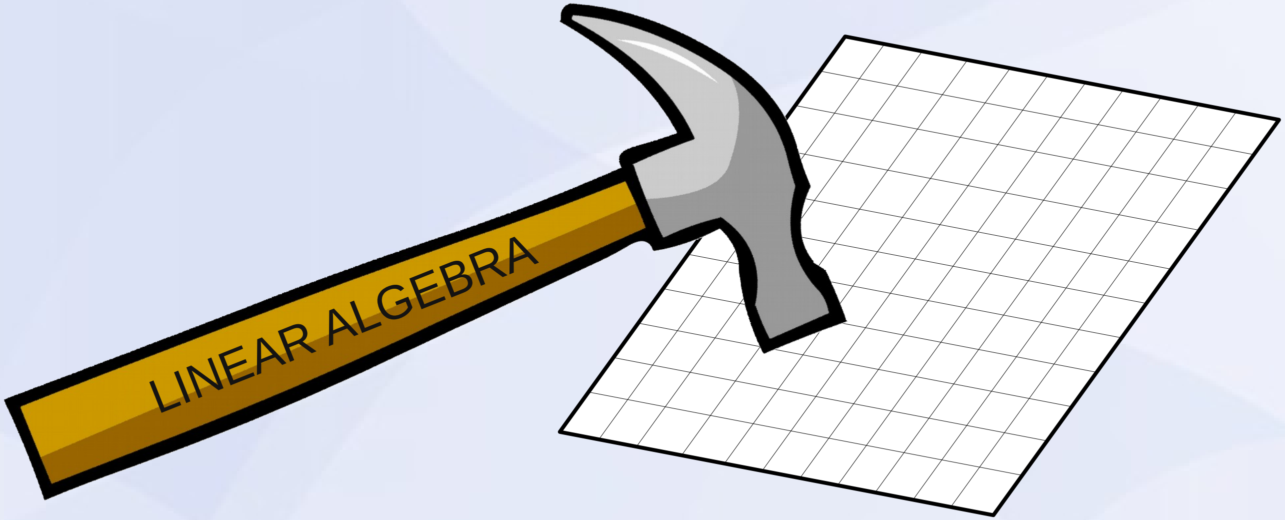
# When All You Have is Linear Algebra, Everything Looks Like a Matrix



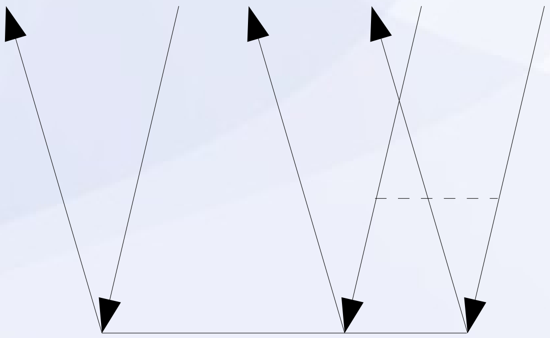
Devin A. Matthews

John F. Stanton

THE UNIVERSITY OF TEXAS AT AUSTIN

# Quantum Chemistry is Just Tensors

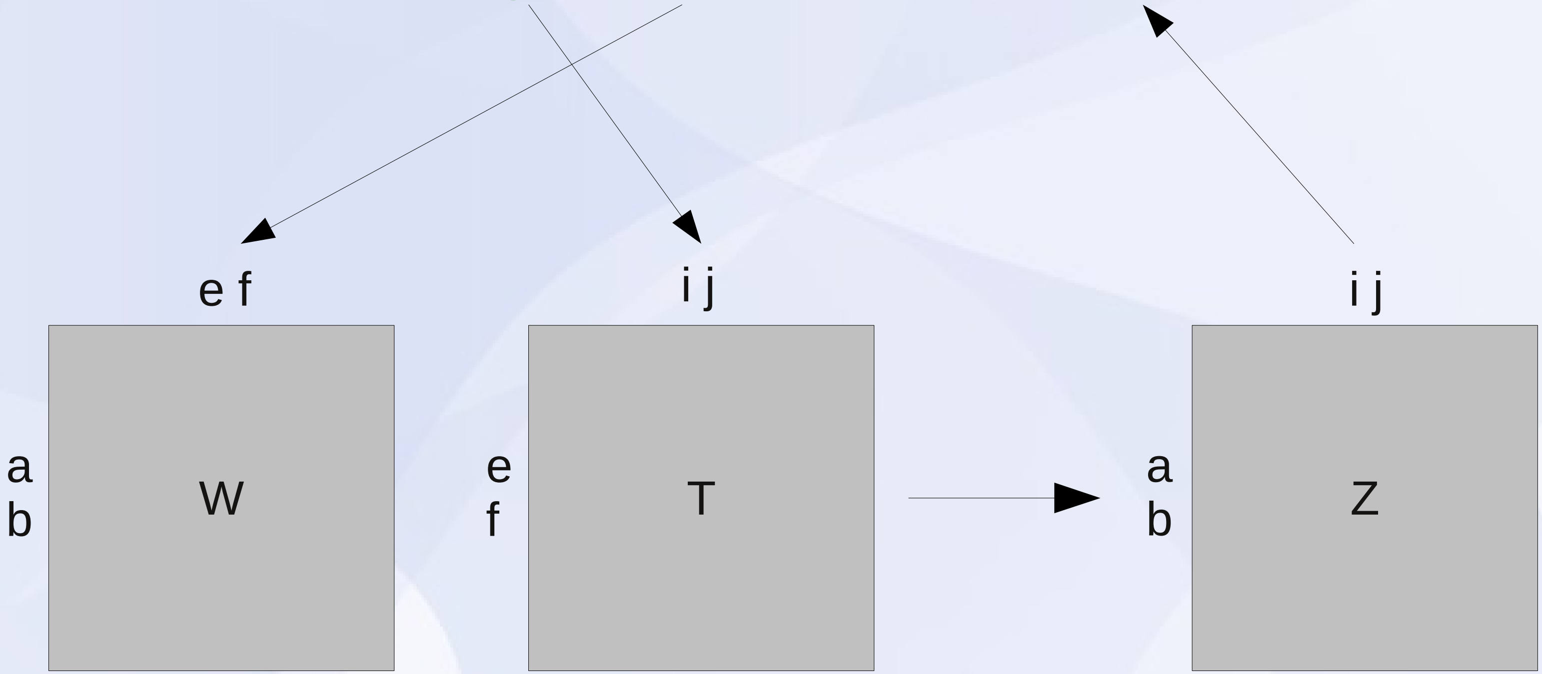
$$\langle \Phi_{ijk}^{abc} | e^{-\hat{T}} \hat{H} e^{\hat{T}} | \Phi_0 \rangle = 0$$



