## Low Rank Bilinear Algorithms for Symmetric Tensor Contractions

Edgar Solomonik

ETH Zurich

SIAM PP, Paris, France April 14, 2016

#### Tensor contractions

For some  $s, t, v \ge 0$ , a tensor contraction of tensors A and B is

$$\textit{\textit{C}}_{\vec{i}\vec{j}} = \sum_{\vec{k}} \textit{\textit{A}}_{\vec{i}\vec{k}} \cdot \textit{\textit{B}}_{\vec{k}\vec{j}}, \quad \text{alternatively written,} \quad \textit{\textit{C}}_{\vec{j}}^{\vec{i}} = \sum_{\vec{k}} \textit{\textit{A}}_{\vec{k}}^{\vec{i}} \cdot \textit{\textit{B}}_{\vec{j}}^{\vec{k}},$$

where 
$$\vec{i} = \{i_1, \dots, i_s\}, \vec{j} = \{j_1, \dots, j_t\}$$
, and  $\vec{k} = \{k_1, \dots, k_v\}$ .

#### Matrix/vector examples:

- (s, t, v) = (0, 0, 1) vector inner product
- (s, t, v) = (1, 0, 1) matrix-vector multiplication
- (s, t, v) = (1, 1, 0) vector outer product
- (s, t, v) = (1, 1, 1) matrix-matrix multiplication
- (s, t, v) = (s, 1, 1) tensor-times-matrix

#### Applications of higher-order tensor contractions

Some applications of contractions of tensors of order at least three:

- tensor factorization algorithms, e.g. alternating least squares
- deep learning convolutional neural networks
- higher-order analysis of probabilistic correlation
- post-Hartree-Fock electronic structure, e.g. coupled cluster
- density matrix renormalization group (DMRG)

## Contractions in Coupled Cluster (CCSD method)

$$\begin{split} W_{ei}^{mn} &= V_{ei}^{mn} + \sum_{f} V_{ef}^{mn} t_{i}^{f}, \\ X_{ij}^{mn} &= V_{ij}^{mn} + P_{j}^{i} \sum_{e} V_{ie}^{mn} t_{i}^{e} + \frac{1}{2} \sum_{ef} V_{ef}^{mn} \tau_{ij}^{ef}, \\ U_{ie}^{am} &= V_{ie}^{am} - \sum_{n} W_{ei}^{mn} t_{n}^{a} + \sum_{f} V_{ef}^{ma} t_{i}^{f} + \frac{1}{2} \sum_{nf} V_{ef}^{mn} T_{in}^{af}, \\ Q_{ij}^{am} &= V_{ij}^{am} + P_{j}^{i} \sum_{e} V_{ie}^{am} t_{i}^{e} + \frac{1}{2} \sum_{ef} V_{ef}^{am} \tau_{ij}^{ef}, \\ Z_{i}^{a} &= f_{i}^{a} - \sum_{m} F_{i}^{m} t_{m}^{a} + \sum_{e} f_{e}^{a} t_{i}^{e} + \sum_{em} V_{ei}^{ma} t_{m}^{e} + \sum_{em} V_{im}^{ae} F_{e}^{m} + \frac{1}{2} \sum_{efm} V_{ef}^{am} \tau_{im}^{ef} \\ &- \frac{1}{2} \sum_{emn} W_{ei}^{mn} T_{mn}^{ea}, \\ Z_{ij}^{ab} &= V_{ij}^{ab} + P_{j}^{i} \sum_{e} V_{ie}^{ab} t_{j}^{e} + P_{b}^{a} P_{j}^{i} \sum_{me} U_{ie}^{am} T_{mj}^{eb} - P_{b}^{a} \sum_{m} Q_{ij}^{am} t_{m}^{b} \\ &+ P_{b}^{a} \sum_{e} F_{e}^{a} T_{ij}^{eb} - P_{j}^{i} \sum_{m} F_{i}^{m} T_{mj}^{ab} + \frac{1}{2} \sum_{ef} V_{ef}^{ab} \tau_{ij}^{ef} + \frac{1}{2} \sum_{mn} X_{ij}^{mn} \tau_{mn}^{ab}, \end{split}$$

where  $P_{y}^{x} f(x, y) := f(x, y) - f(y, x)$ 

### Exploiting symmetry in tensor contractions

Tensor symmetry (e.g.  $A_{ij} = A_{ji}$ ) reduces memory and cost

- for order d tensor, d! less memory
- dot product  $\sum_{i,j} A_{ij} B_{ij} = 2 \sum_{i < j} A_{ij} B_{ij} + \sum_i A_{ii} B_{ii}$
- matrix-vector multiplication  $(A_{ij} = A_{ji})$

$$c_i = \sum_j A_{ij}b_j = \sum_j A_{ij}(b_i + b_j) - \left(\sum_j A_{ij}\right)b_i$$

