Algorithms as Multilinear Tensor Equations

Edgar Solomonik

Department of Computer Science
ETH Zurich

Georgia Institute of Technology, Atlanta GA, USA

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Pervasive paradigms in scientific computing

What commonalities exist among resource-intensive computations in simulation and data analysis?

- multidimensional datasets (observations, discretizations)
- higher-order relations between datasets, i.e. equations, maps, graphs, hypergraphs
- **sparsity** and **symmetry** in structure of relations
- relations lead to solution directly or by acting as an evolutionary (iterative) criterion
- **algebraic descriptions of datasets and relations**

Pervasive paradigms in scientific computing

What type of abstractions are desirable in high performance computing?

- data abstractions should reflect native dimensionality and structure
- global functional abstractions should efficiently orchestrate **communication** and **synchronization**
- **abstractions should enable development of provably efficient algorithms**

Outline

Introduction to tensor computations

Symmetry-preserving tensor algorithms

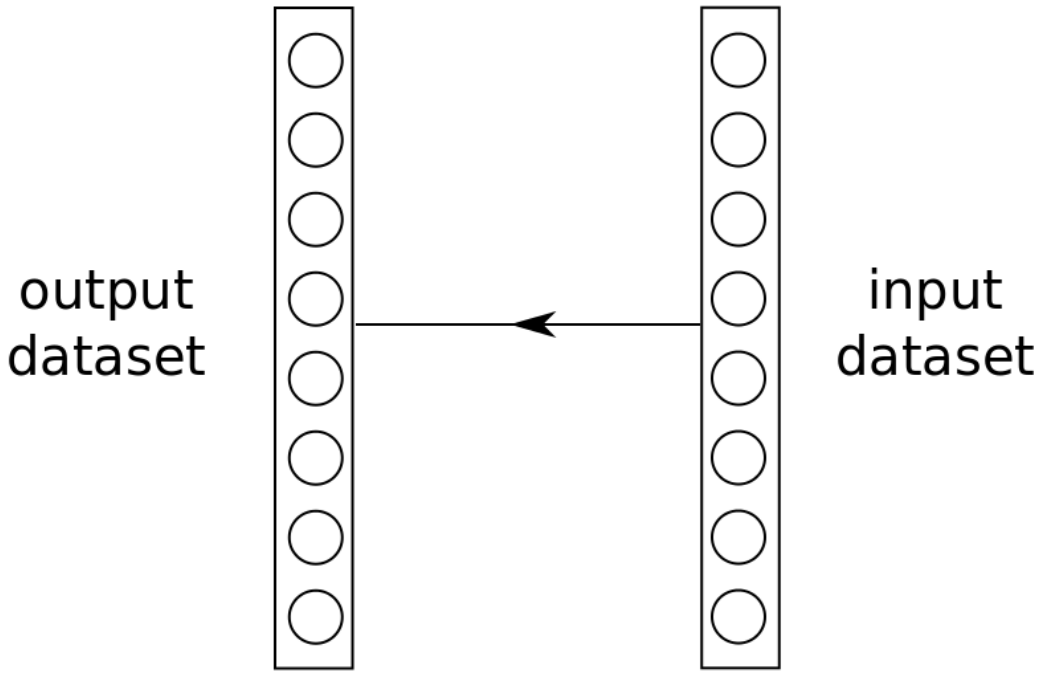
Communication-avoiding parallel algorithms

A massively-parallel tensor framework

Applications to electronic structure calculations

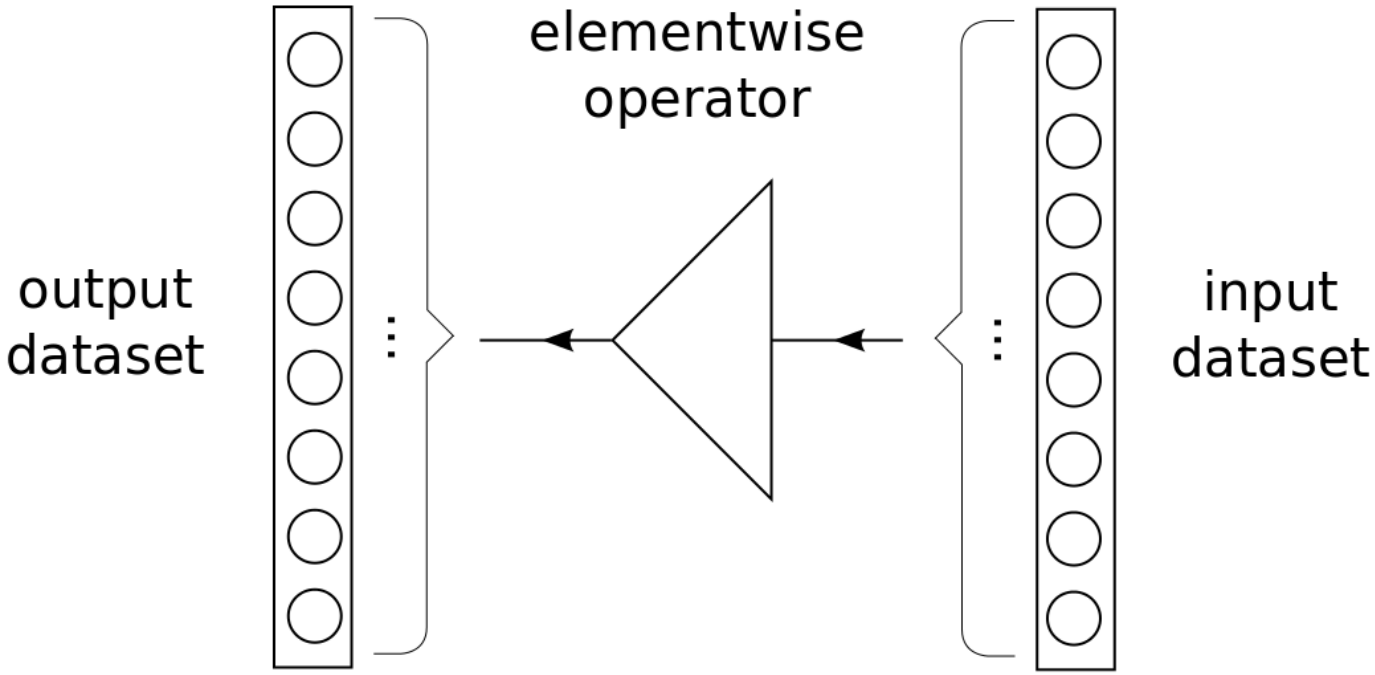
Conclusion

Basic data (vector) parallelism



Basic data (vector) parallelism

$$c_i = f(a_i)$$



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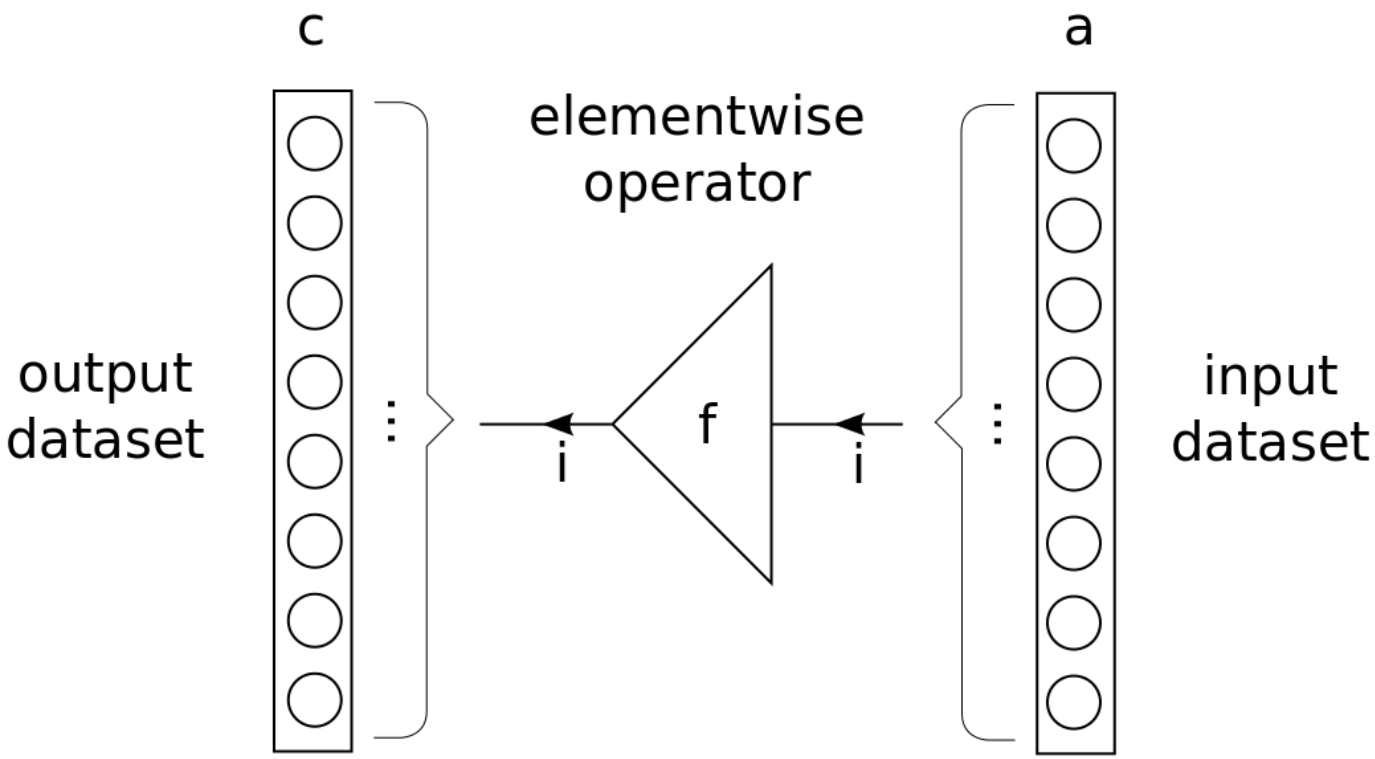
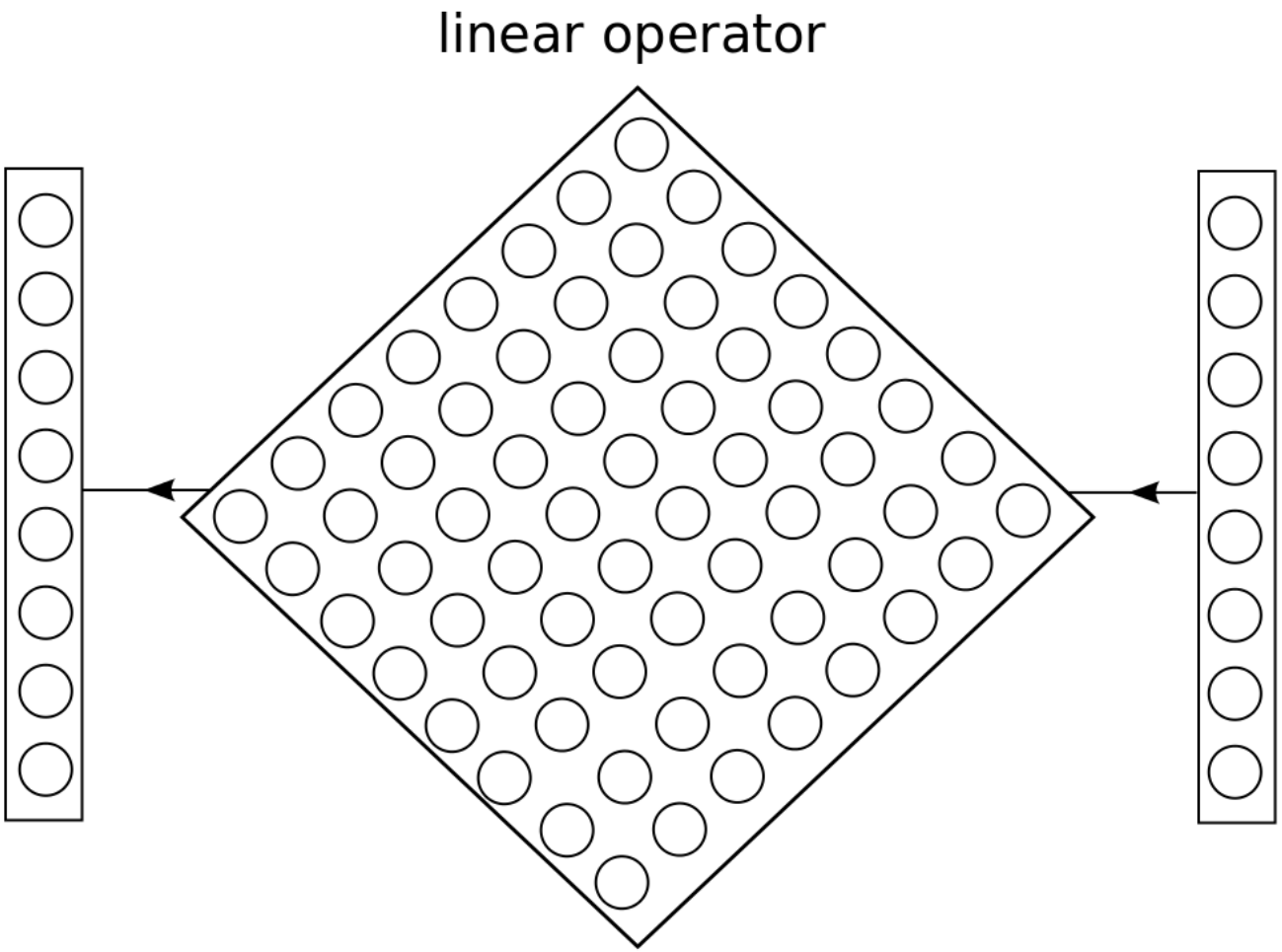