$$\sum_{mn} T_{mnk}^{abc} W_{ij}^{mn} \rightarrow Z_{ijk}^{abc}$$

# And Sometimes Tensors are Like Matrices

$$T_{ij}^{ef} W_{ef}^{ab} \rightarrow Z_{ij}^{ab}$$

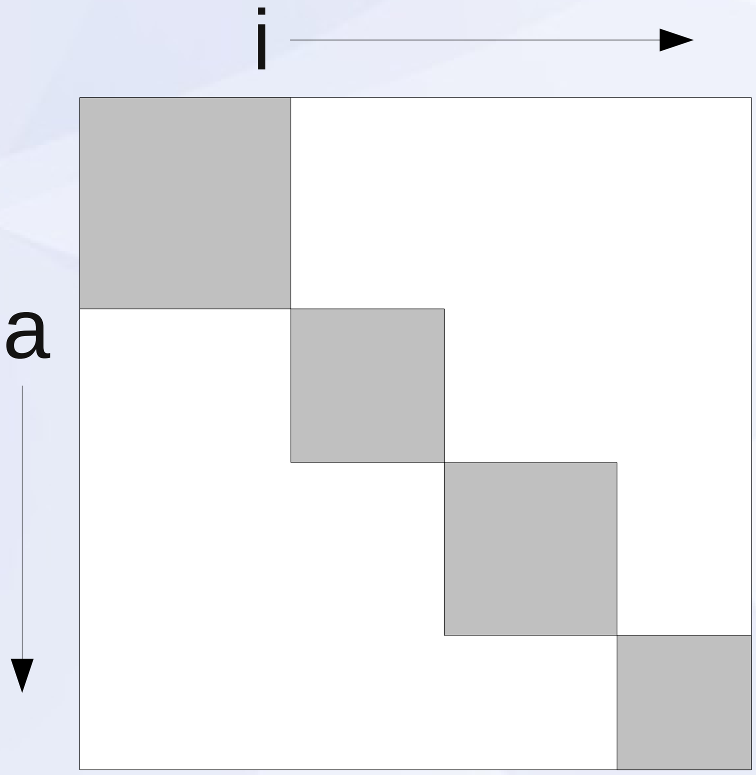


# Additional Complications: DPD

Tensors have block-sparsity due to the spatial symmetry of the molecule. Storage of the non-zero blocks follows a recursive decomposition:

$$T_i^a \longrightarrow$$

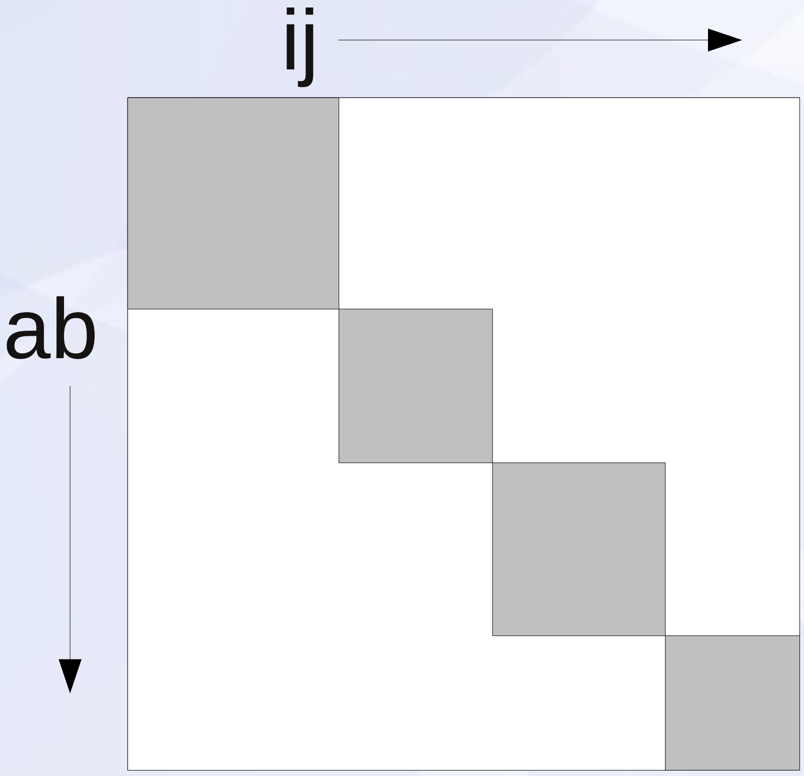
$$\Gamma_a \otimes \Gamma_i = \Gamma_T$$