- $A_{ij}b_j \neq A_{ji}b_i$  but  $A_{ij}(b_i + b_j) = A_{ji}(b_j + b_i) \rightarrow (1/2)n^2$  multiplies
- partially-symmetric case:  $T_{ij}^{ab} = -T_{ji}^{ab}$

$$egin{aligned} W_{ic}^{ak} &= \sum_{j} \sum_{b} T_{ij}^{ab} V_{bc}^{jk} \ &= \sum_{j} \left( \sum_{b} T_{ij}^{ab} (V_{bc}^{ik} + V_{bc}^{jk}) \right) - \sum_{b} \left( \sum_{j} T_{ij}^{ab} \right) V_{bc}^{ik} \end{aligned}$$

•  $Z^{ak}_{ijc} = \sum_b T^{ab}_{ij} (V^{ik}_{bc} + V^{jk}_{bc}) = -Z^{ak}_{jic} o$  2x fewer operations

### Symmetry preserving algorithms

By exploiting symmetry, reduce multiplies (but increase adds)

rank-2 vector outer product

$$C_{ij} = a_i b_j + a_j b_i = (a_i + a_j)(b_i + b_j) - a_i b_i - a_j b_j$$

squaring a symmetric matrix A (or AB + BA)

$$C_{ij} = \sum_{k} A_{ik} A_{kj} = \sum_{k} (A_{ik} + A_{kj} + A_{ij})^{2} - \dots$$

• fully symmetric contraction of order s + v and v + t tensors

$$\frac{(s+t+v)!}{s!t!v!}$$
 fewer multiplies

e.g. cases above are

- (*s*, *t*, *v*) = (1, 1, 0) → reduction by 2X
- $(s, t, v) = (1, 1, 1) \rightarrow \text{reduction by } 6X$

### Applications of symmetry preserving algorithms

#### Extensions and applications:

- numerically stable by forward error bounds and experiments
- for Hermitian tensors, multiplies cost 3X more than adds
  - Hermitian matrix multiplication and tridiagonal reduction (BLAS and LAPACK routines) with 25% fewer operations
- cost reductions in partially-symmetric coupled cluster contractions:
   2X-9X for select contractions, 1.3X, 2.1X for CCSD, CCSDT
- $(2/3)n^3$  multiplies for squaring a *nonsymmetric* matrix

$$egin{aligned} X_{ ext{SY}} &:= rac{1}{2}(X + X^{\mathsf{T}}), \quad X_{ ext{AS}} &:= rac{1}{2}(X - X^{\mathsf{T}}), \ C &= AB + (A^{\mathsf{T}}B^{\mathsf{T}})^{\mathsf{T}} = AB + BA \ &= (A_{ ext{SY}}B_{ ext{SY}})_{ ext{SY}} + (A_{ ext{SY}}B_{ ext{AS}})_{ ext{AS}} + (A_{ ext{AS}}B_{ ext{SY}})_{ ext{AS}} + (A_{ ext{AS}}B_{ ext{SY}})_{ ext{AS}} + (A_{ ext{AS}}B_{ ext{AS}})_{ ext{SY}} \end{aligned}$$