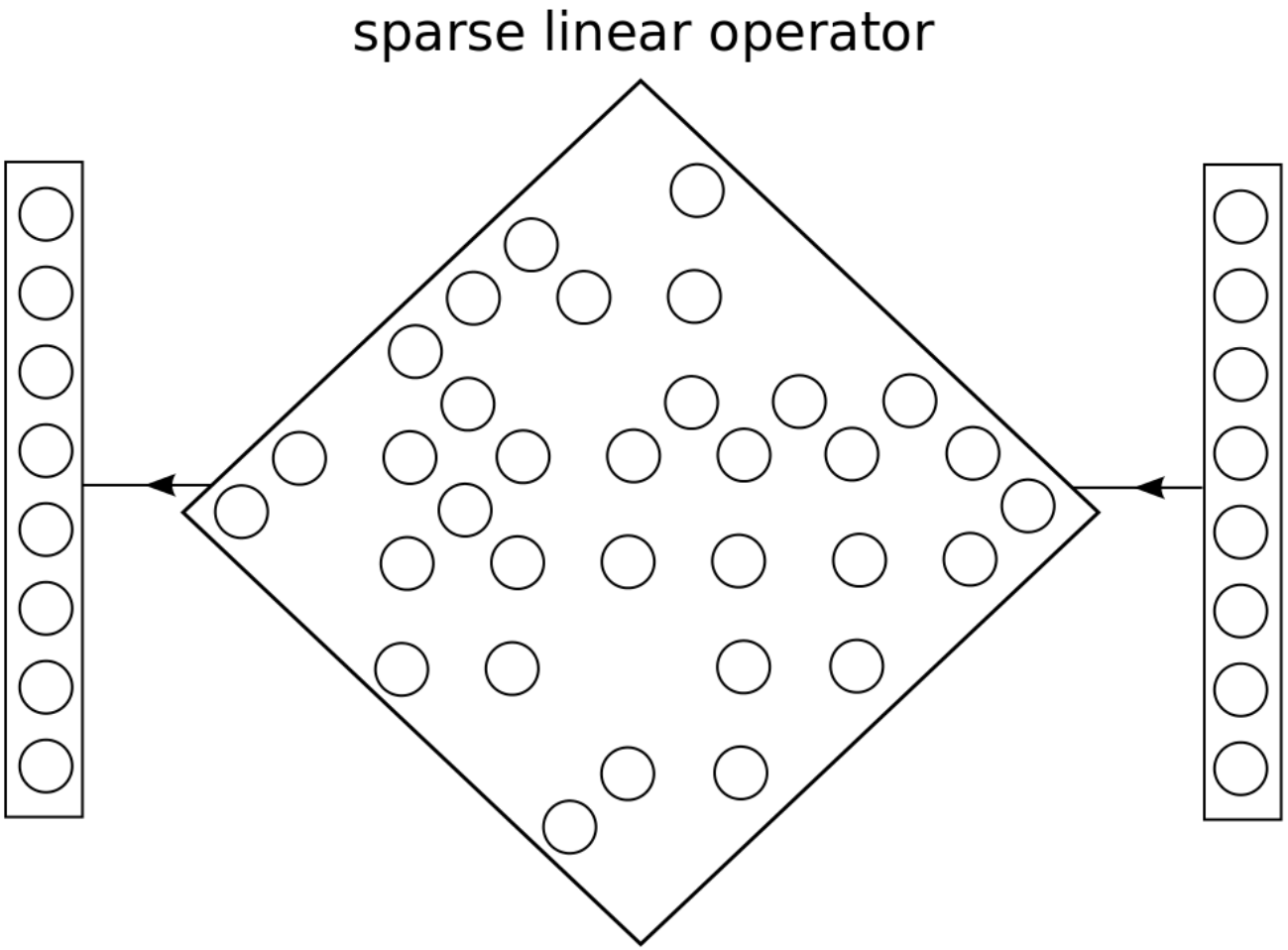
Dense matrix operators

$$\mathbf{c} = \mathbf{A}\mathbf{b}$$



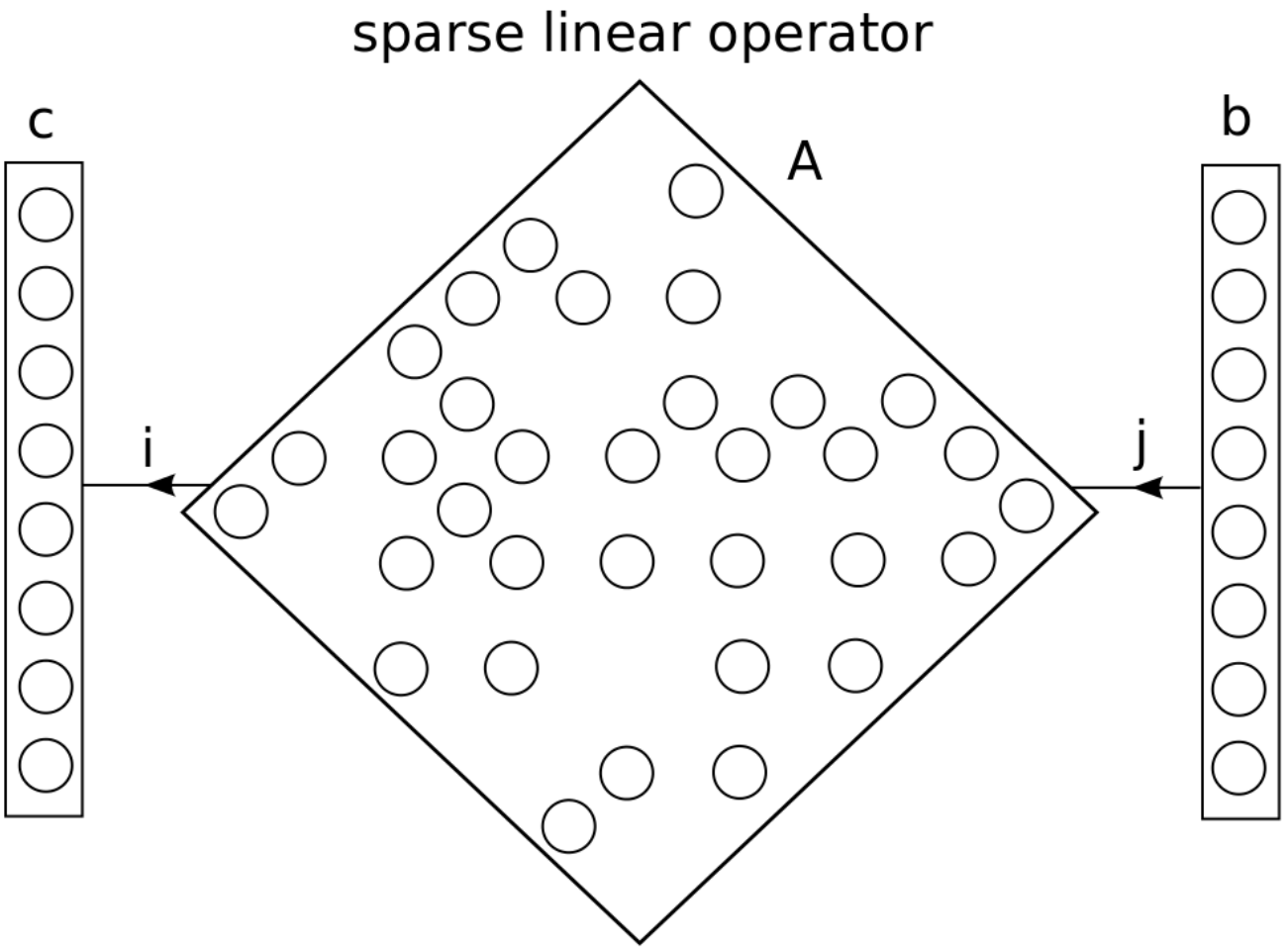
Sparse matrix operators

$$\mathbf{c} = \mathbf{A}\mathbf{b}$$



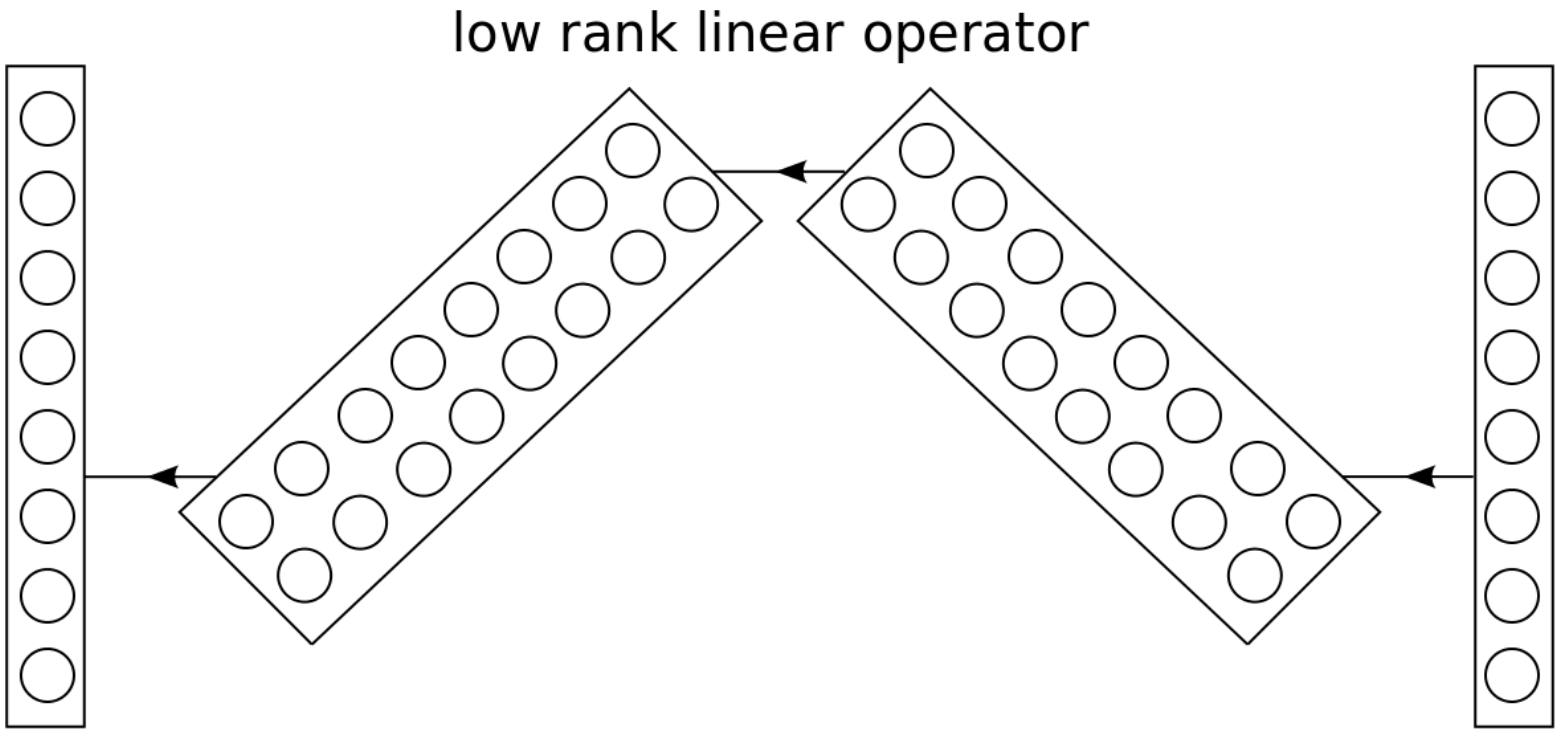
Sparse matrix operators

$$c_i = \sum_j A_{ij} b_j$$