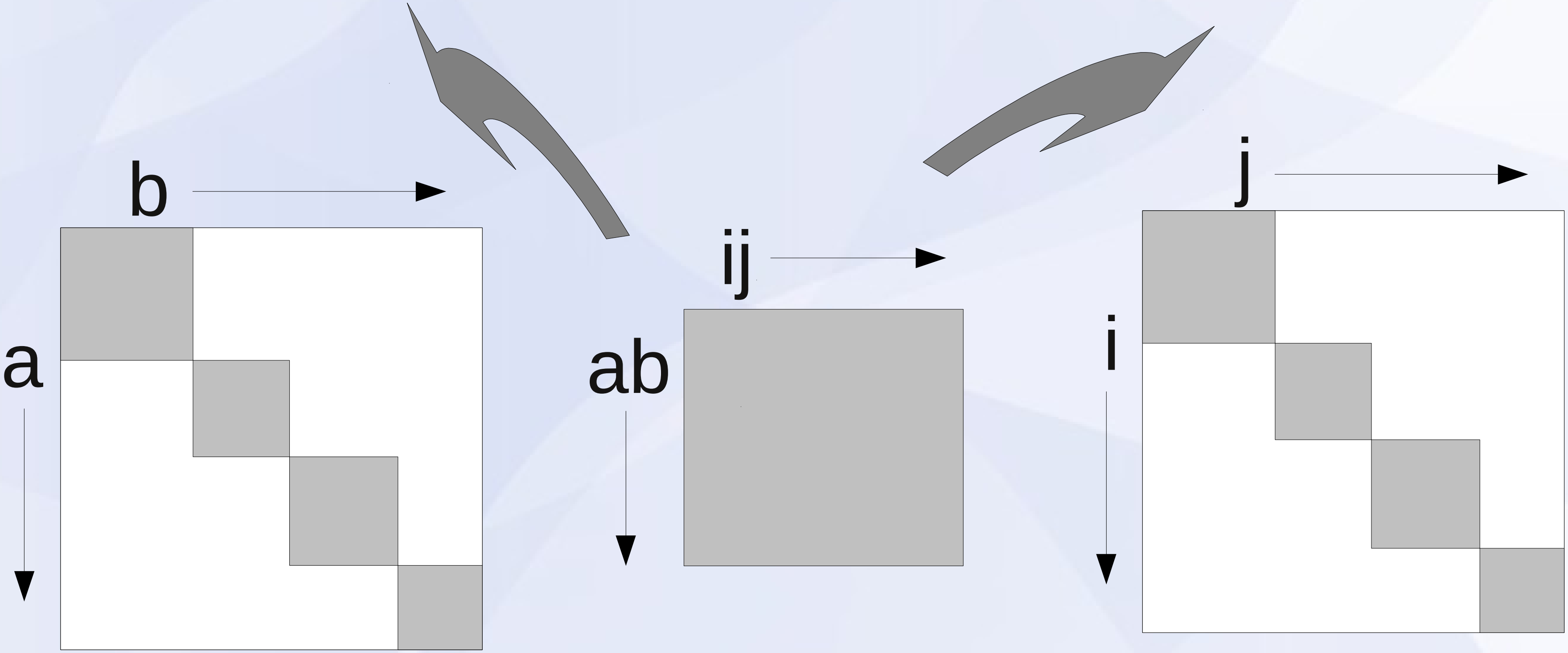
# Additional Complications: DPD

$$T_{ij}^{ab} \longrightarrow$$

$$\Gamma_a \otimes \Gamma_b \otimes \Gamma_i \otimes \Gamma_j = \Gamma_T$$



# Additional Complications: DPD

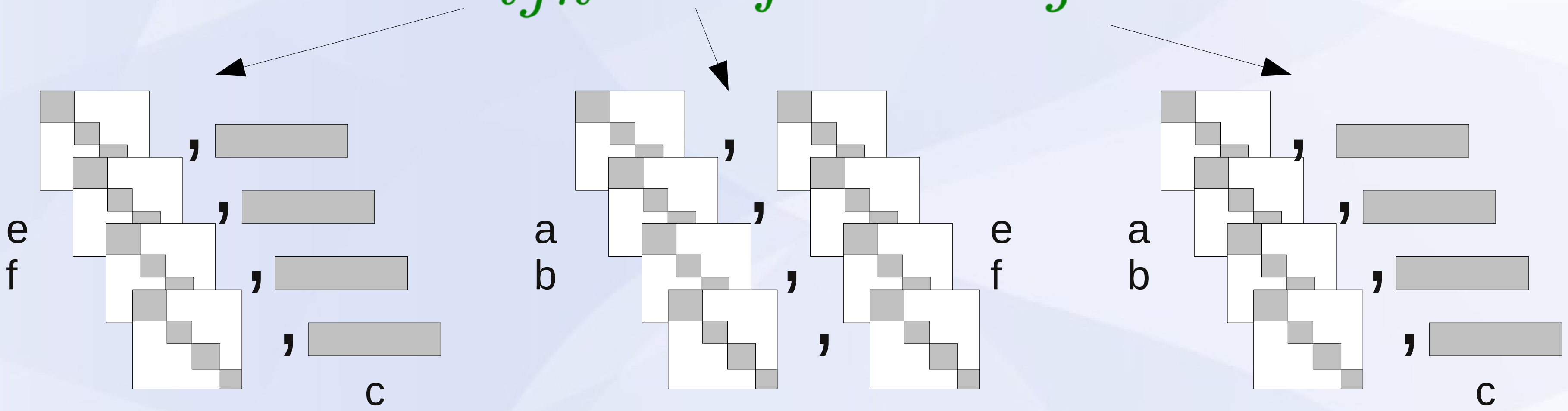


# Sometimes Tensors are Like Matrices

$$T^{efc}_{ijk} W^{ab}_{ef} \rightarrow Z^{abc}_{ijk}$$

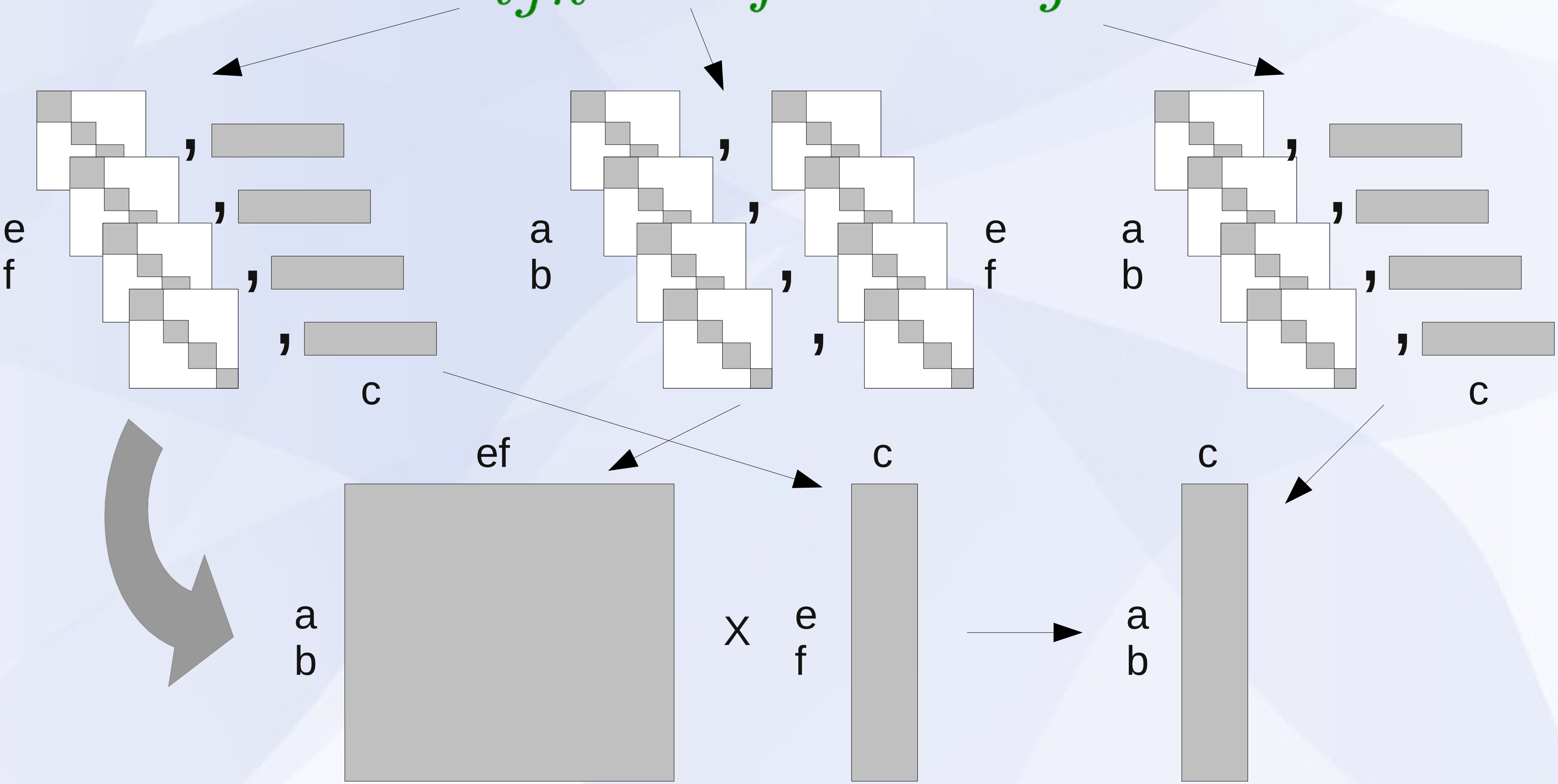