four invocations of (s, t, v) = (1, 1, 1), squaring when A = B

#### Symmetry preserving blocking (sketch)

#### Multiplication of a symmetric matrix *A* and a nonsymmetric matrix *B*:

- classical approach, two choices:
  - treat A as nonsymmetric (unpack if stored as symmetric)
  - multiply by lower-triangle of A then by its transpose
- proposed new approach
  - fold  $n \times n$  matrix A into  $\sqrt{p} \times \frac{n}{\sqrt{p}} \times \sqrt{p} \times \frac{n}{\sqrt{p}}$  tensor T
  - note that  $T_{kl}^{ij} = T_{lk}^{ji}$ , define partially-symmetric  $Y_{kl}^{ij} = T_{kl}^{ij} + T_{lk}^{ij}$  and partially-antisymmetric  $S_{kl}^{ij} = T_{kl}^{ij} T_{lk}^{ij}$
  - use symmetry preserving alg. over indices of dims  $\sqrt{p} \times \sqrt{p}$ , results in p subproblems with symmetric matrices with dims  $\frac{n}{\sqrt{p}} \times \frac{n}{\sqrt{p}}$
- food for thought: keep folding/symmetrizing to 2 × · · · × 2 tensors
   → Hankel matrices (modulo sign interchanges)

#### Bilinear algorithms

Bilinear algorithms<sup>1</sup> for symmetric contractions

• a bilinear algorithm is defined by matrices  $F^{(A)}$ ,  $F^{(B)}$ ,  $F^{(C)}$ ,

$$c = F^{(C)}[(F^{(A)\mathsf{T}}a) \circ (F^{(B)\mathsf{T}}b)]$$

where o is the Hadamard (pointwise) product

- the number of rows in each matrix corresponds to the number of inputs (dimensions of a and b) and outputs (dimension of c)
- for clasiscal  $n \times n$  matrix multiplication  $F^{(A)}$ ,  $F^{(B)}$ ,  $F^{(C)}$  are  $n^2 \times n^3$  and have one unit entry per column
- number of columns in  $F^{(A)}$ ,  $F^{(B)}$ ,  $F^{(C)}$  is the bilinear algorithm rank

Pan, How to Multiply Matrices Faster, Springer, 1984

#### Bilinear algorithms as tensor factorizations

A bilinear algorithm corresponds to a CP tensor decomposition

$$c_{i} = \sum_{r=1}^{R} F_{ir}^{(C)} \left( \sum_{j} F_{jr}^{(A)} a_{j} \right) \left( \sum_{k} F_{kr}^{(B)} b_{k} \right)$$

$$= \sum_{j} \sum_{k} \left( \sum_{r=1}^{R} F_{ir}^{(C)} F_{jr}^{(A)} F_{kr}^{(B)} \right) a_{j} b_{k}$$

$$= \sum_{j} \sum_{k} T_{ijk} a_{j} b_{k} \quad \text{where} \quad T_{ijk} = \sum_{r=1}^{R} F_{ir}^{(C)} F_{jr}^{(A)} F_{kr}^{(B)}$$

For multiplication of  $n \times n$  matrices,

- T is  $n^2 \times n^2 \times n^2$
- classical algorithm has rank  $R = n^3$
- Strassen's algorithm has rank  $R \approx n^{\log_2(7)}$

#### Bilinear algorithms as tensor factorizations

A bilinear algorithm corresponds to a CP tensor decomposition

$$c_{i} = \sum_{r=1}^{R} F_{ir}^{(C)} \left( \sum_{j} F_{jr}^{(A)} a_{j} \right) \left( \sum_{k} F_{kr}^{(B)} b_{k} \right)$$

$$= \sum_{j} \sum_{k} \left( \sum_{r=1}^{R} F_{ir}^{(C)} F_{jr}^{(A)} F_{kr}^{(B)} \right) a_{j} b_{k}$$

$$= \sum_{j} \sum_{k} T_{ijk} a_{j} b_{k} \quad \text{where} \quad T_{ijk} = \sum_{r=1}^{R} F_{ir}^{(C)} F_{jr}^{(A)} F_{kr}^{(B)}$$

For symmetric tensor contractions (not counting diagonals)

- T is  $\binom{n}{s+t} \times \binom{n}{s+v} \times \binom{n}{v+t}$
- classical algorithm has rank  $R = \binom{n}{s} \binom{n}{t} \binom{n}{v}$
- symmetry preserving  $\to R \approx \binom{n}{s+t+\nu}$ , that is  $\frac{(s+t+\nu)!}{s!t!\nu!}$  less

## Expansion in bilinear algorithms

Given  $\Lambda = (F^{(A)}, F^{(B)}, F^{(C)})$ ,  $\Lambda_{\text{sub}} \subseteq \Lambda$  if  $\exists$  projection matrix P, so

$$\Lambda_{\text{sub}} = (F^{(A)}P, F^{(B)}P, F^{(C)}P),$$

the projection matrix extracts #cols(P) columns of each matrix.