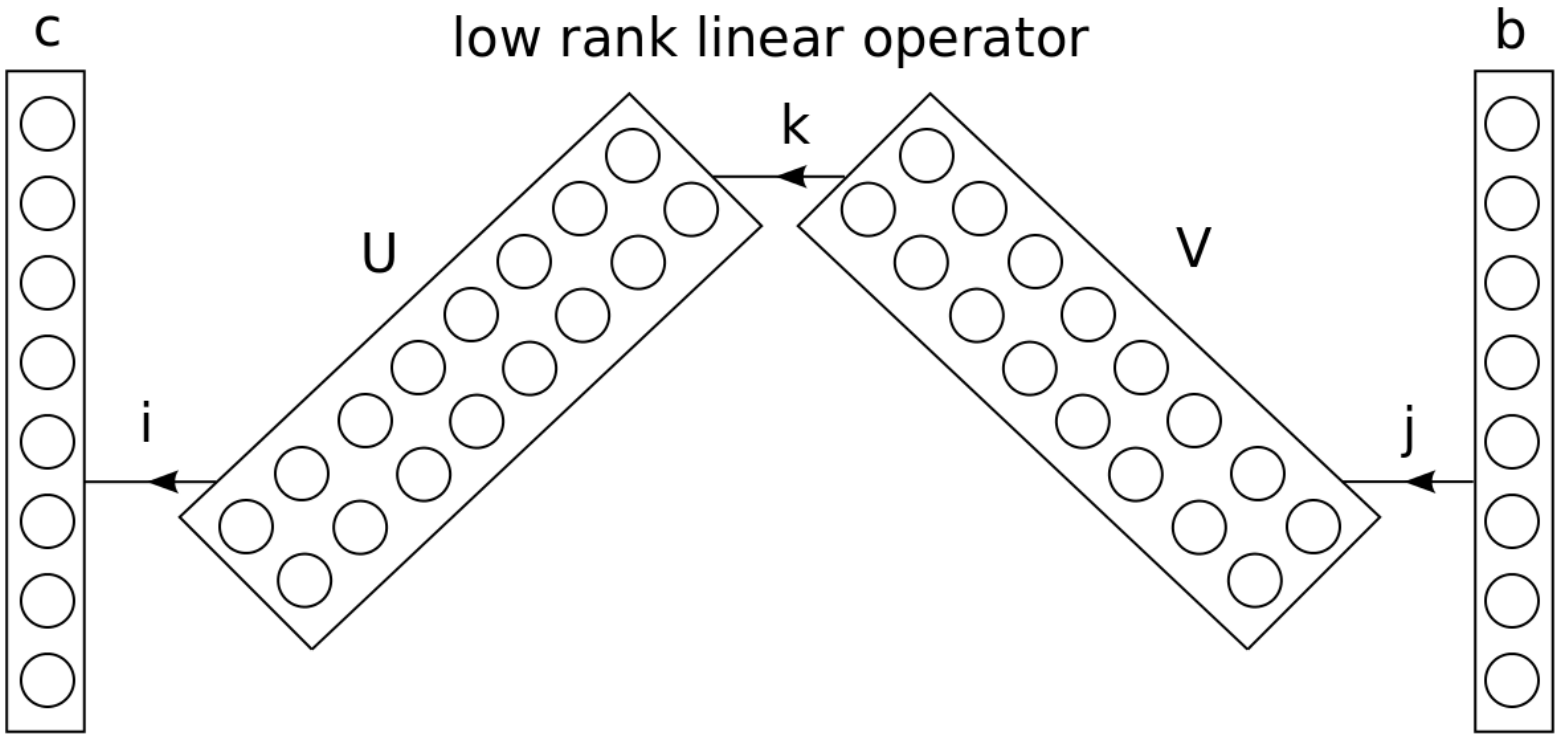
Low-rank matrix factorizations

$$\mathbf{A} = \mathbf{UV} \quad \rightarrow \quad \mathbf{c} = \mathbf{UVb}$$



Low-rank matrix factorizations

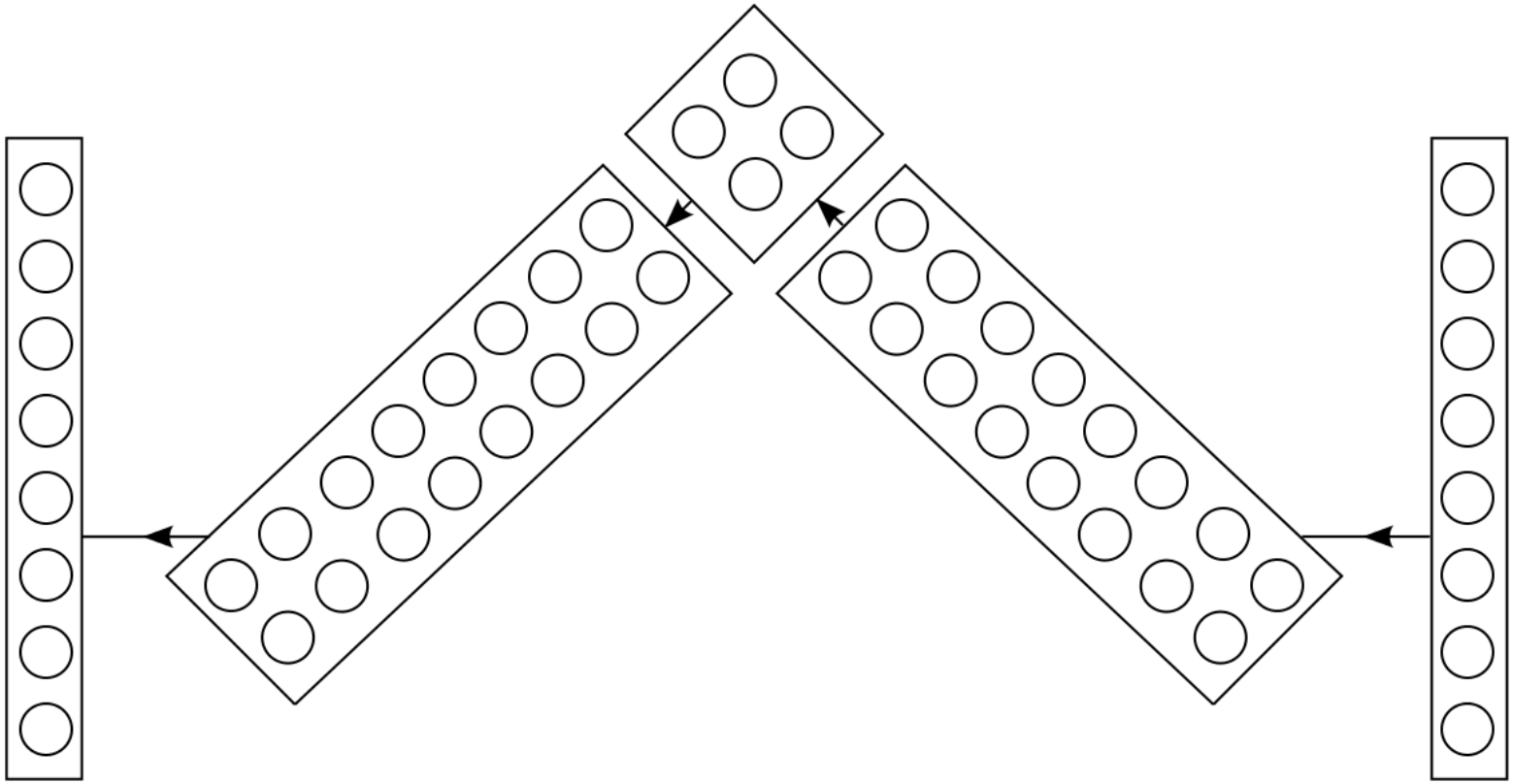
$$A_{ij} = \sum_k U_{ik} V_{kj} \quad \rightarrow \quad c_i = \sum_{j,k} U_{ik} V_{kj} b_j$$



