Supporting Information for "Horizontal Vectorization of Electron Repulsion Integrals"

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1 Compilation/Configure command lines

1.1 simint with AVX

```
CC=icc CXX=icpc cmake -DLIBINT2_PATH=<path_to_libint2> \
                      -DLIBERD_PATH=<path_to_erd> \
                      -DSIMINT_AVX:Bool=True ../
```

1.2 libint2 with AVX

```
../configure --with-cxx=g++ --with-cxxgen=icpc \
             --with-cxxgen-optflags="-xavx -O3" \
             --disable-t1g12-support \
             --disable-g12 --disable-g12dkh \
             --enable-contracted-ints --enable-fma
```

2 Instability in electron transfer

As an example, begin with the electron transfer equation for a $(p_x s|p_x s)$ integral,

$$\Theta^{(0)}_{1010} = \frac{-bX_{AB} + dX_{CD}}{q}\Theta^{(0)}_{1000} + \frac{1}{2q}\Theta^{(0)}_{0000} - \frac{p}{q}\Theta^{(0)}_{2000} \tag{1}$$

where $\Theta^{(0)}_{2000}$ can be obtained from VRR

$$\Theta^{(0)}_{2000} = X_{PA}\Theta^{(0)}_{1000} - \frac{\alpha}{p}X_{PQ}\Theta^{(1)}_{1000} + \frac{i}{2p}\left[\Theta^{(0)}_{0000} - \frac{\alpha}{p}\Theta^{(1)}_{0000}\right] \tag{2}$$

$$\tag{3}$$

If $p \gg q$ and $X_{PA} \approx 0$, then

$$\frac{\alpha}{p} \equiv \frac{pq}{p(p+q)} = \frac{q}{p+q} \approx 0 \tag{4}$$

$$\Theta^{(0)}_{2000} \approx \frac{i}{2p}\Theta^{(0)}_{0000} \tag{5}$$

Therefore, Eq. 1 becomes

$$\Theta^{(0)}_{1010} \approx \frac{-bX_{AB} + dX_{CD}}{q}\Theta^{(0)}_{1000} + \frac{1}{2q}\Theta^{(0)}_{0000} - \frac{p}{q}\frac{1}{2p}\Theta^{(0)}_{0000} \tag{6}$$

This leads to a loss of precision due to the fact that the last two terms in Eq. 1 are approximately equal and the fact that the imprecise subtraction will dominate if the first term is also relatively small.

3 Raw results

Results were obtained on a single thread on an Intel Xeon E5-2698 v3 processor running at 2.30 GHz. Integral screening was not not used. Fused multiply-add was enabled for

Table 1: Number of primitive and contracted quartets for the benchmarked basis sets (with the benzene molecule)

	No. of Contracted Integrals	No. of Primitive Integrals	
Class		ANO-TZ	aug-cc-pVTZ
$(ss\|ss)$	8503056	140283207936	506250000
$(ps\|ss)$	6613488	66015627264	182250000
$(ps\|ps)$	5143824	31066177536	65610000
$(pp\|ss)$	5143824	31066177536	65610000
$(pp\|ps)$	4000752	14619377664	23619600
$(pp\|pp)$	3111696	6879707136	8503056
$(ds\|ss)$	4723920	24755860224	101250000
$(ds\|ps)$	3674160	11649816576	36450000
$(ds\|pp)$	2857680	5482266624	13122000
$(ds\|ds)$	2624400	4368681216	20250000
$(dp\|ss)$	3674160	11649816576	36450000
$(dp\|ps)$	2857680	5482266624	13122000
$(dp\|pp)$	2222640	2579890176	4723920
$(dp\|ds)$	2041200	2055849984	7290000
$(dp\|dp)$	1587600	967458816	2624400
$(dd\|ss)$	2624400	4368681216	20250000
$(dd\|ps)$	2041200	2055849984	7290000
$(dd\|pp)$	1587600	967458816	2624400
$(dd\|ds)$	1458000	770943744	4050000
$(dd\|dp)$	1134000	362797056	1458000
$(dd\|dd)$	810000	136048896	810000
$(dd\|fs)$	583200	256981248	1620000
$(fs\|ss)$	1889568	8251953408	40500000
$(fs\|ps)$	1469664	3883272192	14580000
$(fs\|pp)$	1143072	1827422208	5248800
$(fs\|ds)$	1049760	1456227072	8100000
$(fs\|dp)$	816480	685283328	2916000
$(fs\|fs)$	419904	485409024	3240000
$(fp\|ss)$	1469664	3883272192	14580000
$(fp\|ps)$	1143072	1827422208	5248800
$(fp\|pp)$	889056	859963392	1889568
$(fp\|ds)$	816480	685283328	2916000
$(fp\|dp)$	635040	322486272	1049760
$(fp\|dd)$	453600	120932352	583200
$(fp\|fs)$	326592	228427776	1166400
$(fp\|fp)$	254016	107495424	419904
$(fd\|ss)$	1049760	1456227072	8100000
$(fd\|ps)$	816480	685283328	2916000
$(fd\|pp)$	635040	322486272	1049760
$(fd\|ds)$	583200	256981248	1620000
$(fd\|dp)$	453600	120932352	583200
$(fd\|dd)$	324000	45349632	324000
$(fd\|fs)$	233280	85660416	648000
$(fd\|fp)$	181440	40310784	233280
$(fd\|fd)$	129600	15116544	129600
$(ff\|ss)$	419904	485409024	3240000
$(ff\|ps)$	326592	228427776	1166400
$(ff\|pp)$	254016	107495424	419904
$(ff\|ds)$	233280	85660416	648000
$(ff\|dp)$	181440	40310784	233280
$(ff\|dd)$	129600	15116544	129600
$(ff\|fs)$	93312	28553472	259200
$(ff\|fp)$	72576	13436928	93312
$(ff\|fd)$	51840	5038848	51840
$(ff\|ff)$	20736	1679616	20736