# Sometimes Tensors are Like Matrices

$$T_{ijk}^{efc} W_{ef}^{ab} \rightarrow Z_{ijk}^{abc}$$



# Sometimes Tensors are Like Matrices

$$T^{efc}_{ijk} W^{ab}_{ef} \rightarrow Z^{abc}_{ijk}$$

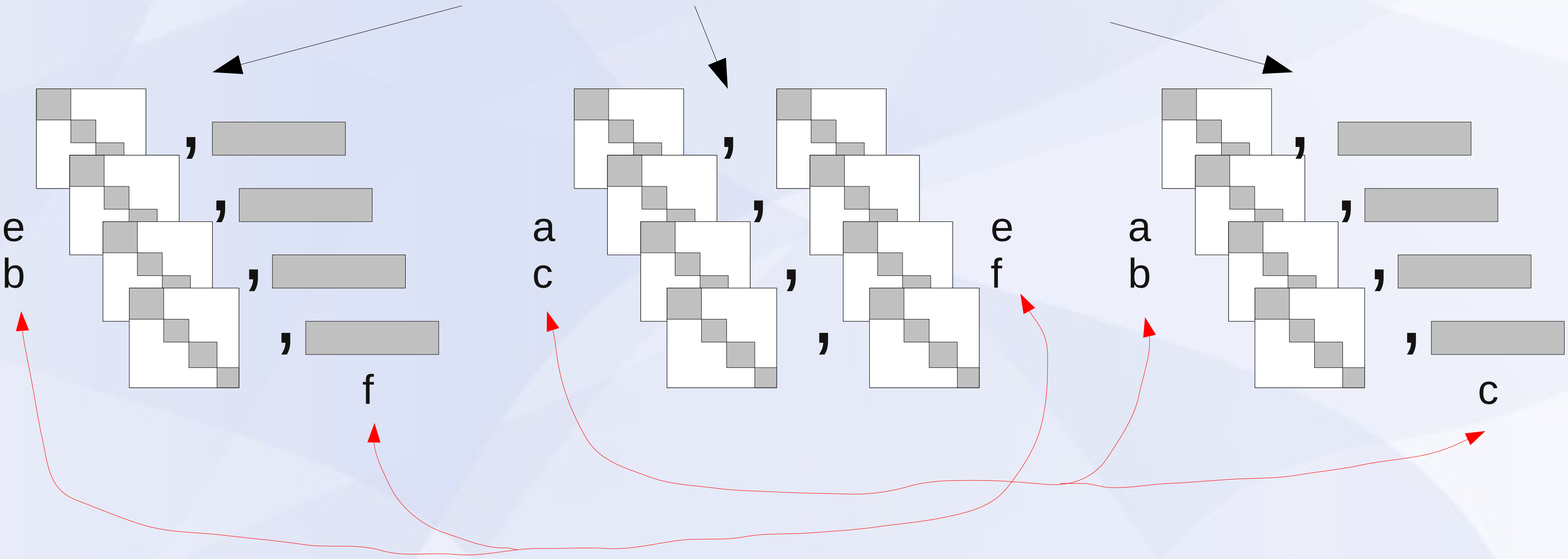


# And Sometimes They Are Not

$$T_{ijk}^{ebf} W_{ef}^{ac} \rightarrow Z_{ijk}^{abc}$$

# And Sometimes They Are Not

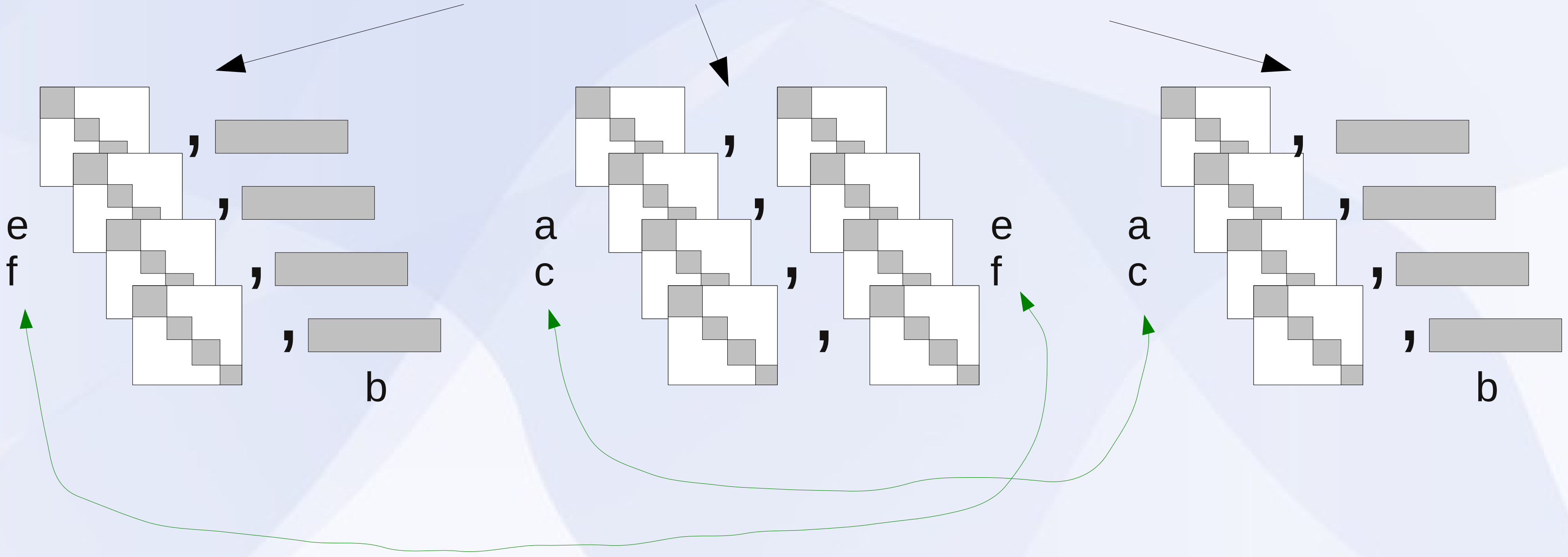
$$T^{ebf}_{ijk} W^{ac}_{ef} \rightarrow Z^{abc}_{ijk}$$