A bilinear algorithm  $\Lambda$  has expansion bound  $\mathcal{E}_{\Lambda}:\mathbb{N}^3\to\mathbb{N},$  if for all

$$\Lambda_{\text{sub}} := (F_{\text{sub}}^{(A)}, F_{\text{sub}}^{(B)}, F_{\text{sub}}^{(C)}) \subseteq \Lambda$$

we have

$$\mathsf{rank}(\Lambda_{\mathsf{sub}}) \leq \mathcal{E}_{\Lambda}\left(\mathsf{rank}(\mathit{F}_{\mathsf{sub}}^{(\mathit{A})}), \mathsf{rank}(\mathit{F}_{\mathsf{sub}}^{(\mathit{B})}), \mathsf{rank}(\mathit{F}_{\mathsf{sub}}^{(\mathit{C})})\right)$$

For matrix mult., Loomis-Whitney inequality  $\to \mathcal{E}_{MM}(x,y,z) = \sqrt{xyz}$  For sym. pres.  $\mathcal{E}_{SP}^{(s,t,v)}(x,y,z) = O\Big(\min\big(x^{\frac{s+t+v}{s+v}},y^{\frac{s+t+v}{t+v}},z^{\frac{s+t+v}{s+t}}\big)\Big)$ 

### Communication in symmetry preserving algorithms

Communication lower bounds based on bilinear algorithm expansion

- horizontal comm. max data sent or received
- vertical comm. max data moved between memory and cache

For contraction of order s + v tensor with order v + t tensor

- matrix-vector-like algorithms (min(s, t, v) = 0)
  - vertical communication dominated by largest tensor
  - horizontal communication asymptotically greater if only unique elements are stored and  $s \neq t \neq v$
- matrix-matrix-like algorithms (min(s, t, v) > 0)
  - vertical and horizontal communication costs asymptotically greater for symmetry preserving algorithm when  $s \neq t \neq v$

#### Conclusion

#### Summary:

- symmetry preserving algorithms reduce cost of contractions
- they have been tested using Cyclops Tensor Framework https://github.com/solomonik/ctf
- rank structure of bilinear algorithms yields communication bounds

#### Future work:

- communication lower bounds for partially-symmetric cases
- high performance implementation

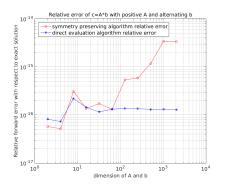
Related work: J. Noga and P. Valiron, Improved algorithm for triple-excitation contributions within the coupled cluster approach, Molecular Physics, 103 (2005).

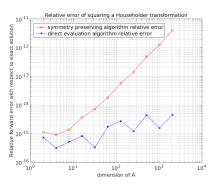
References (for more, email solomonik@inf.ethz.ch):

- E.S. and J. Demmel; Contracting symmetric tensors using fewer multiplications; ETH Zurich, 2015
- E.S., J. Demmel, and T. Hoefler; Communication lower bounds for tensor contraction algorithms; ETH Zurich, 2015

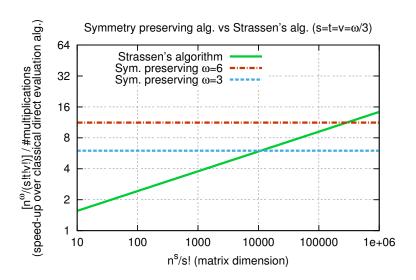
## Backup slides

### Stability of symmetry preserving algorithms





# Symmetry preserving algorithm vs Strassen's algorithm



#### A library for tensor computations

#### Cyclops Tensor Framework

- implicit for loops based on index notation (Einstein summation)
- matrix sums, multiplication, Hadamard product (tensor contractions)
- distributed symmetric-packed/sparse storage via cyclic layout