SIMINT and LIBINT. Permutational symmetry was not taken into account for any library except that only the the given angular momentum classes were benchmarked; that is, no permutational symmetry within a given class was exploited.

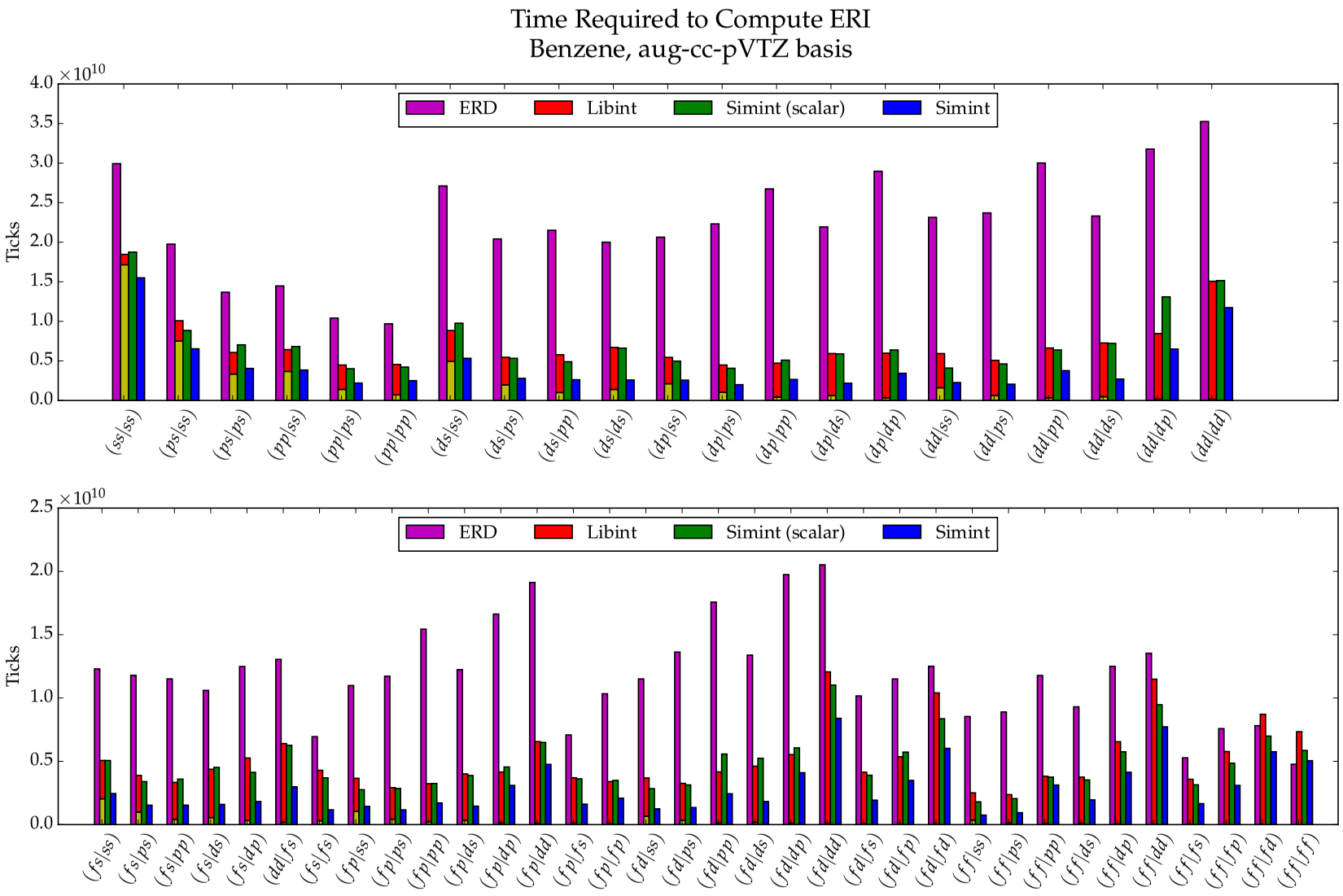

Figure 1: Time to calculate all ERI classes of benzene with the aug-cc-pVTZ basis set. Time is reported as number of processor ticks. For benchmark details, see text. The yellow bars for LIBINT represent the time required to compute prerequisite values (including evaluation of the Boys function).