Low-rank matrix factorizations

$$\mathbf{c} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}\mathbf{b}$$

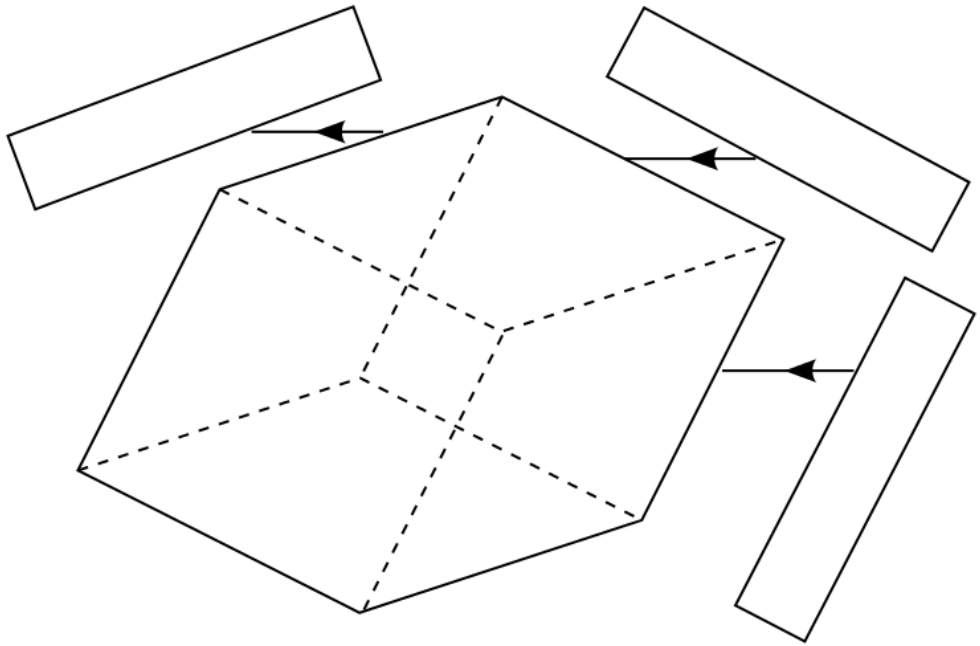
low rank linear operator



Tensor operator

$$d_i = \sum_{j,k} A_{ijk} b_j c_k$$

multilinear operator



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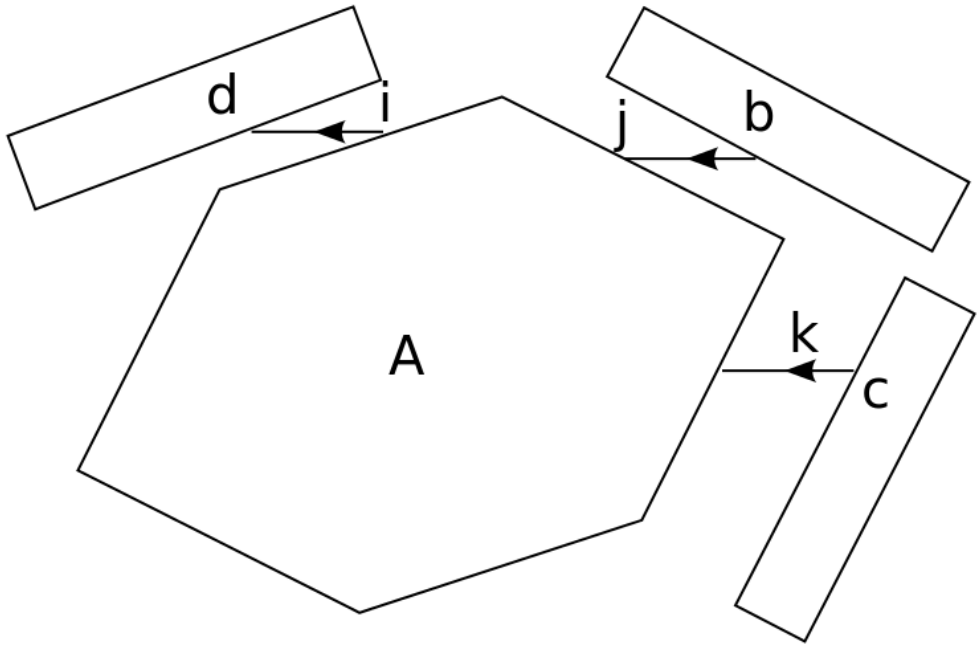
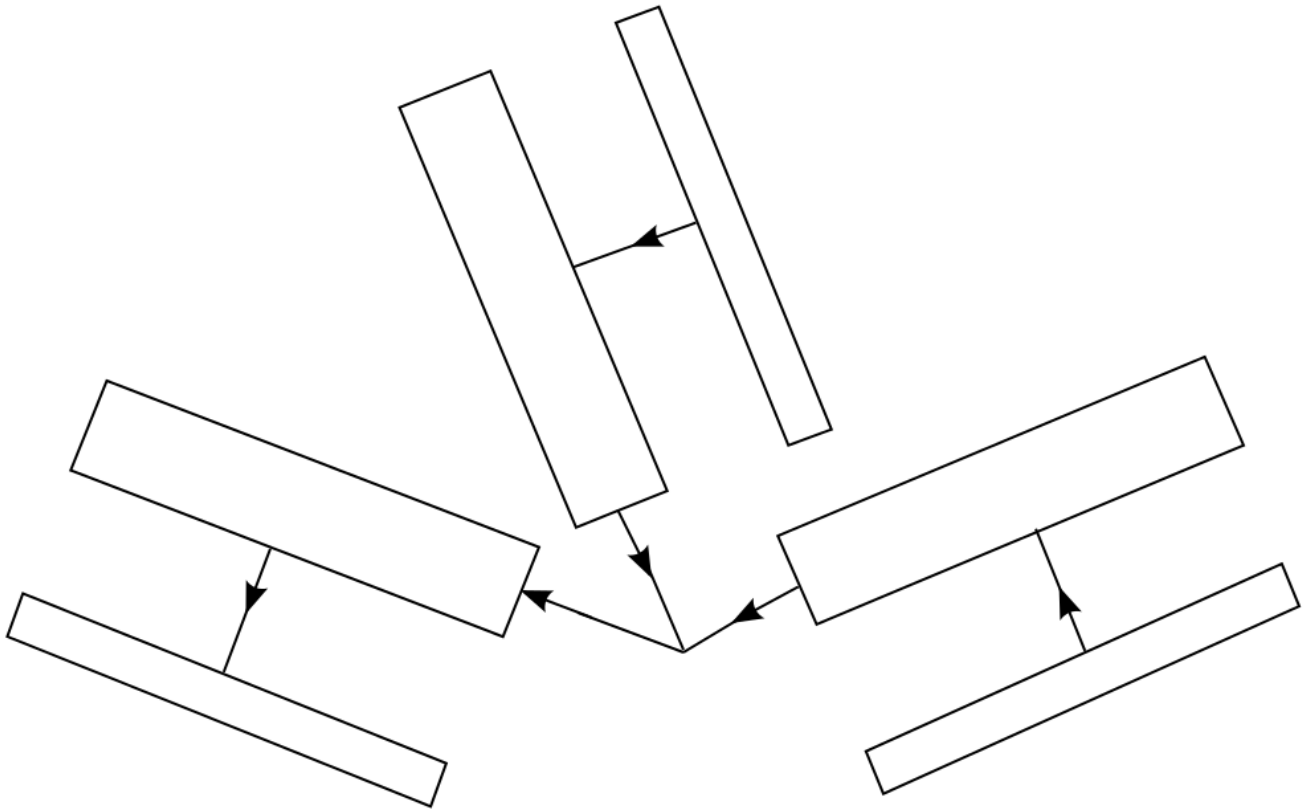


Low-rank tensor factorizations (CP)

$$A_{ijk} = \sum_l U_{il} V_{jl} W_{kl} \quad \rightarrow \quad d_i = \sum_{j,k,l} U_{il} V_{jl} W_{kl} b_j c_k$$

multilinear low rank operator



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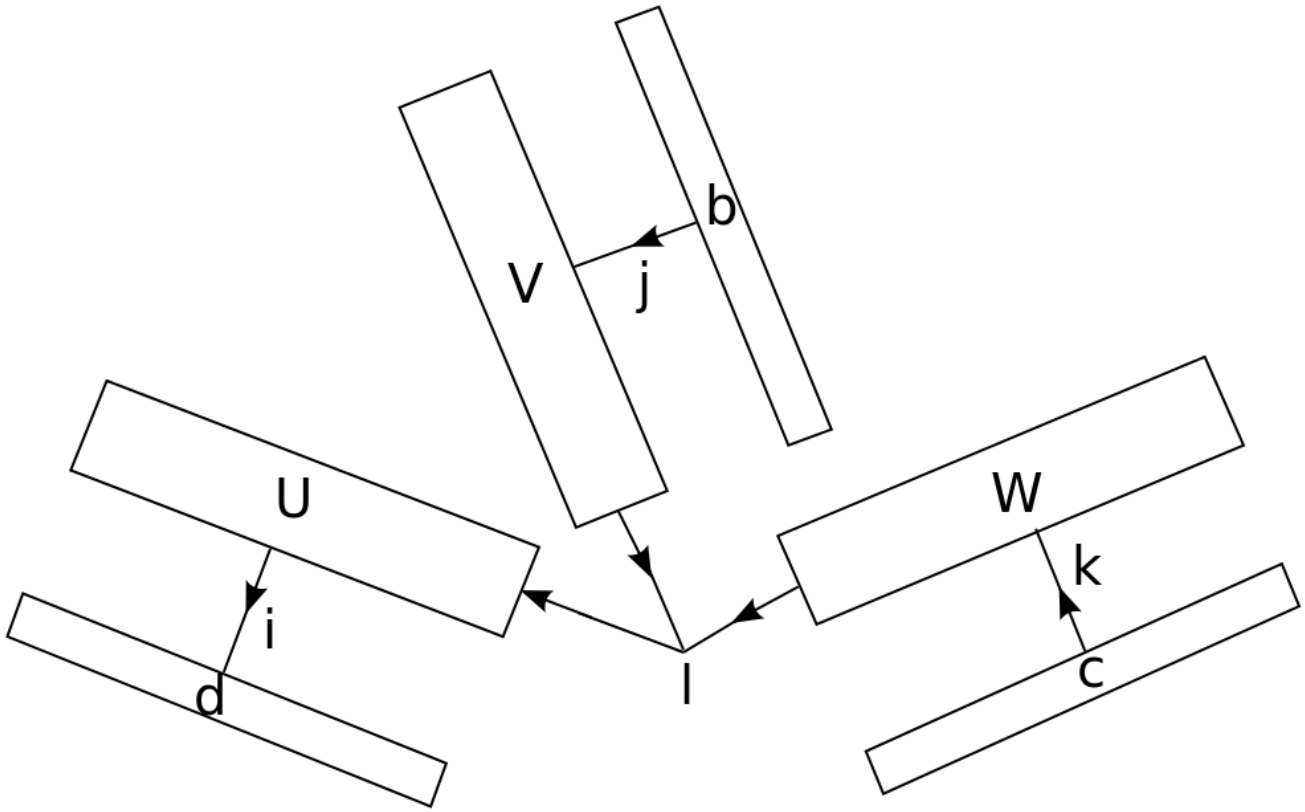
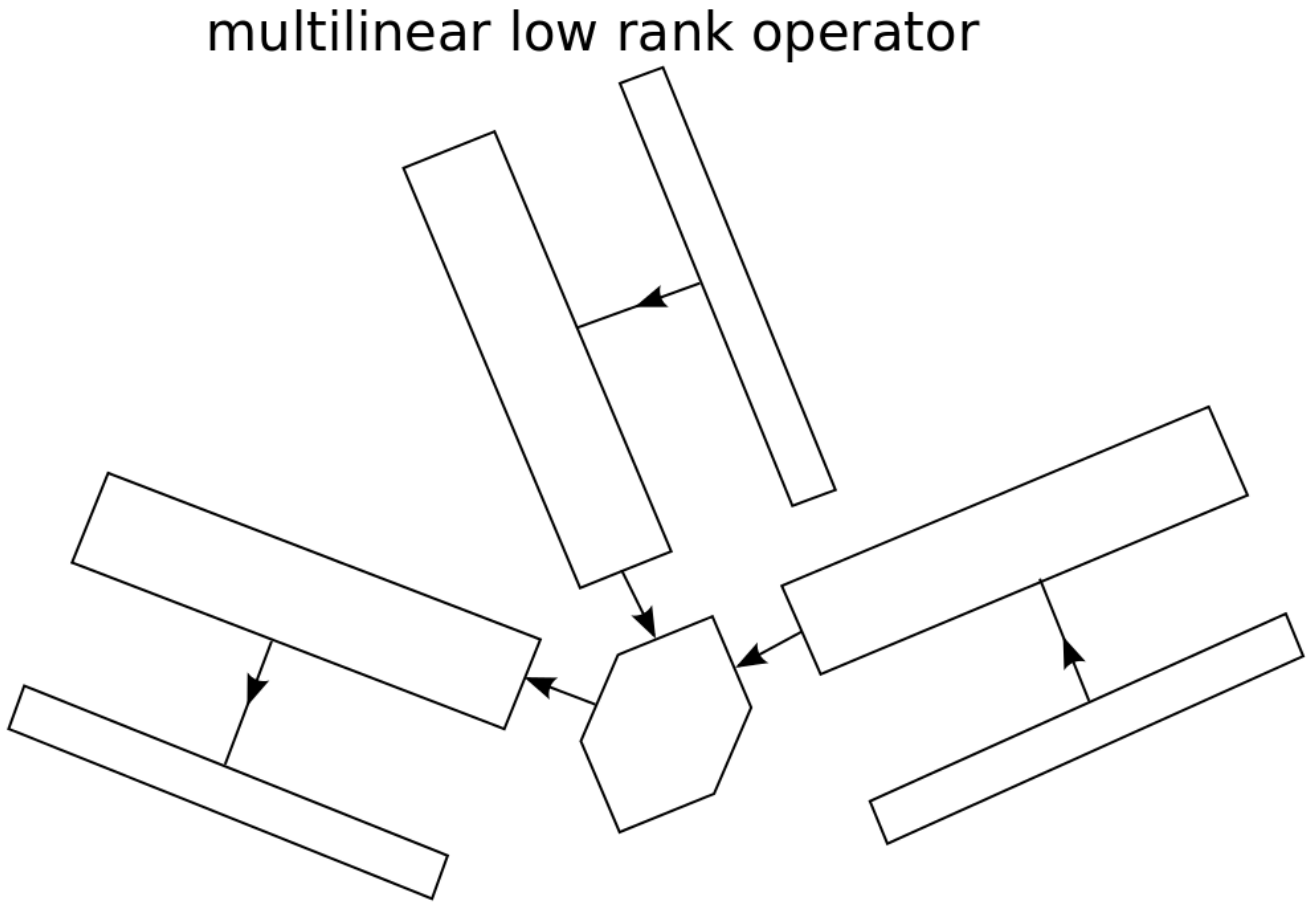
multilinear low rank operator