Jacobi iteration (solves Ax = b iteratively) example code snippet

#### Coupled cluster using CTF

Extracted from Aquarius (Devin Matthews' code, https://github.com/devinamatthews/aquarius)

```
FMI["mi"] += 0.5*WMNEF["mnef"]*T2["efin"];
WMNIJ["mnij"] += 0.5*WMNEF["mnef"]*T2["efij"];
FAE["ae"] -= 0.5*WMNEF["mnef"]*T2["afmn"];
WAMEI["amei"] -= 0.5*WMNEF["mnef"]*T2["afin"];

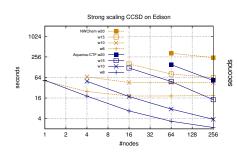
Z2["abij"] = WMNEF["ijab"];
Z2["abij"] += FAE["af"]*T2["fbij"];
Z2["abij"] -= FMI["ni"]*T2["abnj"];
Z2["abij"] += 0.5*WABEF["abef"]*T2["efij"];
Z2["abij"] += 0.5*WMNIJ["mnij"]*T2["abmn"];
Z2["abij"] -= WAMEI["amei"]*T2["ebmj"];
```

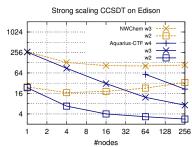
CTF is used within Aquarius, QChem, VASP, and Psi4

#### Comparison with NWChem

NWChem is the most commonly-used distributed-memory quantum chemistry method suite

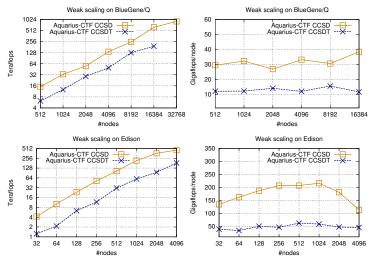
- provides Coupled Cluster methods: CCSD and CCSDT
- derives equations via Tensor Contraction Engine (TCE)
- generates contractions as blocked loops leveraging Global Arrays





### Coupled cluster on IBM BlueGene/Q and Cray XC30

CCSD up to 55 (50) water molecules with cc-pVDZ CCSDT up to 10 water molecules with cc-pVDZ<sup>a</sup>



<sup>&</sup>lt;sup>a</sup>S., Matthews, Hammond, Demmel, JPDC, 2014

### Coupled cluster methods

Coupled cluster provides a systematically improvable approximation to the manybody time-independent Schrödinger equation  $H|\Psi\rangle=E|\Psi\rangle$ 

- the Hamiltonian has one- and two- electron components H = F + V
- Hartree-Fock (SCF) computes mean-field Hamiltonian: F, V
- Coupled-cluster methods (CCSD, CCSDT, CCSDTQ) consider transitions of (doubles, triples, and quadruples) of electrons to unoccupied orbitals, encoded by tensor operator,

$$T = T_1 + T_2 + T_3 + T_4$$

- they use an exponential ansatz for the wavefunction,  $\Psi = e^T \phi$  where  $\phi$  is a Slater determinant
- expanding  $0 = \langle \phi' | H | \Psi \rangle$  yields nonlinear equations for  $\{T_i\}$  in F, V

$$0 = V_{ij}^{ab} + P(a,b) \sum_{e} T_{ij}^{ae} F_{e}^{b} - \frac{1}{2} P(i,j) \sum_{mnef} T_{im}^{ab} V_{ef}^{mn} T_{jn}^{ef} + \dots$$

where P is an antisymmetrization operator

#### Vertical communication in bilinear algorithms

Any schedule on a sequential machine with a cache of size H for  $\Lambda = (F^{(A)}, F^{(B)}, F^{(C)})$  with expansion bound  $\mathcal{E}_{\Lambda}$  has vertical communication cost,

$$Q_{\Lambda} \geq \max \left[ \frac{2 \operatorname{rank}(\Lambda) H}{\mathcal{E}_{\Lambda}^{\max}(H)}, \#\operatorname{rows}(F^{(A)}) + \#\operatorname{rows}(F^{(B)}) + \#\operatorname{rows}(F^{(C)}) \right]$$

where 
$$\mathcal{E}^{\max}_{\Lambda}(H) := \max_{c^{(A)}, c^{(B)}, c^{(C)} \in \mathbb{N}, c^{(A)} + c^{(B)} + c^{(C)} = 3H} \mathcal{E}_{\Lambda}(c^{(A)}, c^{(B)}, c^{(C)})$$

