T_1.

Table S6. Speedups and parallelization ratios for energy calculations of DIMER at the CASCI(16,16)/6-31G** level of theory.

Number of CPUs	Number of threads	Number of cores	Elapsed time[sec]				Speedup[a,b]			
			Total	Integral transformation	Fock matrix generation	Eigenvalue problem	Total	Integral transformation	Fock matrix generation	Eigenvalue problem
256	8	2048	691.328	308.495	5.516	289.848	1.000	1.000	1.000	1.000
512	8	4096	529.307	145.659	3.081	171.417	1.306	2.118	1.790	1.691
1024	8	8192	466.399	105.787	2.033	142.372	1.482	2.916	2.713	2.036

Serial fraction[%][a,c]				Parallelization ratio[%][a]			
Total	Integral transformation	Fock matrix generation	Eigenvalue problem	Total	Integral transformation	Fock matrix generation	Eigenvalue problem
—	—	—	—	—	—	—	—
0.0553	-0.0026	0.0065	0.0109	99.9447	100.0026	99.9935	99.9891
0.0637	0.0069	0.0092	0.0231	99.9363	99.9931	99.9908	99.9769

[a] Speedup, serial fraction, and parallelization ratio were evaluated on the basis of the elapsed time measured with 2048 core processors.

[b] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with 2048 core processors was used as T_1.

[c] Serial fraction was evaluated by using eq. 5.

[d] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with 2048 core processors was used as T_1.

Table S7. Speedups and parallelization ratios for force calculations of DIMER at the HF/cc-pVDZ level of theory.

Number of CPUs	Number of threads	Number of cores	Elapsed time[sec]			Speedup[a]			Serial fraction[%][b]			Parallelization ratio[%][c]		
			Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral
1	1	1	55866.363	1366.995	54498.802	1.000	1.000	1.000	—	—	—	—	—	—
1	8	8	6909.150	172.495	6735.949	8.086	7.925	8.091	-0.1517	0.1355	-0.1602	100.1517	99.8645	100.1602
2	8	16	3467.883	86.162	3381.134	16.110	15.865	16.118	-0.0454	0.0565	-0.0490	100.0454	99.9435	100.0490
4	8	32	1738.001	43.394	1694.092	32.144	31.502	32.170	-0.0145	0.0510	-0.0170	100.0145	99.9490	100.0170
8	8	64	885.490	22.065	862.910	63.091	61.954	63.157	0.0229	0.0524	0.0212	99.9771	99.9476	99.9788
16	8	128	449.616	11.380	437.715	124.254	120.127	124.508	0.0237	0.0516	0.0221	99.9763	99.9484	99.9779
32	8	256	229.790	6.129	223.142	243.119	223.031	244.234	0.0208	0.0580	0.0189	99.9792	99.9420	99.9811
64	8	512	119.173	3.489	115.157	468.782	391.846	473.255	0.0180	0.0600	0.0160	99.9820	99.9400	99.9840
128	8	1024	64.038	2.153	61.368	872.400	635.000	888.071	0.0170	0.0599	0.0150	99.9830	99.9401	99.9850
256	8	2048	36.330	1.953	33.425	1537.740	699.868	1630.466	0.0162	0.0941	0.0125	99.9838	99.9059	99.9875
512	8	4096	22.742	1.347	20.105	2456.563	1014.558	2710.729	0.0163	0.0742	0.0125	99.9837	99.9258	99.9875
1024	8	8192	14.401	1.132	12.236	3879.423	1207.309	4454.078	0.0136	0.0706	0.0102	99.9864	99.9294	99.9898
2048	8	16384	10.394	1.120	8.455	5375.072	1220.981	6446.052	0.0125	0.0758	0.0094	99.9875	99.9242	99.9906
4096	8	32768	8.231	0.945	5.830	6787.285	1447.136	9347.254	0.0117	0.0661	0.0076	99.9883	99.9339	99.9924
8192	8	65536	7.459	1.086	5.235	7489.404	1258.595	10411.361	0.0118	0.0779	0.0081	99.9882	99.9221	99.9919
16384	8	131072	9.153	0.985	4.406	6103.336	1387.374	12368.753	0.0156	0.0713	0.0073	99.9844	99.9287	99.9927

[a] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with a single core processor was used as T_1.

[b] Serial fraction was evaluated by using eq. 5.

[c] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with a single core processor was used as T_1.

Table S8. Comparison of speedup and parallelization ratios for force calculations of DIMER between 64 (64 CPUs x 1 thread) and 512 (64 CPUs x 8 threads) core processors at the HF/cc-pVDZ level of theory.