Low-rank tensor factorizations (Tucker)

$$A_{ijk} = \sum_{l,m,n} T_{lmn} U_{il} V^{jm} W^{kn} \quad \rightarrow \quad d_i = \sum_{j,k,l,m,n} T_{lmn} U_{il} V_{jm} W_{jn} b_j c_k$$



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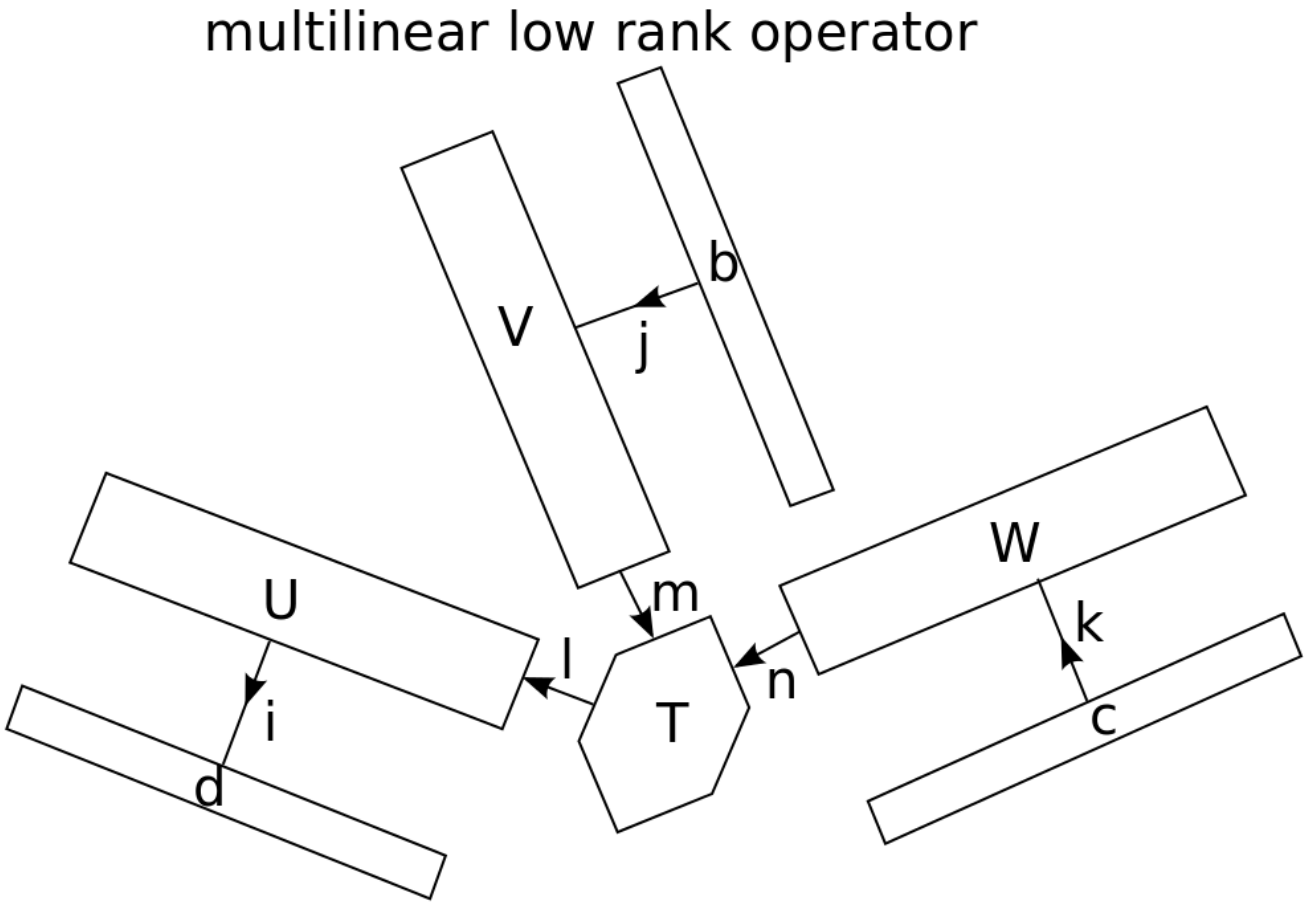
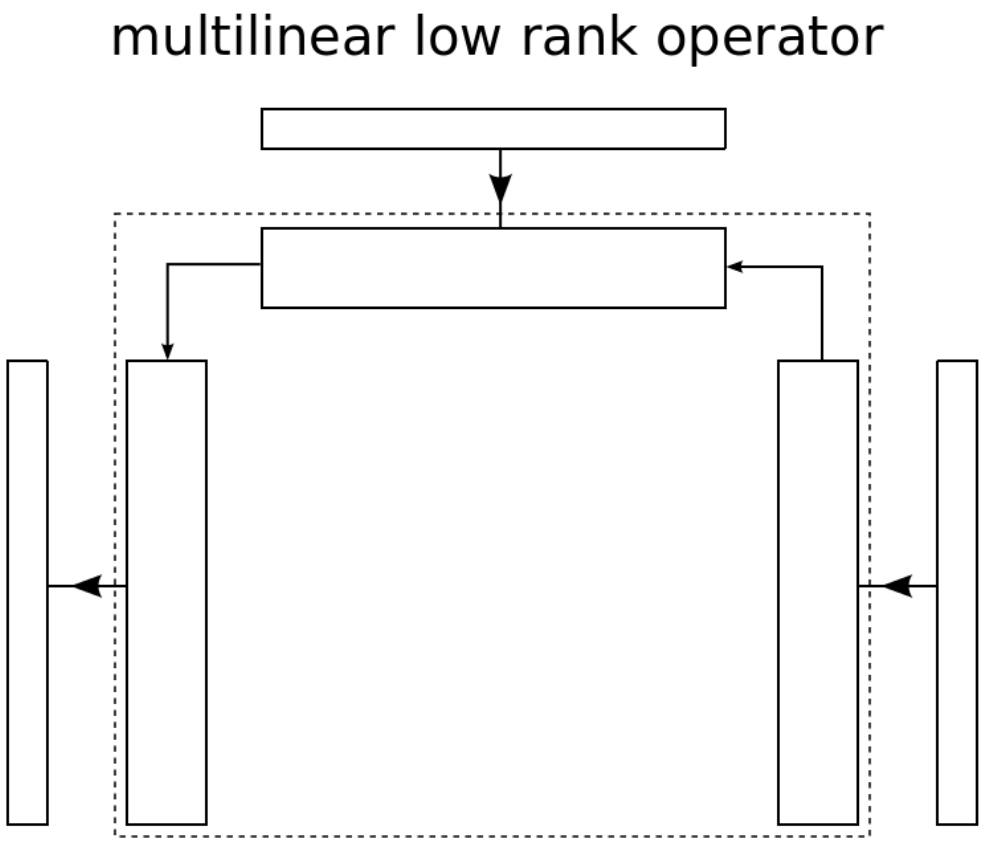


Low-rank tensor factorizations (TT)

$$A_{ijk} = \sum_{l,m} U_{il} V_{ljm} W_{mk} \quad \rightarrow \quad \sum_{j,k,l,m} U_{il} V_{ljm} W_{mk} b_j c_k$$



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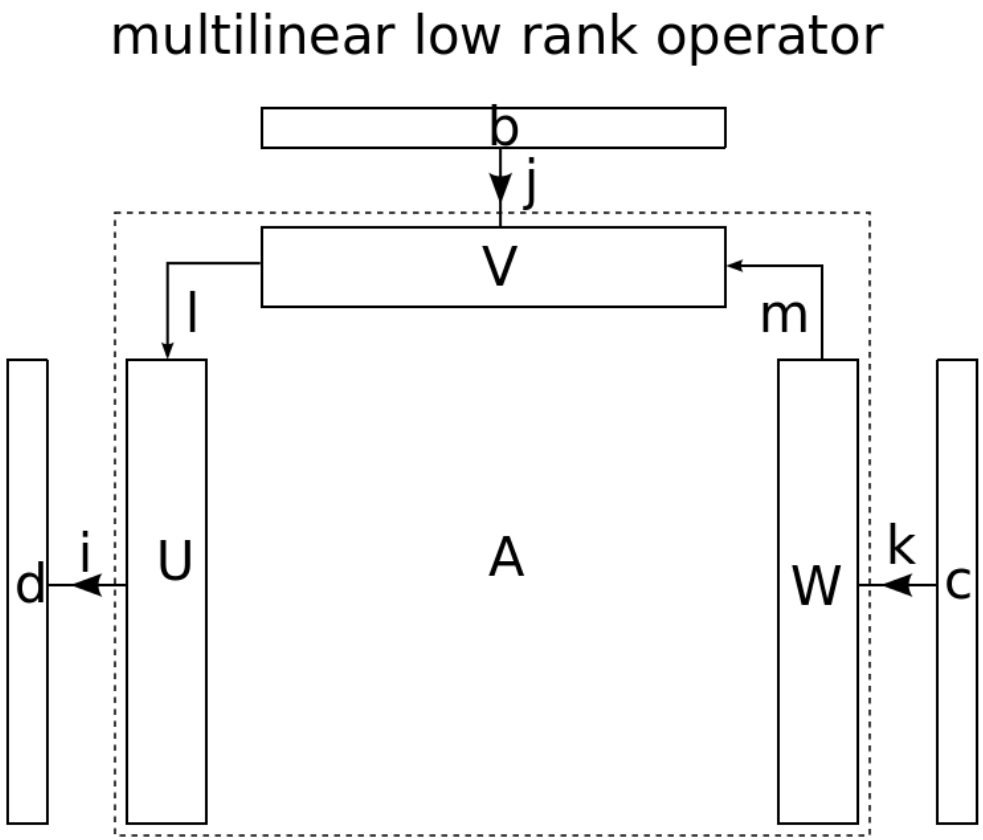
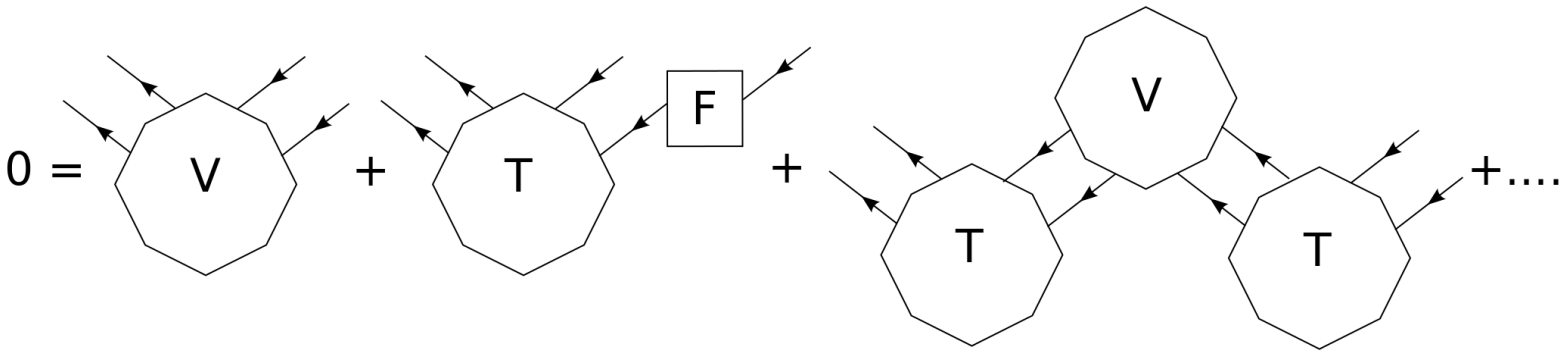