### Vertical communication in matrix multiplication

For the classical (non-Strassen-like) matrix multiplication algorithm of m-by-k matrix A with k-by-n matrix B into m-by-n matrix C,

$$\mathcal{E}_{\mathsf{MM}}(c^{(A)},c^{(B)},c^{(C)}) = (c^{(A)}c^{(B)}c^{(C)})^{1/2}$$

further, we have

$$\mathcal{E}_{\mathrm{MM}}^{\mathrm{max}}(H) = \max_{c^{(A)}, c^{(B)}, c^{(C)} \in \mathbb{N}, c^{(A)} + c^{(B)} + c^{(C)} < 3H} (c^{(A)}c^{(B)}c^{(C)})^{1/2} = H^{3/2}$$

so we obtain the expected bound,

$$\begin{aligned} Q_{\text{MM}} &\geq \max \left[ \frac{2 \operatorname{rank}(\text{MM}) H}{\mathcal{E}_{\text{MM}}^{\text{max}}(H)}, \# \operatorname{rows}(F^{(A)}) + \# \operatorname{rows}(F^{(B)}) + \# \operatorname{rows}(F^{(C)}) \right] \\ &= \max \left[ \frac{2 \operatorname{mnk}}{\sqrt{H}}, \operatorname{mk} + \operatorname{kn} + \operatorname{mn} \right] \end{aligned}$$

#### Horizontal communication in bilinear algorithms

Any load balanced schedule on a parallel machine with p processes of  $\Lambda = (F^{(A)}, F^{(B)}, F^{(C)})$  with expansion bound  $\mathcal{E}_{\Lambda}$  has horizontal communication cost,

$$W_{\Lambda} \geq c^{(A)} + c^{(B)} + c^{(C)}$$

for some (communicated amounts)  $c^{(A)}, c^{(B)}, c^{(C)} \in \mathbb{N}$  such that,

$$\operatorname{\mathsf{rank}}(\Lambda)/p \leq \mathcal{E}_{\Lambda}(c^{(A)} + \#\operatorname{\mathsf{rows}}(F^{(A)})/p, \ c^{(B)} + \#\operatorname{\mathsf{rows}}(F^{(B)})/p, \ c^{(C)} + \#\operatorname{\mathsf{rows}}(F^{(C)})/p)$$

#### Horizontal communication in matrix multiplication

For the classical (non-Strassen-like) matrix multiplication algorithm of m-by-k matrix A with k-by-n matrix B into m-by-n matrix C on a parallel machine of p processors,

$$W_{\text{MM}} = \Omega\left(W_{\text{O}}(\min(m, n, k), \operatorname{median}(m, n, k), \max(m, n, k), p)\right)$$

where

$$W_{O}(x, y, z, p) = \begin{cases} \left(\frac{xyz}{p}\right)^{2/3} &: p > yz/x^{2} \\ x\left(\frac{yz}{p}\right)^{1/2} &: yz/x^{2} \ge p > z/y \\ xy &: z/y \ge p \end{cases}$$

# Communication lower bounds for direct evaluation of symmetric contractions

An expansion bound on  $\Psi^{(s,t,v)}$  is

$$\mathcal{E}_{\Psi}^{(s,t,v)}(c^{(A)},c^{(B)},c^{(C)})=q\left(c^{(A)}c^{(B)}c^{(C)}\right)^{1/2},$$

where 
$$q = \left[\binom{s+v}{s}\binom{v+t}{v}\binom{s+t}{s}\right]^{1/2}$$
.

Therefore, the same (asymptotically) horizontal and vertical communication lower bounds apply for  $\Psi^{(s,t,v)}$  as for a matrix multiplication with dimensions  $n^s \times n^t \times n^v$ .