Number of CPUs	Number of threads	Number of cores	Elapsed time[sec]			Speedup[a,b]		
			Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral
64	1	64	948.643	23.281	924.846	1.000	1.000	1.000
64	8	512	119.173	3.489	115.157	7.960	6.673	8.031

Serial fraction[%][a,c]			Parallelization ratio[%][a,d]		
Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral
—	—	—	—	—	—
0.0011	0.0456	-0.0009	99.9989	99.9544	100.0009

[a] Speedup, serial fraction, and parallelization ratio were evaluated on the basis of the elapsed time measured with 64 core processors.

[b] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with 64 core processors was used as T_1.

[c] Serial fraction was evaluated by using eq. 5.

[d] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with 64 core processors was used as T_1.

Table S9. Speedup and parallelization ratios of force calculations of DIMER at the B3LYP/cc-pVDZ level of theory.

Number of CPUs	Number of threads	Number of cores	Elapsed time[sec]			Speedup[a]			Serial fraction[%][b]			Parallelization ratio[%][c]		
			Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral
1	1	1	57456.397	1367.819	56087.529	1.000	1.000	1.000	—	—	—	—	—	—
1	8	8	7099.900	171.568	6927.539	8.093	7.972	8.096	-0.1634	0.0494	-0.1699	100.1634	99.9506	100.1699
2	8	16	3726.127	86.030	3485.639	15.420	15.899	16.091	0.2508	0.0422	-0.0377	99.7492	99.9578	100.0377
4	8	32	1875.301	43.286	1744.087	30.638	31.599	32.159	0.1433	0.0409	-0.0159	99.8567	99.9591	100.0159
8	8	64	957.335	21.943	863.837	60.017	62.336	64.928	0.1053	0.0424	-0.0227	99.8947	99.9576	100.0227
16	8	128	484.818	11.262	441.570	118.511	121.458	127.018	0.0630	0.0424	0.0061	99.9370	99.9576	99.9939
32	8	256	249.014	6.005	219.130	230.736	227.768	255.955	0.0429	0.0486	0.0001	99.9571	99.9514	99.9999
64	8	512	129.212	3.847	112.522	444.666	355.597	498.457	0.0296	0.0861	0.0053	99.9704	99.9139	99.9947
128	8	1024	68.926	2.409	57.419	833.594	567.851	976.816	0.0223	0.0785	0.0047	99.9777	99.9215	99.9953
256	8	2048	36.738	1.352	28.602	1563.951	1011.786	1960.982	0.0151	0.0500	0.0022	99.9849	99.9500	99.9978
512	8	4096	23.546	1.096	18.859	2440.187	1247.992	2974.001	0.0166	0.0557	0.0092	99.9834	99.9443	99.9908
1024	8	8192	16.768	1.223	13.876	3426.456	1118.870	4042.147	0.0170	0.0772	0.0125	99.9830	99.9228	99.9875
2048	8	16384	13.715	1.153	10.789	4189.263	1185.916	5198.529	0.0178	0.0782	0.0131	99.9822	99.9218	99.9869
4096	8	32768	12.394	1.132	9.348	4635.970	1208.062	5999.909	0.0185	0.0797	0.0136	99.9815	99.9203	99.9864
8192	8	65536	11.291	1.306	8.204	5088.483	1047.126	6836.358	0.0181	0.0940	0.0131	99.9819	99.9060	99.9869
16384	8	131072	9.873	0.798	7.508	5819.641	1713.486	7470.565	0.0164	0.0576	0.0126	99.9836	99.9424	99.9874

[a] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with a single core processor was used as T_1.

[b] Serial fraction was evaluated by using eq. 5.

[c] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with a single core processor was used as T_1.

Table S10. Comparison of speedups and parallelization ratios for force calculations of DIMER between 64 (64 CPUs x 1 thread) and 512 (64 CPUs x 8 threads) core processors at the B3LYP/cc-pVDZ level of theory.

Number of CPUs	Number of threads	Number of cores	Elapsed time[sec]			Speedup[a,b]		
			Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral
64	1	64	1020.217	23.280	900.466	1.000	1.000	1.000
64	8	512	129.212	3.847	112.522	7.896	6.052	8.003

Serial fraction[%][a,c]			Parallelization ratio[%][a,d]		
Total	1-electron integral	2-electron integral	Total	1-electron integral	2-electron integral
—	—	—	—	—	—
0.0030	0.0752	-0.0001	99.9970	99.9248	100.0001

[a] Speedup, serial fraction, and parallelization ratio were evaluated on the basis of the elapsed time measured with 64 core processors.

[b] Speedup was evaluated by using eq. 3. Here, the elapsed time measured with 64 core processors was used as T_1.

[c] Serial fraction was evaluated by using eq. 5.

[d] Parallelization ratio was evaluated by using eq. 4. Here, the elapsed time measured with 64 core processors was used as T_1.