Supporting Information
Performance Portability of Electron Repulsion Integrals and Their Related Methods across Peta to Exascale Architectures

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Table S1 The average of maximum time per RHF iteration and the standard deviation of the RHF SP algorithm for water clusters, H_2O_n, n=50, 80, 100, and 200 calculated at RHF/6-31G using GPU code. The calculations were performed using one compute node on various computer clusters and compilers. The data are corresponded to Fig. 4 in the main text.

# waters	Average of maximum time per RHF iteration (s)					
	V100/ XLF 6 GPUs	V100/ NVHPC 6 GPUs	A100/ NVHPC 4 GPUs	A100/ CCE 4 GPUs	PVC/ oneAPI 12 tiles	MI-250X/ CCE 8 GCDs
50	6.25	0.54	0.45	0.85	2.26	0.17
80	14.68	1.32	1.04	2.04	4.28	0.27
100	17.35	1.57	1.24	2.42	4.93	0.29
200	181.43	15.21	12.27	20.90	37.84	1.87
Standard deviation (SD)						
50	0.01	0.01	0.01	0.04	0.02	0.01
80	0.01	0.00	0.01	0.07	0.01	0.01
100	0.07	0.00	0.01	0.09	0.02	0.00
200	1.09	0.04	0.04	0.74	0.07	0.02

Table S2 The average of maximum time per RHF iteration and the standard deviation of the RHF SPD algorithm for water clusters, H_2O_n, n= 30-100 calculated at RHF/6-31+G(d) using GPU code. The calculations were performed using one compute node on various computer clusters and compilers. The data are corresponded to Fig. 5 in the main text.

# waters	Average of maximum time per RHF iteration (s)					
	V100/ XLF 6 GPUs	V100/ NVHPC 6 GPUs	A100/ NVHPC 4 GPUs	A100/ CCE 4 GPUs	PVC/ oneAPI 12 tiles	MI-250X/ CCE 8 GCDs
30	19.78	1.47	1.24	2.07	10.15	1.01
40	46.15	3.75	2.89	4.82	18.15	2.04
50	82.54	6.92	5.27	8.59	25.70	2.78
60	128.59	10.92	8.26	13.22	33.86	3.81
70	161.94	14.02	10.63	16.42	38.68	4.51
80	250.79	21.83	16.30	24.92	55.10	6.54
90	283.50	24.75	18.53	28.46	62.15	7.09
100	328.73	29.15	21.40	32.77	68.58	7.76

Table S3 The average of maximum time per RHF iteration and the standard deviation (second) for the 100-watercluster at RHF/6-31G using the SP scheme using CPU MPI, CPU MPI/OpenMP, and GPU codes on various hardware and different compiler vendors. The data are corresponded to Fig. 6 in the main text.

Version	Average of maximum time per RHF iteration (s)					
	V100/ XLF	V100/ NVHPC	A100/ NVHPC	A100/ CCE	MI-250X/ CCE	PVC/ oneAPI
CPU MPI	35.47	26.38	16.52	19.84	32.17	13.54
CPU MPI/OMP	17.80	23.15	26.12	18.86	68.34	15.24
GPU	17.35	1.57	1.24	2.42	4.93	0.29
Standard deviation (SD)						
CPU MPI	0.11	3.35	0.15	0.17	0.02	0.03
CPU MPI/OMP	0.62	1.56	0.02	0.08	0.21	0.01
GPU	0.07	0.00	0.01	0.09	0.02	0.00

Table S4 The average of maximum time per RHF iteration and the standard deviation (second) for the 80-watercluster at RHF/6-31+G(d) using the SPD scheme using CPU MPI, CPU MPI/OpenMP, and GPU codes on various hardware and different compiler vendors. The data are corresponded to Fig. 7 in the main text.

Version	Average of maximum time per RHF iteration (s)					
	V100/ XLF	V100/ NVHPC	A100/ NVHPC	A100/ CCE	MI-250X/ CCE	PVC/ oneAPI
CPU MPI	126.84	121.74	73.09	81.98	139.13	59.37
CPU MPI/OMP	87.30	114.71	73.09	119.95	435.65	69.20
GPU	250.79	21.83	16.30	24.92	55.10	6.54
Standard deviation (SD)						
CPU MPI	0.57	8.73	0.35	0.91	0.18	0.04
CPU MPI/OMP	2.76	2.78	0.35	0.04	7.81	0.79
GPU	0.36	0.02	0.08	0.17	0.21	0.16

Table S5 Total time (seconds) for RHF/6-31G calculations for 100-water cluster and RHF/6-31+G(d) calculations for 80-water cluster with respect to the number of GPUs on various hardware and compilers. The data are corresponded to GPU speed-up and percent efficiency shown in Fig. 8 and 9 in the main text.

#GPU	Total RHF wall time (s)					
	V100/XLF	V100/NVHPC	A100/NVHPC	A100/CCE	PVC/oneAPI	MI-250X/CCE
RHF/6-31G calculations for 100-water cluster						
1	1029.91	88.91	48.54	89.02	41.28	288.21
2	600.27	52.5	29.32	54.92	17.59	178.02
4	312.87	28.54	16.25	30.9	8.45	102.7
6	212.1	20.21			5.97	73.61
8					4.76	58.06
10					4.06	
12					3.6	
RHF/6-31+G(d) calculations for 80-water cluster						
1	N/A*	1504.61	759.22	1016.63	1068.91	3990.12
2	N/A*	816.69	424.84	598.08	507.68	2315.61
4	4933.28	424.55	225.25	327.52	241.24	1281.41
6	3254.69	286.03			166.19	915.86
8					130.32	711.92
10					101.39	
12					85.27	

* The calculations exceed two-hour limit on the OLCF Summit policy.

Table S6 Wall times for RHF, CPHF and TDHF calculations of d-tubocurarine molecule using CPU MPI, CPU MPI/OpenMP, and GPU codes on various hardware and different compiler vendors. The data are corresponded to Fig. 10 and 11 in the main text.

method	version	Wall time (s)				
		V100/ NVHPC 6 GPUs	A100/ NVHPC 4 GPUs	A100/ CCE 4 GPUs	PVC/ oneAPI 12 tiles	MI-250X/ CCE 8 GCDs
RHF	CPU MPI/OMP	66.90	74.11	17.37	32.82	205.80
	CPU MPI	58.44	17.77	32.15	23.31	57.41
	GPU	7.17	6.50	9.78	10.57	59.91
CPHF	CPU MPI/OMP	68.72	78.61	19.55	35.14	226.32
	CPU MPI	63.47	20.57	37.11	27.15	64.30
	GPU	9.80	9.05	9.43	14.36	75.19
TDHF	CPU MPI/OMP	1053.12	1081.43	260.34	482.17	3037.93
	CPU MPI	965.21	275.62	487.13	360.44	833.81
	GPU	108.90	97.50	121.29	138.16	657.60