# And Sometimes They Are Not

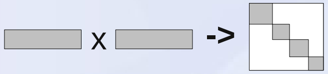
$$T^{ebf}_{ijk} W^{ac}_{ef} \rightarrow Z^{abc}_{ijk}$$

$$T^{efb}_{ikj} W^{ac}_{ef} \rightarrow Z^{acb}_{ikj}$$

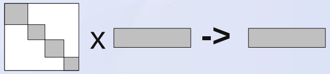


# DPD+GEMM Toolbox

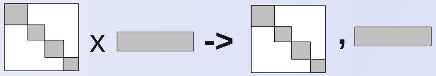
1x1 → 2



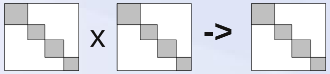
2x1 → 1



2x1 → 3

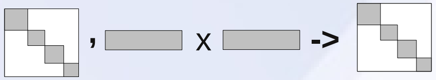


2x2 → 2



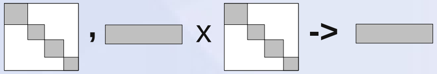
2x2 → 4

3x1 → 2

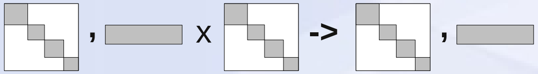


3x1 → 4

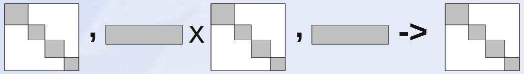
3x2 → 1



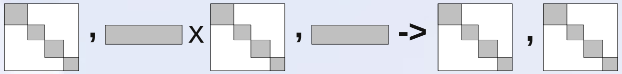
3x2 → 3



3x3 → 2

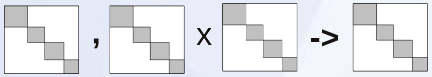


3x3 → 4

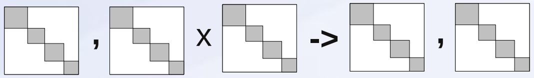


4x1 → 3

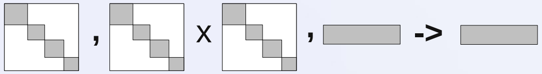
4x2 → 2



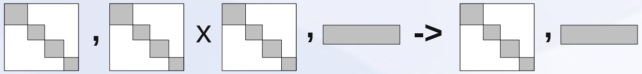
4x2 → 4



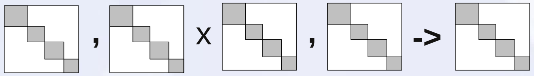
4x3 → 1



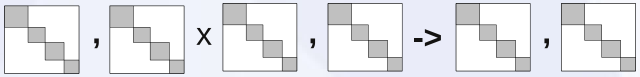
4x3 → 3



4x4 → 2



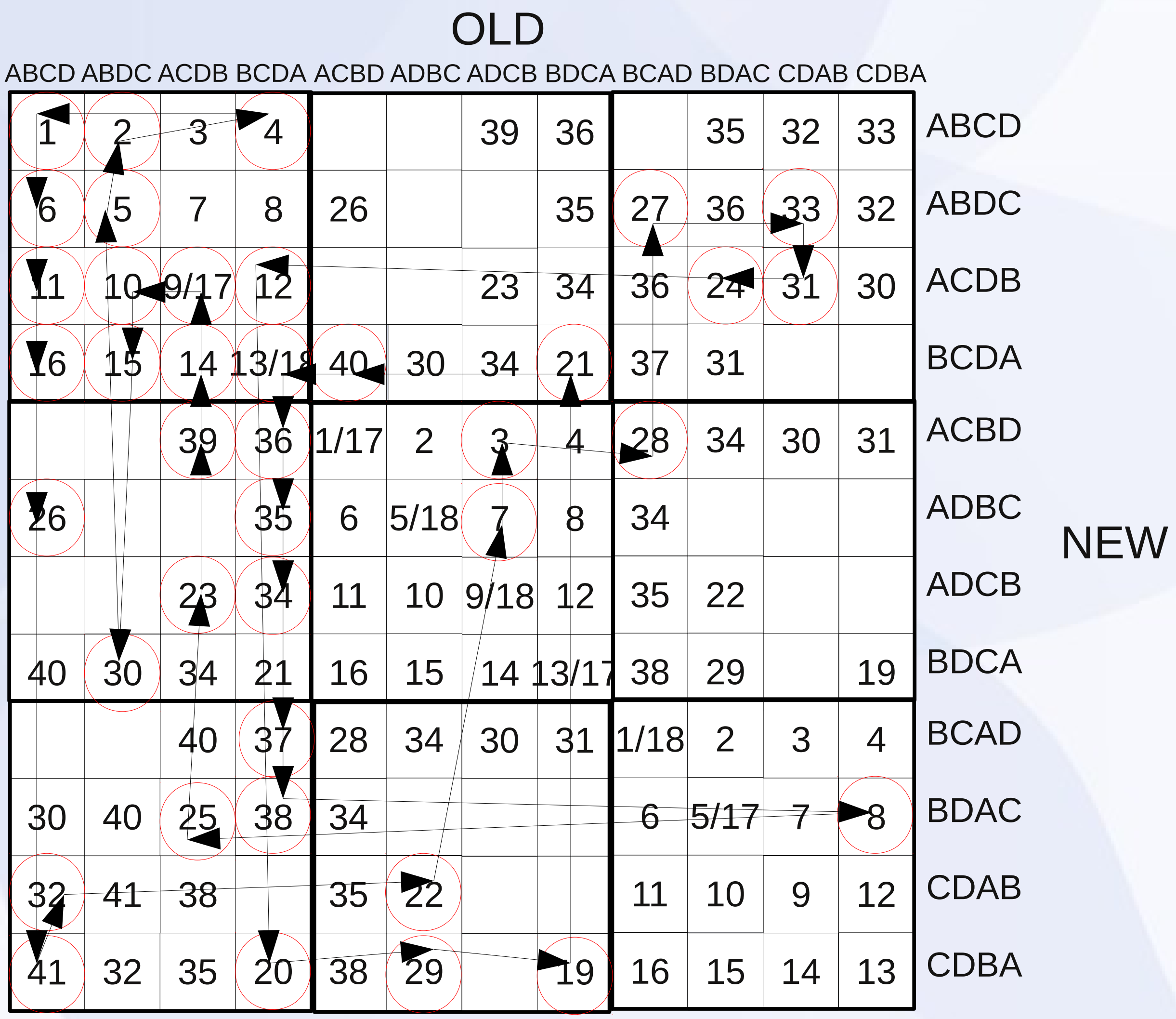
4x4 → 4



# CCSDTQ Magic Cycle

Minimum number of transposes required to make all necessary contractions amenable to GEMM.

