Mixed-Precision CCSD

ZHE WANG

01/09

T_1 equation:

$$t_i^a D_i^a = f_{ia} + \sum_e t_i^e \mathscr{F}_{ae} - \sum_m t_m^a \mathscr{F}_{mi} + \sum_{me} t_{im}^{ae} \mathscr{F}_{me}$$
$$- \sum_{nf} t_n^f \langle na \| if \rangle - \tfrac{1}{2} \sum_{mef} t_{im}^{ef} \langle ma \| ef \rangle$$
$$- \tfrac{1}{2} \sum_{men} t_{mn}^{ae} \langle nm \| ei \rangle. \qquad (1)$$

T_2 equation:

$$t_{ij}^{ab} D_{ij}^{ab} = \langle ij \| ab \rangle + P_-(ab) \sum_e t_{ij}^{ae} \left(\mathscr{F}_{be} - \tfrac{1}{2} \sum_m t_m^b \mathscr{F}_{me} \right)$$
$$- P_-(ij) \sum_m t_{im}^{ab} \left(\mathscr{F}_{mj} + \tfrac{1}{2} \sum_e t_j^e \mathscr{F}_{me} \right)$$
$$+ \tfrac{1}{2} \sum_{mn} \tau_{mn}^{ab} \mathscr{W}_{mnij} + \tfrac{1}{2} \sum_{ef} \tau_{ij}^{ef} \mathscr{W}_{abef}$$
$$+ P_-(ij) P_-(ab) \sum_{me} (t_{im}^{ae} \mathscr{W}_{mbej} - t_i^e t_m^a \langle mb \| ej \rangle$$
$$+ P_-(ij) \sum_e t_i^e \langle ab \| ej \rangle - P_-(ab) \sum_m t_m^a \langle mb \| ij \rangle.$$
$$(2)$$

Single-precision calculation

1-3 recover iterations in double-precision

Calculate contractions in single-precision

Sum up the terms in T-amplitude equations in double-precision

Stanton, J. F.; Gauss, J.; Watts, J. D.; Bartlett, R. J., A direct product decomposition approach for symmetry exploitation in many−body methods. I. Energy calculations. *The Journal of Chemical Physics* **1991,** *94*, 4334-4345.

Pokhilko, P.; Epifanovsky, E.; Krylov, A. I., Double Precision Is Not Needed for Many-Body Calculations: Emergent Conventional Wisdom. *Journal of Chemical Theory and Computation* **2018,** *14*, 4088-4096

Table1. Performance of CCSD calculation for water molecule clusters in double/mixed/single-precision (Results were from Python script)

# of water molecules	Double-precision(dp)				Mixed-precision(mp)				single-precision(sp)								
	Time/s	Iterations	Time/iteration	Accuracy	Time /s	Iterations	Time/ iteration	Accuracy	Time/s	Iterations	Time/iteration	Accuracy	Speedup(mp)	Speedup(sp)	Speedup / iteration (mp)	Speedup / iteration (sp)	mp vs. sp
1	0.19	17	0.011176471	6	0.16	17	0.00962963	6	0.16	18	0.008888889	5	0.842105263	0.842105263	0.861598441	0.795321637	1.083333333
2	2.69	15	0.179333333	6	1.64	15	0.109333333	6	1.52	15	0.101333333	5	0.609665428	0.565055762	0.609665428	0.565055762	1.078947368
3	23.28	16	1.455	6	13.14	16	0.82125	6	11.57	15	0.771333333	4	0.56443299	0.496993127	0.56443299	0.530126002	1.06471478
4	122.95	16	7.684375	6	61.97	15	4.131333333	5	60.47	16	3.779375	2	0.504026027	0.491825946	0.537627762	0.491825946	1.093126068
5	428.63	17	25.21352941	6	239.43	17	14.00765795	6	209.77	16	13.110625	5	0.558593659	0.489396449	0.555561172	0.519983727	1.068420304
6	1211.93	17	71.29	6	617.63	16	38.601875	6	621.28	17	35.85712418	4	0.509625143	0.512636868	0.541476715	0.502975511	1.076546875

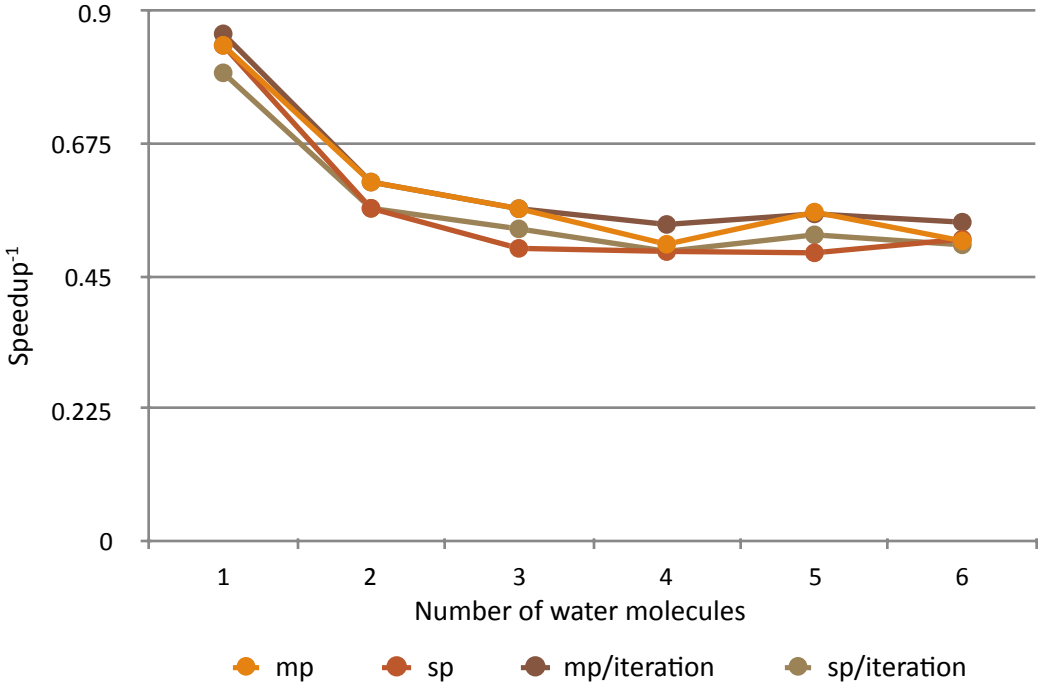

Fig1. The speedup of mixed-precision and single-precision CCSD calculation. The comparison was made between the overall time and time/iteration The smaller value in the y-axis means the calculation is faster.