Tensor contractions in electronic structure methods

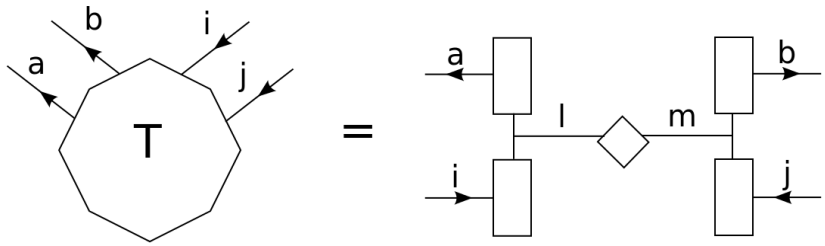
Amplitude equation snippet from coupled cluster doubles model

$$0 = V_{abij} + \sum_{k} T_{abik} F_{kj} + \sum_{k,l,m,n} T_{abkl} V_{klmn} T_{mnij} + \dots$$



Tensor hypercontraction representation[a]

$$T_{abij} = \sum_{l,m} \psi_{al} \phi_{jl} Z_{lm} \phi_{jm} \psi_{bm}$$



[a] Hohenstein, Parrish, Sherrill, Martinez, JCP, 2012

Structured tensor computations

Challenges for matrix/tensor algebraic abstractions

- data and relation sparsity $\rightarrow$ tensor sparsity
- low-order representations of data $\rightarrow$ tensor decompositions
- implicitly defined relations $\rightarrow$ implicit tensor representations
- data and relation equivalences $\rightarrow$ tensor symmetries

Exploiting symmetry in tensors

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[1]

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

- rank-2 vector outer product[1]

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

- squaring a symmetric matrix (or $AB + BA$)[1]

$$C_{ij} = \sum_k A_{ik}A_{kj} = \sum_k (A_{ik} + A_{kj} + A_{ij})^2 - \ldots$$

- for order ω contraction, $\omega!$ fewer multiplications [1]

[1] S., Demmel; Technical Report, ETH Zurich, 2015.

Symmetry preserving algorithms

By exploiting symmetry, we can reduce the number of multiplications at the cost of more additions[2]

- partially symmetric contractions
  - symmetry preserving algorithm can be nested over each index group
  - reduction in multiplications implies reduction in nested calls
  - cost reductions: 1.3 for CCSD, 2.1 for CCSDT
- algorithms generalize to most antisymmetric tensor contractions
- for Hermitian tensors, multiplication cost 3X more than addition
  - BLAS routines: `hemm` and `her2k` as well as LAPACK routines like `hetrd` (tridiagonal reduction) may be done with 25% fewer operations
- achieves $(2/3)n^3$ bilinear rank for squaring a nonsymmetric matrix, assuming elementwise commutativity
- allows blocking of symmetric contractions into smaller (anti)symmetric contractions

[2] S., Demmel; Technical Report, ETH Zurich, 2015.

Beyond computation cost

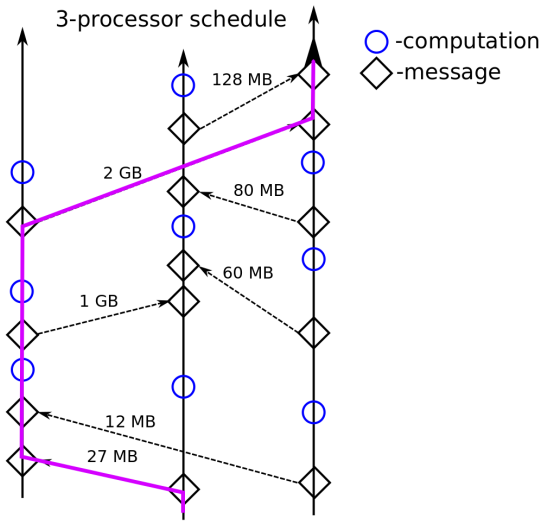
Algorithms should be not only work-efficient but communication-efficient

- data movement and synchronization cost more energy than flops
- two types of data movement: vertical (intranode memory–cache) and horizontal (internode network transfers)
- parallel algorithm design involves tradeoffs between computation, communication, and synchronization
- lower bounds and parameterized algorithms provide optimal solutions within a well-defined tuning space

Cost model for parallel algorithms

Given a schedule that specifies all work and communication tasks on p processors, we consider the following costs, accumulated along chains of tasks (as in $\alpha - \beta$, BSP, and LogGP models),

- F – computation cost
- Q – vertical communication cost
- W – horizontal communication cost
- S – synchronization cost



Communication lower bounds: previous work

Multiplication of $n \times n$ matrices

- horizontal communication lower bound[3] $W_{\text{MM}} = \Omega\left(\frac{n^2}{p^{2/3}}\right)$
- memory-dependent horizontal communication lower bound[4] $W_{\text{MM}} = \Omega\left(\frac{n^3}{p\sqrt{M}}\right)$
- with $M = cn^2/p$ memory, can hope to obtain $W = O(n^2/\sqrt{cp})$ communication
- standard parallel libraries (ScaLAPACK, Elemental) optimal only for $c = 1$

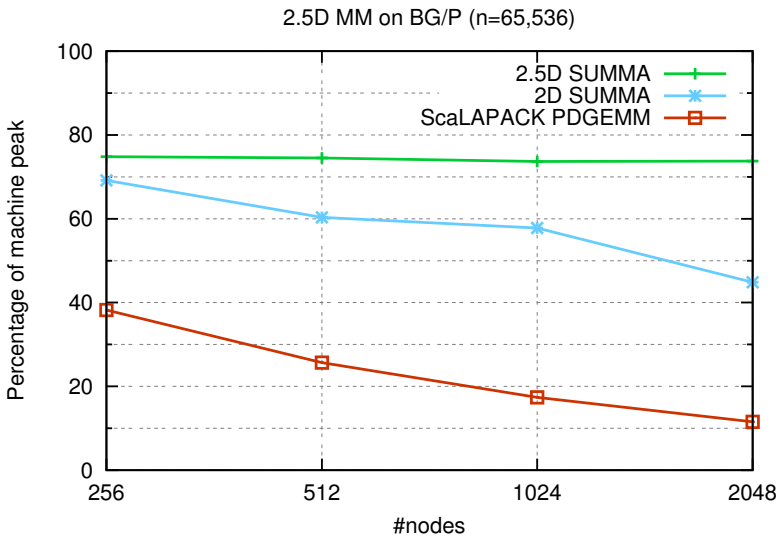
[3] Aggarwal, Chandra, Snir, TCS, 1990

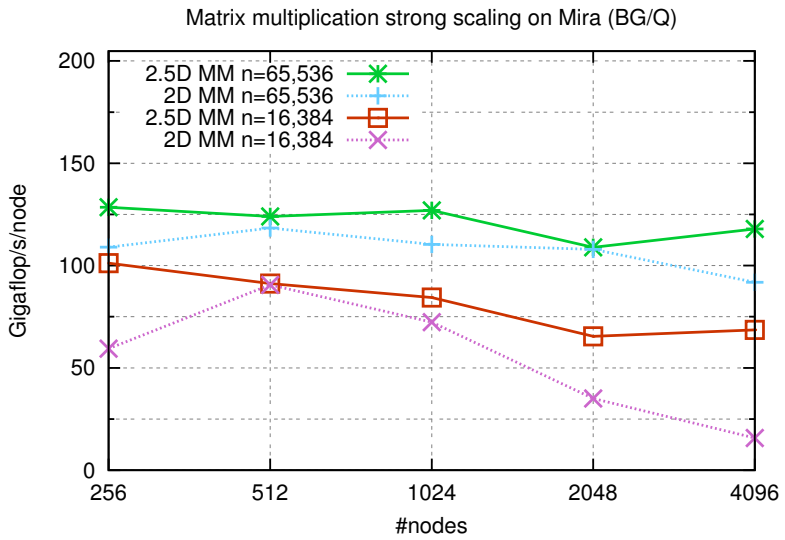
[4] Irony, Toledo, Tiskin, JPDC, 2004

Communication-efficient matrix multiplication

Communication-optimal algorithms for matrix multiplication have been studied extensively[5]

They continue to be attractive on modern architectures[6]





[5] Berntsen, Par. Comp., 1989; Agarwal, Chandra, Snir, TCS, 1990; Agarwal, Balle, Gustavson, Joshi, Palkar, IBM, 1995; McColl, Tiskin, Algorithmica, 1999; ...

[6] S., Bhatele, Demmel, SC, 2011

Synchronization cost lower bounds

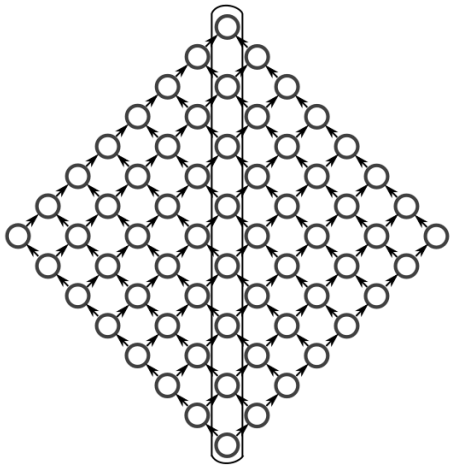
Unlike matrix multiplication, many algorithms in numerical linear algebra have polynomial depth

- synchronization cost bounds[7] $S_{\text{MM}} = \Theta\left(\frac{n^3}{pM^{3/2}}\right)$
- algorithms for Cholesky, LU, QR, SVD have additional dependencies
- lowering computation and communication costs, requires additional synchronization

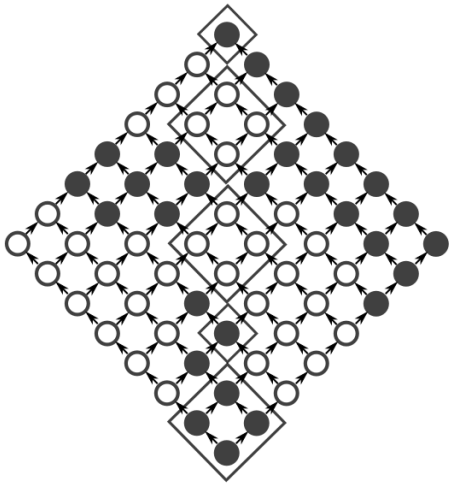
[7] Ballard, Demmel, Holtz, Schwartz, SIAM JMAA, 2011

Tradeoffs in the diamond DAG

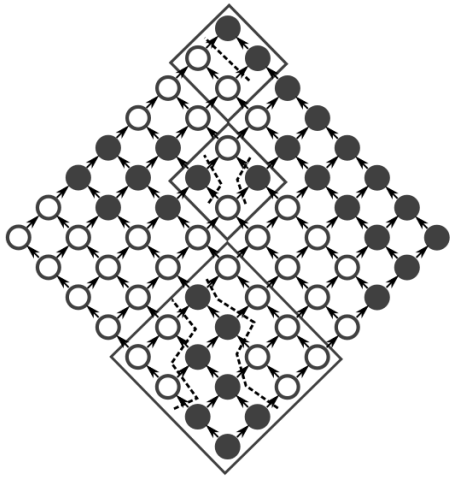
For the $n \times n$ diamond DAG, there is a tradeoff between computation and synchronization costs[8] $F \cdot S = \Omega(n^2)$



Dependency chain P



Monochrome dependency intervals



Multicolored dependency intervals

We generalize such tradeoffs to consider horizontal communication and arbitrary (polynomial or exponential) interval expansion[9]

[8] Papadimitriou, Ullman, SIAM JC, 1987

[9] S., Carson, Knight, Demmel, SPAA 2014 (extended version, JPDC 2016)

Tradeoffs involving synchronization

We apply tradeoff lower bounds to dense linear algebra algorithms, represented via dependency hypergraphs.[a]

For triangular solve with an $n \times n$ matrix

$$F_{\text{TRSV}} \cdot S_{\text{TRSV}} = \Omega\left(n^2\right)$$

For Cholesky of an $n \times n$ matrix

$$F_{\text{CHOL}} \cdot S_{\text{CHOL}}^2 = \Omega\left(n^3\right) \qquad W_{\text{CHOL}} \cdot S_{\text{CHOL}} = \Omega\left(n^2\right)$$

Proof employs classical Loomis-Whitney inequality.