Spin-summation must be repeated for each transpose since it does not preserve the full symmetry.



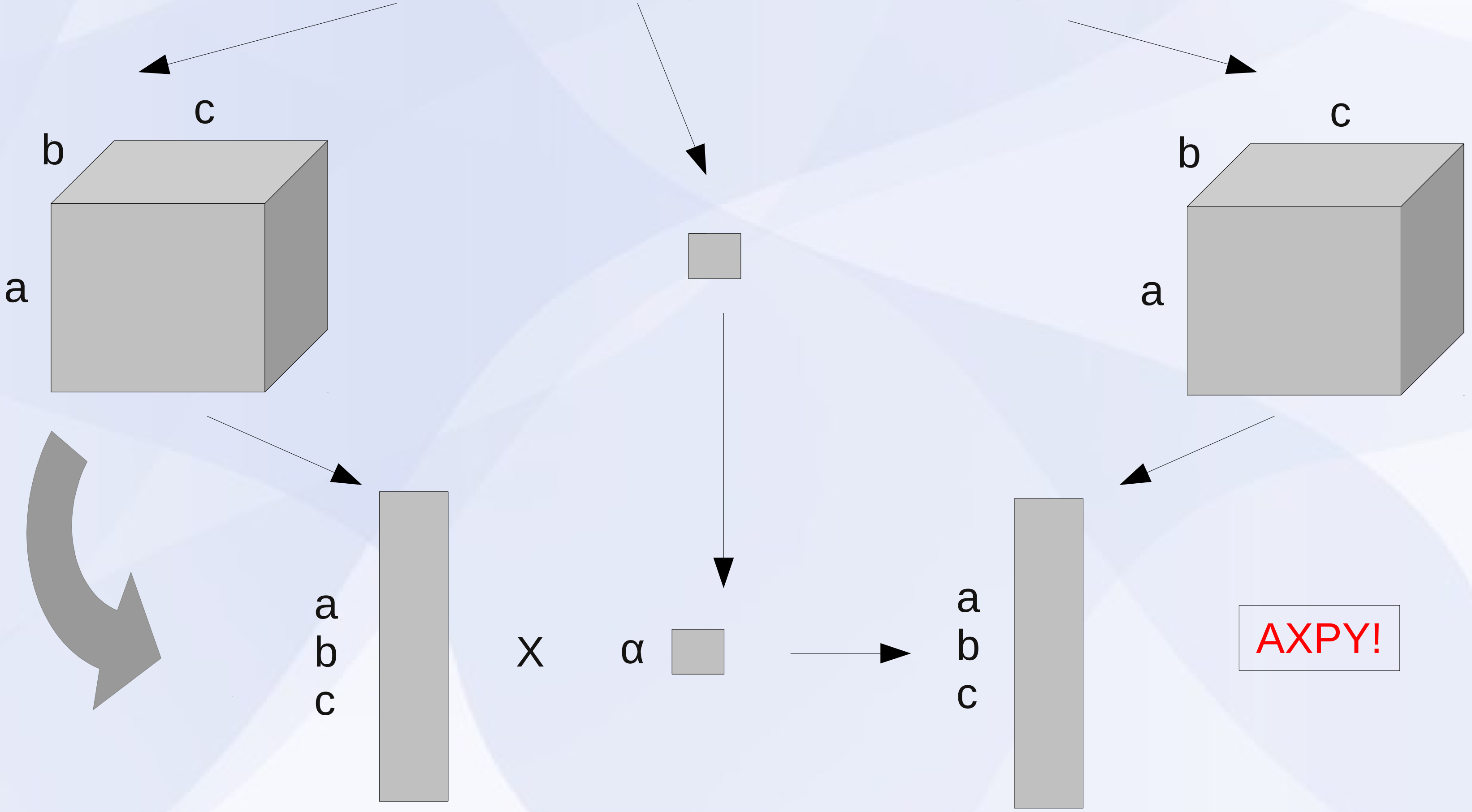
OLD

| | ABCD | ABDC | ACDB | BCDA | ACBD | ADBC | ADCB | BDCA | BCAD | BDAC | CDAB | CDBA |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ABCD | 1 | 2 | 3 | 4 | | | 39 | 36 | | 35 | 32 | 33 |
| ABDC | 6 | 5 | 7 | 8 | 26 | | | 35 | 27 | 36 | 33 | 32 |
| ACDB | 11 | 10 | 9/17 | 12 | | | 23 | 34 | 36 | 24 | 31 | 30 |
| BCDA | 16 | 15 | 14 | 13/18 | 40 | 30 | 34 | 21 | 37 | 31 | | |
| ACBD | | | 39 | 36 | 1/17 | 2 | 3 | 4 | 28 | 34 | 30 | 31 |
| ADBC | 26 | | | 35 | 6 | 5/18 | 7 | 8 | 34 | | | |
| ADCB | | | 23 | 34 | 11 | 10 | 9/18 | 12 | 35 | 22 | | |
| BDCA | 40 | 30 | 34 | 21 | 16 | 15 | 14 | 13/17 | 38 | 29 | | 19 |
| BCAD | | | 40 | 37 | 28 | 34 | 30 | 31 | 1/18 | 2 | 3 | 4 |
| BDAC | 30 | 40 | 25 | 38 | 34 | | | | 6 | 5/17 | 7 | 8 |
| CDAB | 32 | 41 | 38 | | 35 | 22 | | | 11 | 10 | 9 | 12 |
| CDBA | 41 | 32 | 35 | 20 | 38 | 29 | | 19 | 16 | 15 | 14 | 13 |