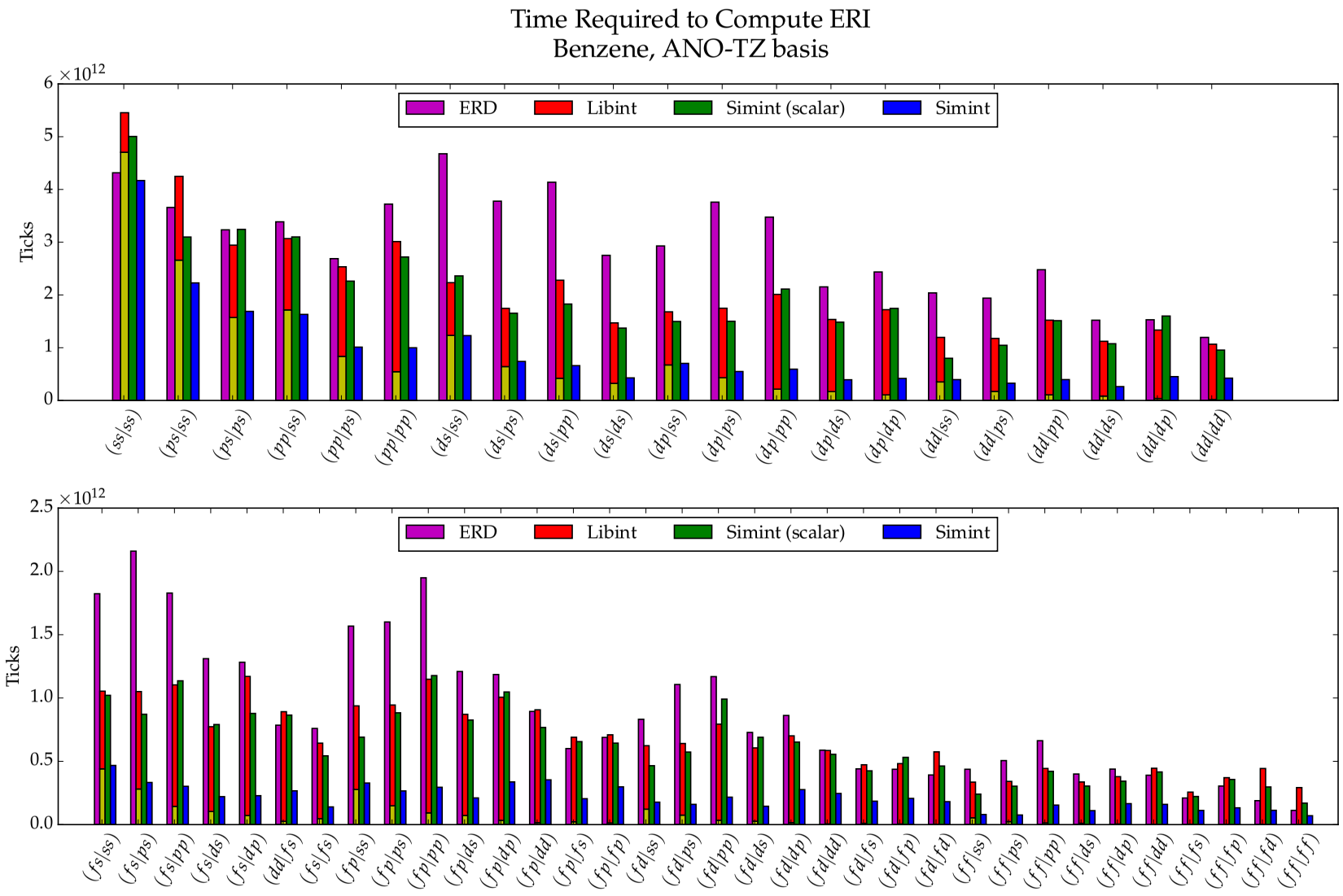

Figure 2: Time to calculate varioius ERI classes of benzene with the ANO-TZ basis set. Time is reported as number of processor ticks. For benchmark details, see text. The yellow bars for LIBINT represent the time required to compute prequisite values (including evaluation of the Boys function).