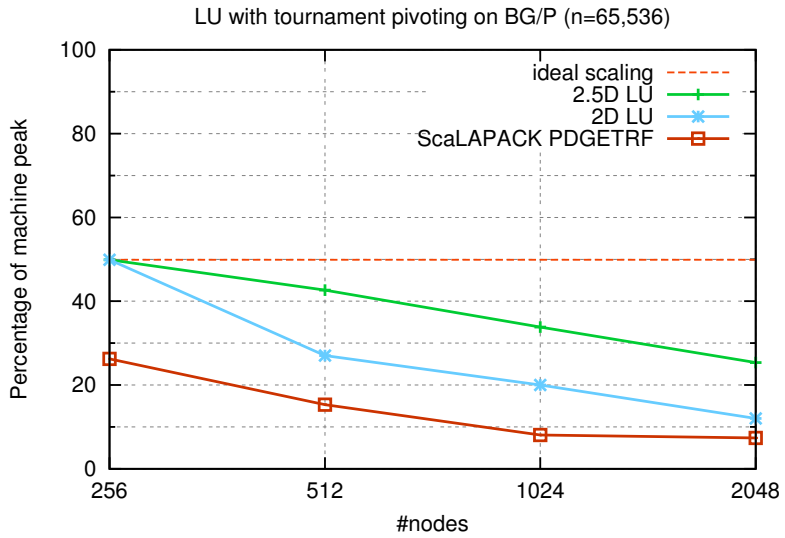
For any $R \subset \mathbb{N} \times \mathbb{N} \times \mathbb{N}$, three projections of R onto $\mathbb{N} \times \mathbb{N}$ have total size at least $|R|^{2/3}$

[a] S., Carson, Knight, Demmel, SPAA 2014 (extended version, JPDC 2016)

Communication-efficient LU factorization

For any $c \in [1, p^{1/3}]$, use cn^2/p memory per processor and obtain

$$W_{\mathrm{LU}} = O(n^2/\sqrt{cp}), \qquad S_{\mathrm{LU}} = O(\sqrt{cp})$$



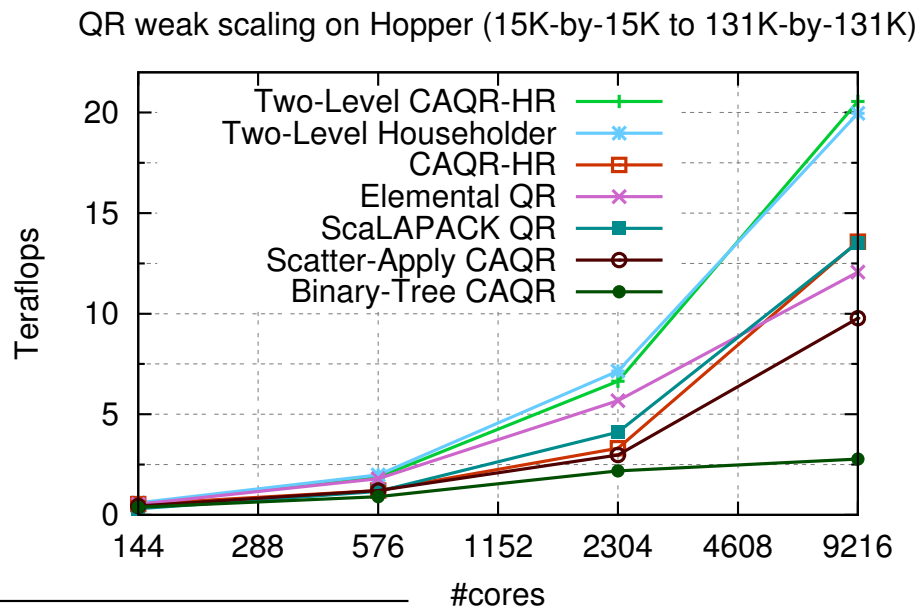
- LU with pairwise pivoting[10] extended to tournament pivoting [11]
- first implementation of a communication-optimal LU algorithm

[10] Tiskin, FGCS, 2007

[11] S., Demmel, Euro-Par, 2011

Communication-efficient QR factorization

- $W_{\mathrm{QR}} = O(n^2/\sqrt{cp}), S_{\mathrm{QR}} = O(\sqrt{cp})$ using Givens rotations[12]
- Householder form can be reconstructed quickly from TSQR[13]
- optimal QR communication and synchronization (modulo log factors) costs can be obtained with Householder representation[14]
- Householder aggregation yields performance improvements



[12] Tiskin, FGCS, 2007

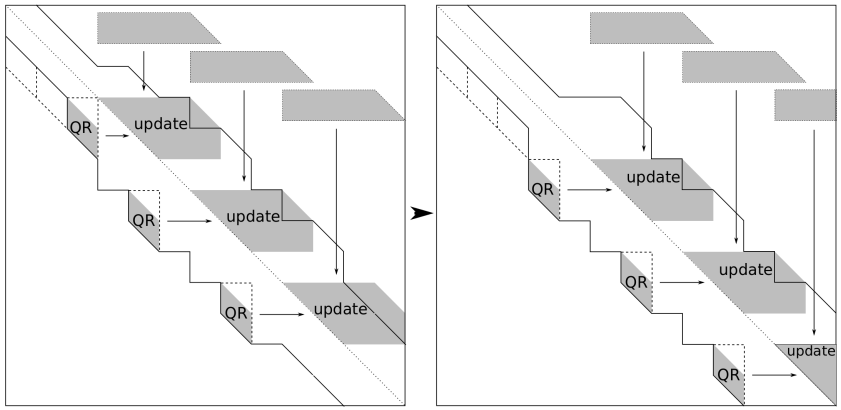
[13] Ballard, Demmel, Grigori, Jacquelin, Nguyen, Diep, S., IPDPS, 2014

[14] S., UCB, 2014

Communication-efficient eigenvalue computation

For the dense symmetric matrix eigenvalue problem

- $W_{\text{SE}} = O(n^2/\sqrt{cp}), S_{\text{QR}} = O(\sqrt{cp}\log^2 p)$ [15]
- optimal horizontal communication can be obtained with left-looking algorithm and aggregation, however, requires more vertical communication
- successive band reduction can be used to minimize both communication costs



[15] S., UCB, 2014. S., Hoefler, Demmel, in preparation

Synchronization tradeoffs in stencils

Our lower bound analysis extends also to sparse iterative methods.[16]
For computing s applications of a $(2m+1)^d$-point stencil

$$F_{\text{St}} \cdot S_{\text{St}}^d = \Omega\left(m^{2d} \cdot s^{d+1}\right) \qquad W_{\text{St}} \cdot S_{\text{St}}^{d-1} = \Omega\left(m^d \cdot s^d\right)$$

proof requires generalization of Loomis-Whitney inequality to order d set and order $d-1$ projections

- time-blocking lowers synchronization and vertical communication costs, but raises horizontal communication
- we suggest alternative approach that minimizes vertical and horizontal communication, but not synchronization

[16] S., Carson, Knight, Demmel, SPAA 2014 (extended version, JPDC 2016)

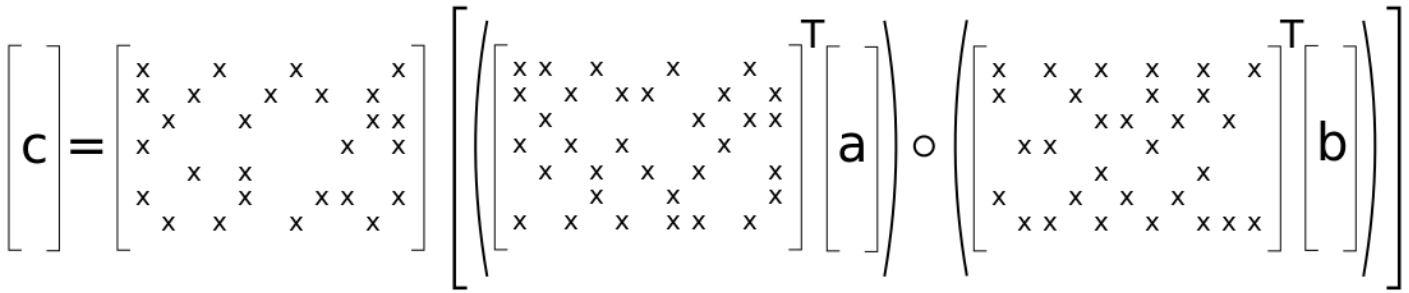
Beyond the Loomis-Whitney inequalities

Loomis-Whitney inequalities are not sufficient for all computations

- symmetry preserving tensor contraction algorithms have arbitrary order projections from order d set
- bilinear algorithms[17] provide a more general framework
- 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 $\circ$ is the Hadamard (pointwise) product



- communication lower bounds can be formulated in terms of rank[18]

[17] Pan, Springer, 1984

[18] S., Hoefler, Demmel, in preparation

Communication cost of symmetry preserving algorithms

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

- Υ is the nonsymmetric contraction algorithm
- Ψ is the best previously known algorithm
- Φ is the symmetry preserving algorithm

Asymptotic communication lower bounds based on bilinear expansion[a] (H–cache size, p–#processors, n–dimension):

s	t	v	F_Υ	F_Ψ	F_Φ	$Q_{\Upsilon,\Psi}$	Q_Φ	W_Υ	W_Ψ	W_Φ
1	1	0	n^2	n^2	$\frac{n^2}{2}$	n^2	n^2	$\frac{n}{p^{1/2}}$	$\frac{n}{p^{1/2}}$	$\frac{n}{p^{1/2}}$
2	1	0	n^3	$\frac{n^3}{2}$	$\frac{n^3}{6}$	n^3	n^3	n	$\frac{n^2}{p^{2/3}}$	$\frac{n^2}{p^{2/3}}$
2	2	0	n^4	$\frac{n^4}{4}$	$\frac{n^4}{24}$	n^4	n^4	$\frac{n^2}{p^{1/2}}$	$\frac{n^2}{p^{1/2}}$	$\frac{n^2}{p^{1/2}}$
1	1	1	n^3	n^3	$\frac{n^3}{6}$	$\frac{n^3}{H^{1/2}}$	$\frac{n^3}{H^{1/2}}$	$\frac{n^2}{p^{2/3}}$	$\frac{n^2}{p^{2/3}}$	$\frac{n^2}{p^{2/3}}$
2	1	1	n^4	$\frac{n^4}{2}$	$\frac{n^4}{24}$	$\frac{n^4}{H^{1/2}}$	$\frac{n^4}{H^{1/3}}$	n^2	n^2	$\frac{n^3}{p^{3/4}}$
2	2	2	n^6	$\frac{n^6}{8}$	$\frac{n^6}{720}$	$\frac{n^6}{H^{1/2}}$	$\frac{n^6}{H^{1/2}}$	$\frac{n^4}{p^{2/3}}$	$\frac{n^4}{p^{2/3}}$	$\frac{n^4}{p^{2/3}}$