NEW

# Inefficient "GEMM"'s

$$T^{abc}_{mnk} W^{mn}_{ij} \rightarrow Z^{abc}_{ijk}$$



# The Real Impact

Speedup of NCC (new code) relative to MRCC:

| | HSOH | $H_2O$ | $H_2C_4H_2$ | $O_3$ | $FO_3^-$ |
|---|---|---|---|---|---|
| CCSDTQ | 6.2 | 4.4 | 5.2 | 6.2 | 4.9 |
| CCSDT(Q) | 33.1 | 102.6 | 18.2 | 28.7 | 17.2 |

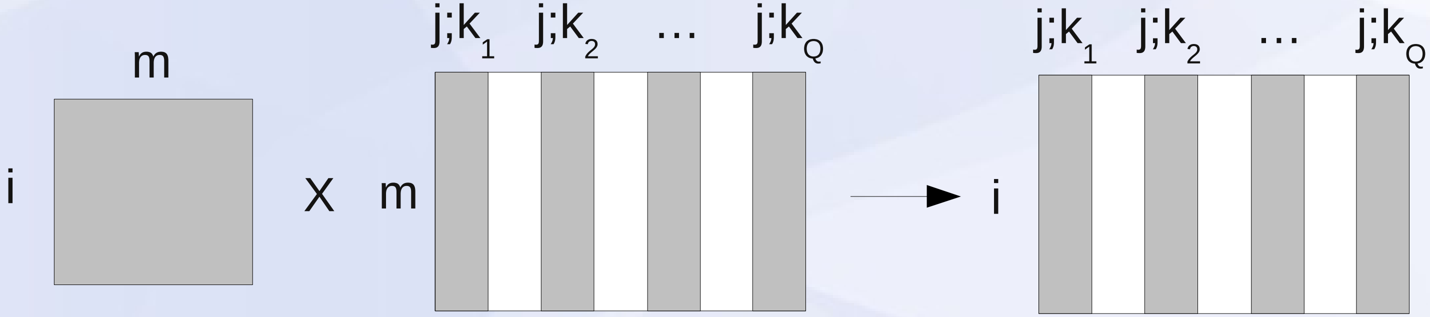
| Timing breakdown of (Q) by low-level operation | |
|---|---|
| Level 1 BLAS | 2.4% |
| Level 2 BLAS | 2.0% |
| Level 3 BLAS | 47.9% |
| Disk I/O | < 0.1% |
| Spin-summation | 3.7% |
| Transpose | 41.1% |

| Timing breakdown by low-level operation | |
|---|---|
| Level 1 BLAS | 10.9% |
| Level 2 BLAS | 0.9% |
| Level 3 BLAS | 45.5% |
| Disk I/O | 3.4% |
| Spin-summation | 13.0% |
| Transpose | 26.3% |

# How BLIS Can Help

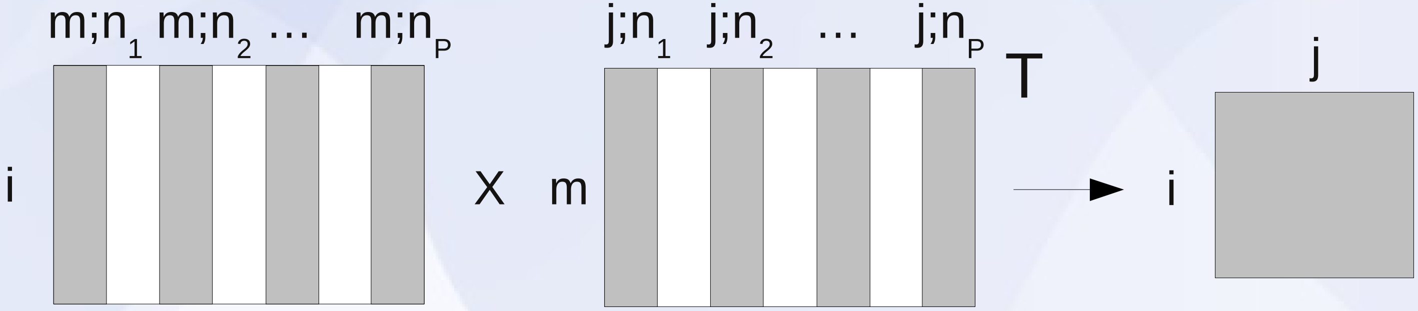
“Stacked GEMM”

$$C_{ij;k} := \beta C_{ij;k} + \alpha \sum_{m} A_{im} B_{mj;k}$$

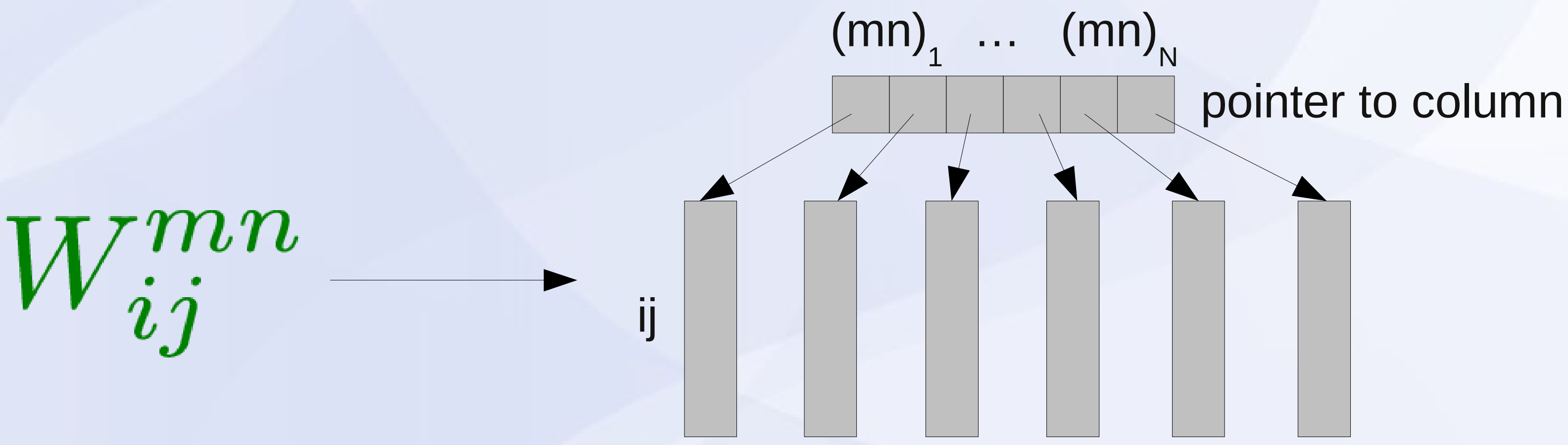


“Summed GEMM”