# Communication lower bounds for direct evaluation of symmetric contractions

Another expansion bound on  $\Psi^{(s,t,0)}$  (when v=0) is

$$\mathcal{E}_{\Psi}^{(s,t,0)}(c^{(A)},c^{(B)},c^{(C)}) = \left(\binom{\omega}{s} - 1\right)c^{(C)} + \min\left((c^{(A)})^{\omega/s},(c^{(B)})^{\omega/t},c^{(C)}\right)$$

There are also symmetric bounds when s=0 or t=0. When exactly one of s, t, v is zero, any load balanced schedule of  $\Psi^{(s,t,v)}$  on a parallel machine with p processors has horizontal communication cost.

$$extbf{\textit{W}}_{\Psi} = \Omega \left( ( extit{\textit{n}}^{\omega}/ extit{\textit{p}})^{\mathsf{max}( extit{\textit{s}},t, extit{\textit{v}})/\omega} 
ight)$$

This can be greater than the corresponding nonsymmetric bound,

$$W_{\Psi} = \Omega\left((n^{\omega}/p)^{1/2}\right)$$

# Communication lower bounds for the symmetry preserving algorithm

An expansion bound on  $\Phi^{(s,t,v)}$  is

$$\mathcal{E}_{\Phi}^{(s,t,v)}(c^{(A)},c^{(B)},c^{(C)}) = \min\left(\left(inom{\omega}{t}c^{(A)}
ight)^{rac{\omega}{s+v}}, \ \left(inom{\omega}{s}c^{(B)}
ight)^{rac{\omega}{s+t}}, \ \left(inom{\omega}{v}c^{(C)}
ight)^{rac{\omega}{s+t}}
ight)$$

This yields communication bounds with  $\kappa := \max(s + v, v + t, s + t)$ ,

$$Q_{\Phi} = \Omega \left( \frac{n^{\omega} H}{H^{\omega/\kappa}} + n^{\kappa} \right) \qquad W_{\Phi} = \begin{cases} \Omega \left( (n^{\omega}/p)^{\kappa/\omega} \right) &: s, t, v > 0 \\ \Omega \left( (n^{\omega}/p)^{\max(s,t,v)/\omega} \right) &: \kappa = \omega \end{cases}$$

#### Nesting of bilinear algorithms

Given two bilinear algorithms:

$$\begin{split} &\Lambda_1 = & (F_1^{(A)}, F_1^{(B)}, F_1^{(C)}) \\ &\Lambda_2 = & (F_2^{(A)}, F_2^{(B)}, F_2^{(C)}) \end{split}$$

We can nest them by computing their tensor product

$$\begin{split} &\Lambda_1 \otimes \Lambda_2 := & (F_1^{(A)} \otimes F_2^{(A)}, F_1^{(B)} \otimes F_2^{(B)}, F_1^{(C)} \otimes F_2^{(C)}) \\ & \text{rank}(\Lambda_1 \otimes \Lambda_2) = & \text{rank}(\Lambda_1) \cdot \text{rank}(\Lambda_2) \end{split}$$

### Communication lower bounds for nested algorithms

Conjecture: if bilinear algorithms  $\lambda_1$  and  $\lambda_2$  have expansion bounds  $\mathcal{E}_1$  and  $\mathcal{E}_2$ , then  $\lambda_1 \otimes \lambda_2$  has expansion bound,  $\mathcal{E}_{12}(c^{(A)}, c^{(B)}, c^{(C)})$ 

$$= \max_{\substack{c_1^{(A)}, c_1^{(B)}, c_1^{(C)}, c_2^{(A)}, c_2^{(B)}, c_2^{(C)} \in \mathbb{N} \\ c_1^{(A)}c_2^{(A)} = c^{(A)}, c_1^{(B)}c_2^{(B)} = c^{(B)}, c_1^{(C)}c_2^{(C)} = c^{(C)}}} \left[ \mathcal{E}_1(c_1^{(A)}, c_1^{(B)}, c_1^{(C)}) \mathcal{E}_2(c_2^{(A)}, c_2^{(B)}, c_2^{(C)}) \mathcal{E}_2(c_2^{(A)}, c_2^{(B)}, c_2^{(C)}) \right]$$

Simplified conjecture: consider matrices A and B, such that for some  $\alpha, \beta \in [0, 1]$  and any  $k \in \mathbb{N}$ 

- any subset of k columns of A has rank at least  $k^{\alpha}$
- any subset of k columns of B has rank at least  $k^{\beta}$

then any subset of  $k \in \mathbb{N}$  columns of  $A \otimes B$  has rank at least  $k^{\min(\alpha,\beta)}$ 

The first conjecture would provide lower bounds for the nested algorithms we wish to use for partially-symmetric coupled-cluster contractions.