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

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- **Problem**

$$(\mu\nu|\lambda\sigma) = \sum_{p=1}^{N_\mu}\sum_{q=1}^{N_\nu}\sum_{r=1}^{N_\lambda}\sum_{s=1}^{N_\sigma} d_{\mu p}\, d_{\nu q}\, d_{\lambda r}\, d_{\sigma s}\, [pq|rs]$$

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

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

$$\vec{\mathbf{R}}_{\mathbf{kl}} = \vec{\mathbf{R}}_{\mathbf{k}} - \vec{\mathbf{R}}_{\mathbf{l}},\ \vec{\mathbf{R}}_{\mathbf{P}} = \frac{\alpha_1\vec{\mathbf{R}}_{\mathbf{1}} + \alpha_2\vec{\mathbf{R}}_{\mathbf{2}}}{A},\ \vec{\mathbf{R}}_{\mathbf{Q}} = \frac{\alpha_3\vec{\mathbf{R}}_{\mathbf{3}} + \alpha_4\vec{\mathbf{R}}_{\mathbf{4}}}{B},$$

$$K_{ij}\left(\vec{\mathbf{R}}_{ij}\right) = exp\left(-\frac{\alpha_i\alpha_j}{\alpha_i + \alpha_j}\left[\vec{\mathbf{R}}_i - \vec{\mathbf{R}}_j\right]^2\right)$$

- # Solution

	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