



Example of Tensor Operations in Quantum Chemistry and Material

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Example contraction (non-aligned)

$$T_{ij}^{ab} \leftarrow \sum_{e,f,m} V_{ef}^{am} \times T_{ijm}^{efb}$$

$$T_{ij}^{ab}(B_{ij}) \leftarrow \sum_{B_3, B_{ef}, ef, m} V_{ef}^{am}(B_{ef}) \times T_{ijm}^{efb}(B_{ef}, B_{ij}, B_3) \times F_{abm}(B_{ij}, B_{ef}, B_3)$$

Blas version (single block)

$$T_{ij}^{ab} \leftarrow \sum_{ef,m} V_{ef}^{am} \times T_{ijm}^{efb} \times F_{abm}$$

- Unpack: $T_{ij}^{ab} \rightarrow T_2(a, ij, b), V_{ef}^{am} \rightarrow V(a, ef, m)$
- Tensor transpose: $T_{ijm}^{efb} \rightarrow T_3(ef, m, ij, b)$
- Intermediate update: $\forall b, X_b(a, ef, m) = V(a, ef, m)F(a, m, b)$
- Xgemm: $\forall b, T_2(b) \leftarrow X_b T_3(b)$
- Pack: $T_2(a, ij, b) \rightarrow T_{ij}^{ab}$