

# 1E03 Parallel computation of the four-center molecular integral over the Slater-type orbitals

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## 1. Introduction

Up to present, we have developed efficient algorithms [1-2] for the calculation of all of the one-electron as well as the two-electron integrals with the Slater-type orbitals (STO). Especially, one of us (K.I.) has developed the ACE-b3k3 algorithm [2] for the four-center two-electron integrals with the STO-NG expansions. The ACE-b3k3 algorithm has been implemented in our program for the molecular integrals with STO (SMILES 2007) [1]. Recently, one of us (K.I.) has developed a parallel version of his ACE-b3k3 algorithm. We have already presented a part of the present efficiency of the parallel calculation for the four-center (two-electron) electron-repulsion integrals (ERIs) at the 13<sup>th</sup> International Congress of Quantum Chemistry (ICQC) held at the Helsinki University during June 22-27, 2009 [3]. A part of the present results is shown in Table I. As seen in Table I, we may conclude that ab initio calculation for middle size molecules with a good STO basis sets are currently an actual possibility. The next step is clearly the parallel computation of the derivatives of the four-center ERIs over STOs. The derivatives with respect to the nuclear coordinates are necessary, for example, for the geometry optimization of a molecule, for the calculation of the intrinsic reaction coordinates (IRC), and so on. In this report, we show a new algorithm for the derivatives.

## 2. A new algorithm special for the derivatives

A part of the results of the present new algorithm is shown in Table II. As seen in Table II, the total computer time for ERI + 12 kinds of derivatives is only slightly more than that for ERI only.

## 3. References

- [1] Fernández Rico, J.; López, R.; Ema, I.; Ramírez, G. *Int. J. Quantum Chem.* 2008, 108, 1415-1421.
- [2] Ishida, K. *J. Chem. Phys.* 2000, 113, 7818-7829.
- [3] Ishida, K; López, R.; Fernández Rico, J. Abstract #B49, 13<sup>th</sup> ICQC.

**Table I.** Computer time of all four-center ERIs over STOs for several molecules

Molecule	SMILES 2007	Parallel computation
Basis (# of STOs)	single processor	with 64 processors
Methanol CH <sub>3</sub> OH (18 electrons; C <sub>s</sub> )		
VB1 (62 STOs)	79 sec.	3.6 sec. (22 times faster)
VB2 (130 STOs)	990 sec.	35 sec. (28 times faster)
VB3 (244 STOs)	7928 sec.	270 sec. (29 times faster)
Naphthalene C <sub>10</sub> H <sub>8</sub> (68 electrons; C-C=1.40 and C-H=1.01; D <sub>2h</sub> )		
VB1 (238 STOs)	9293 sec.	591 sec. (16 times faster)
Adenine C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> (70 electrons; C <sub>s</sub> )		
VB1 (220 STO2)	19490 sec.	1095 sec. (19 times faster)
Di-silicon hexa-chloride Si <sub>2</sub> Cl <sub>6</sub> (130 electrons; D <sub>3d</sub> )		
ZVB2 (336 STOs)	2652 sec.	231 sec. (11 times faster)

The basis set VB1 is a “triple-zeta + polarization”

Each basis set of VB2 and ZVB2 is a “quadruple zeta + double polarization”

The basis set VB3 is a “quintuple zeta + triple polarization”

**Table II.** Comparison of the present parallel algorithm with a new parallel algorithm for the four-center ERIs and its first derivatives over STOs in the case of (2p2p|2p2p)

	The parallel for 81 ERIs	New parallel for both 81x(ERI + 12 Derivatives)
Preparation time	41 μsec.	28 μsec.
Computation 1 time	121 μsec.	190 μsec.
Communication time	42 μsec.	31 μsec.
Computation 2 time	8 μsec.	34 μsec.
Total time	212 μsec.	283 μsec.

For all parallel computation, 64 processors were used.

Computation time was measured with a HITAC sr11000 computer.

The communication time depends on the computer hardware used.