Evaluation of two-electron repulsion integrals over Gaussian basis functions on SRC-6 reconfigurable computer

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• Problem

$$\langle \mu \nu | \lambda \sigma \rangle = \sum_{p=1}^{N_\mu} \sum_{q=1}^{N_\nu} \sum_{r=1}^{N_\lambda} \sum_{s=1}^{N_\sigma} d_{\mu p} d_{\nu q} d_{\lambda r} d_{\sigma s} [p q | r s]$$

$$[s_1 s_2 | s_3 s_4] = \frac{\pi^3}{AB \sqrt{A + B}} K_{12}(\vec{R}_{12}) K_{34}(\vec{R}_{34}) F_0 \left( \frac{A B}{A + B} [\vec{R}_P - \vec{R}_Q]^2 \right)$$

$$A = \alpha_1 + \alpha_2, \quad B = \alpha_3 + \alpha_4, \quad F_0 (t) = \frac{erf (\sqrt{t})}{\sqrt{t}},$$

$$\vec{R}_{kl} = \vec{R}_k - \vec{R}_l, \quad \vec{R}_P = \frac{\alpha_1 \vec{R}_1 + \alpha_2 \vec{R}_2}{A}, \quad \vec{R}_Q = \frac{\alpha_3 \vec{R}_3 + \alpha_4 \vec{R}_4}{B},$$

$$K_{ij} (\vec{R}_{ij}) = \exp \left( - \frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j} [\vec{R}_i - \vec{R}_j]^2 \right)$$
for (shell1 = 0; shell1 < totNumShells; shell1++) {
    for (shell2 = shell1; shell2 < totNumShells; shell2++) {
        for (shell3 = shell1; shell3 < totNumShells; shell3++) {
            for (shell4 = shell3; shell4 < totNumShells; shell4++) {
                allprims = cs1_numPrimitives * cs2_numPrimitives * cs3_numPrimitives * cs4_numPrimitives;
                for (i = 0; i < allprims; i++) {
                    p_product = I1*I2*I3 * Coeff1*Coeff2*Coeff3*Coeff4;
                }
            }
        }
    }
}

Device Utilization Summary:
Number of MULT18X18s               46 out of 444    10%
Number of RAMB16s                     64 out of 444     14%
Number of SLICEs                    15677 out of 44096  35%

Model 1
# of atoms              30
Basis set              6-311G
# of integrals         528,569,315
# of reduction elements 3,146,010
SRC-6 host (sec)           70.55
SRC-6 MAP E (sec)           25.42
Speedup               2.8x

Model 2
# of atoms              64
Basis set              STO-6G
# of integrals         2,861,464,320
# of reduction elements 2,207,920
SRC-6 host (sec)           518.90
SRC-6 MAP E (sec)           42.85
Speedup               12.1x

 SRC-6 MAP E processor