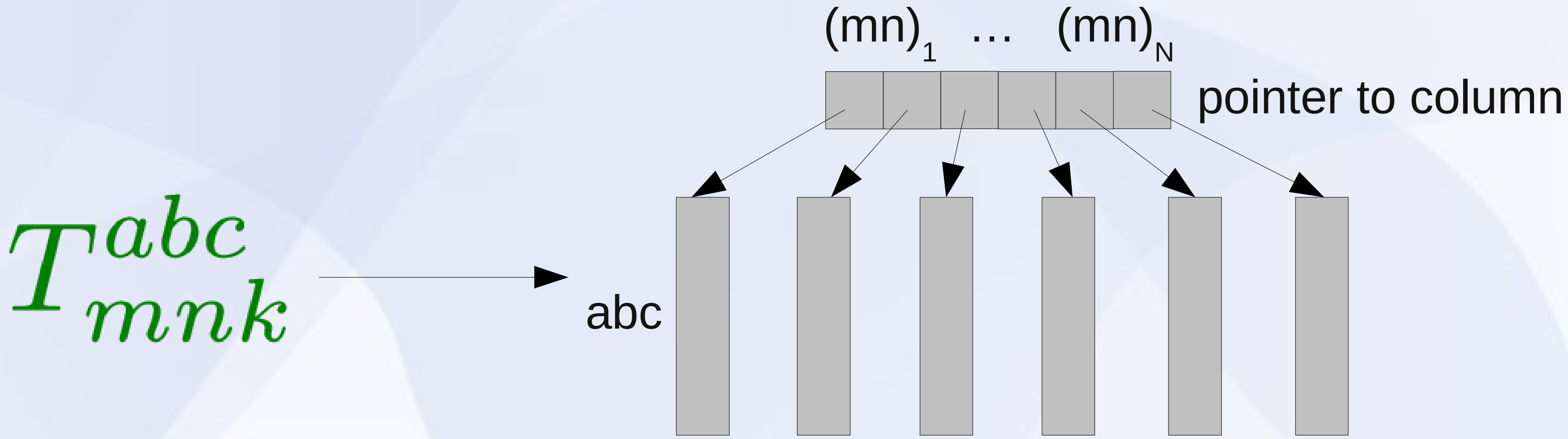
$$C_{ij} := \beta C_{ij} + \alpha \sum_{mn} A_{im;n} B_{mj;n}$$



# How BLIS Can Help

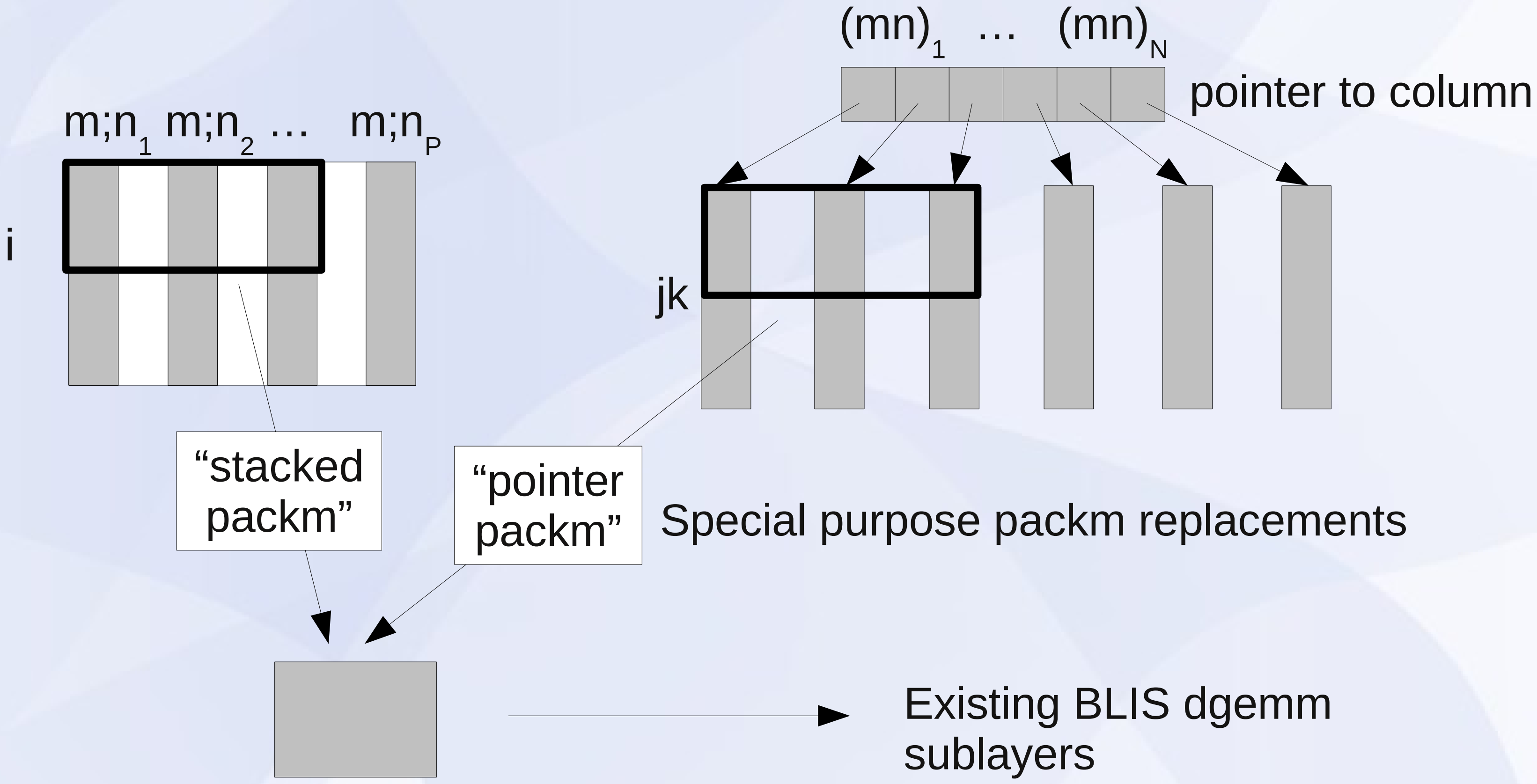


$$W_{ij}^{mn}$$



$$T_{mnk}^{abc}$$

# How BLIS Can Help



Special purpose packm replacements

Existing BLIS dgemm sublayers

packed panel/block

# Thanks

- Stanton Group
- FLAME Group
- Esp.: Field van Zee

NSF

DOE
CSGF