[a] S., Hoefler, Demmel, ETHZ, 2014

Open theoretical problems

- lower bounds for multiplication of a sparse and a dense matrix
- lower bounds for nested bilinear algorithms
- broader parameterizations of algorithmic representations needed for QR and SVD lower bounds

Tensor algebra as a programming abstraction

Cyclops Tensor Framework[19]

- contraction/summation/functions of tensors
- distributed symmetric-packed/sparse storage via cyclic layout
- parallelization via MPI+OpenMP(+CUDA)

[19] S., Hammond, Demmel, UCB, 2011. S., Matthews, Hammond, Demmel, IPDPS, 2013

Tensor algebra as a programming abstraction

Cyclops Tensor Framework

- contraction/summation/functions of tensors
- distributed symmetric-packed/sparse storage via cyclic layout
- parallelization via MPI+OpenMP(+CUDA)

Jacobi iteration example code snippet

```
void Jacobi(Matrix<> A, Vector<> b, int n){
  Matrix<> R(A);
  R["ii"] = 0.0;
  Vector<> x(n), d(n), r(n);
  Function<> inv([](double & d){ return 1./d; });
  d["i"] = inv(A["ii"]); // set d to inverse of diagonal of A
  do {
    x["i"] = d["i"]*(b["i"]-R["ij"]*x["j"]);
    r["i"] = b["i"]-A["ij"]*x["j"]; // compute residual
  } while (r.norm2() > 1.E-6); // check for convergence
}
```

Tensor algebra as a programming abstraction

Cyclops Tensor Framework

- contraction/summation/functions of tensors
- distributed symmetric-packed/sparse storage via cyclic layout
- parallelization via MPI+OpenMP(+CUDA)

Møller-Plesset perturbation theory (MP3) code snippet

```
Z["abij"] += Fab["af"]*T["fbij"];
Z["abij"] -= Fij["ni"]*T["abnj"];
Z["abij"] += 0.5*Vabcd["abef"]*T["efij"];
Z["abij"] += 0.5*Vijkl["mnij"]*T["abmn"];
Z["abij"] -= Vaibj["amei"]*T["ebmj"];
```

Betweenness centrality

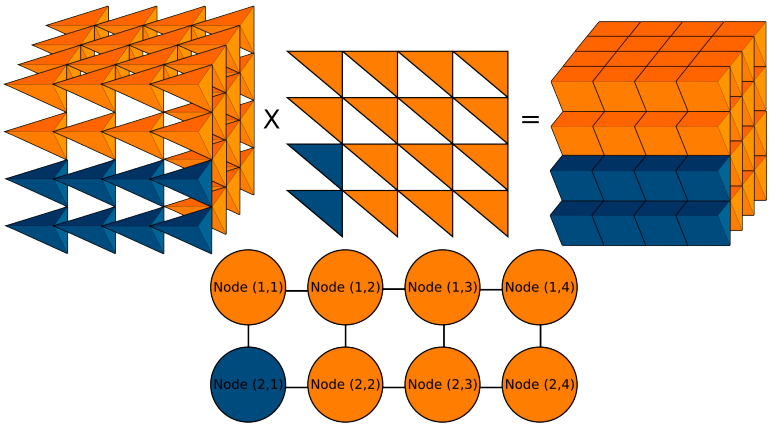
Betweenness centrality code snippet, for k of n nodes

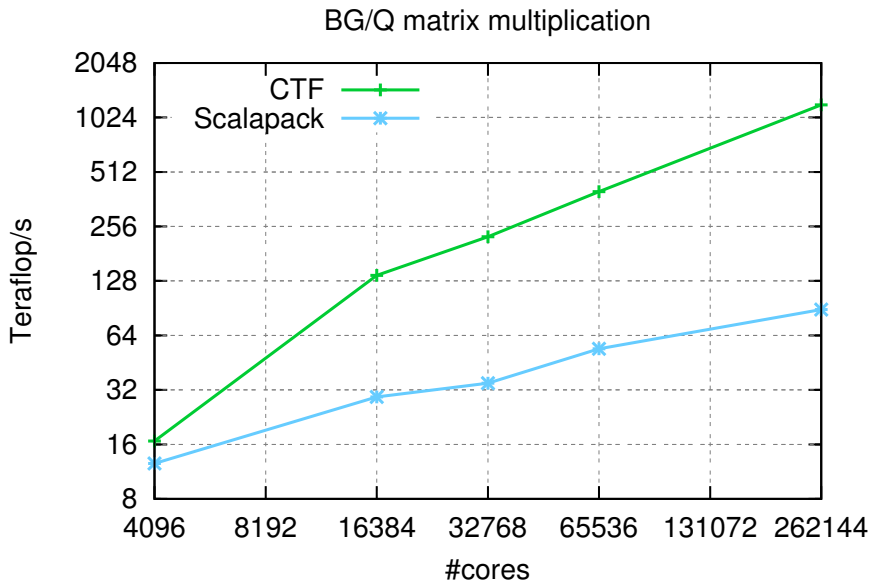
```
void btwn_central(Matrix<int> A, Matrix<path> P, int n, int k)
  Monoid<path> mon(...,
                   [](path a, path b){
                     if (a.w<b.w) return a;
                     else if (b.w<a.w) return b;
                     else return path(a.w, a.m+b.m);
                   }, ...);

  Matrix<path> Q(n,k,mon); // shortest path matrix
  Q["ij"] = P["ij"];

  Function<int,path> append([](int w, path p){
                       return path(w+p.w, p.m);
                     }; );

  for (int i=0; i<n; i++)
    Q["ij"] = append(A["ik"],Q["kj"]);
  ...
}
```

Performance of CTF for dense computations

CTF is highly tuned for massively-parallel machines

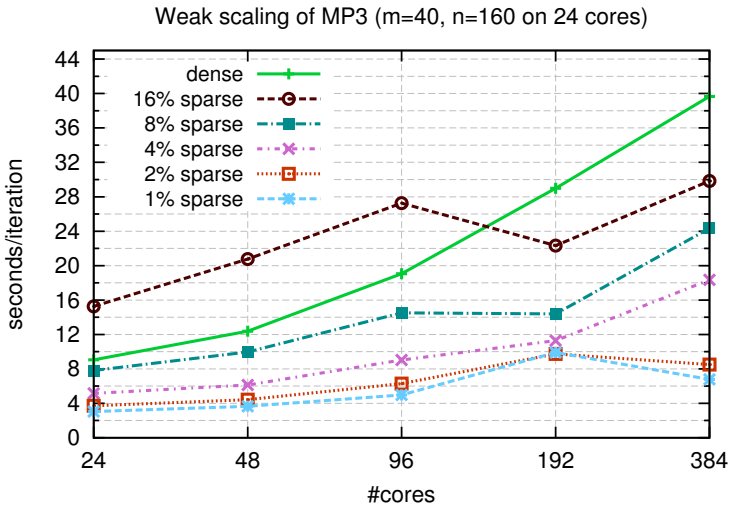
- virtualized multidimensional processor grids
- topology-aware mapping and collective communication
- performance-model-driven decomposition done at runtime
- optimized redistribution kernels for tensor transposition

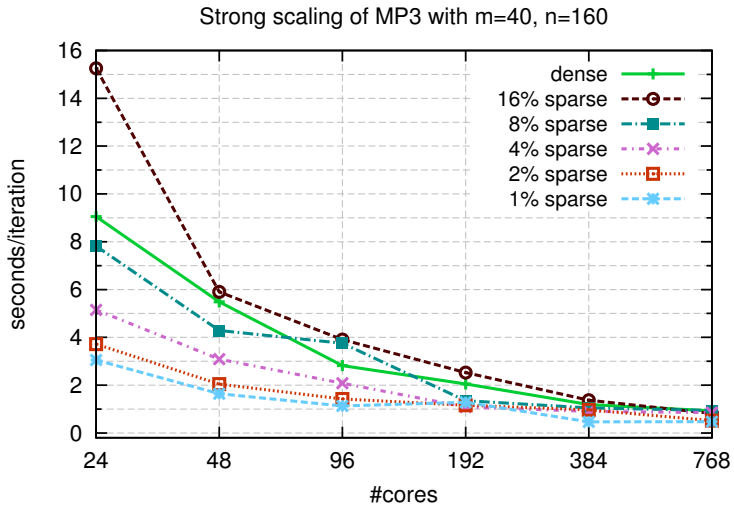




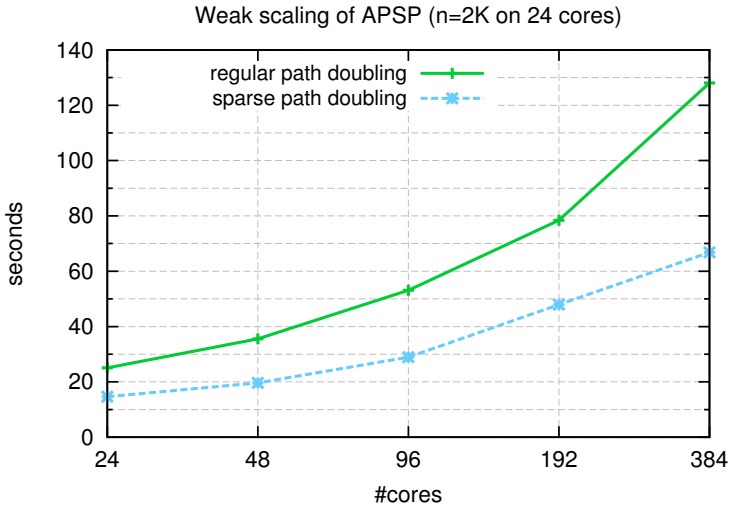
Performance of CTF for sparse computations

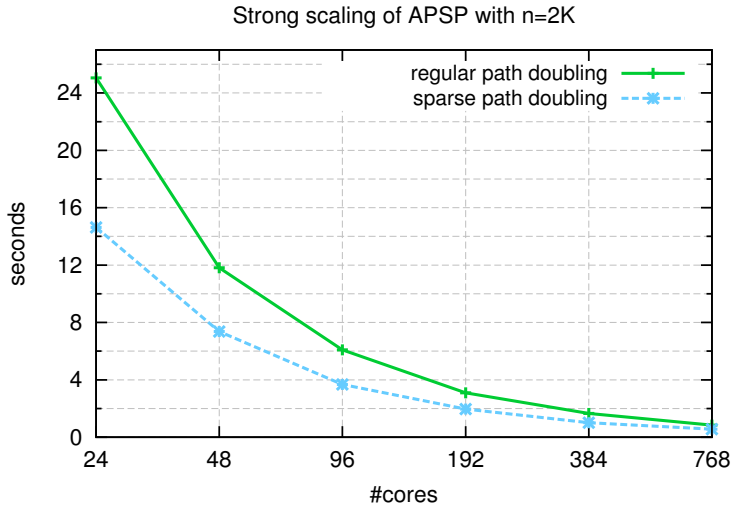
MP3 leveraging sparse-dense tensor contractions[a]





All-pairs shortest-paths based on path doubling with sparsification

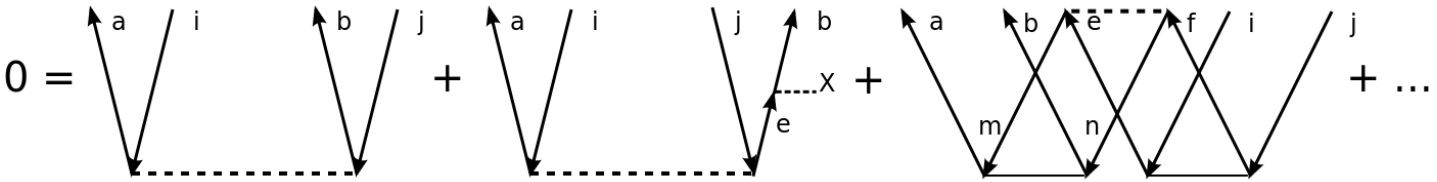




Post-Hartree-Fock (HF) methods

Accurate models of electronic correlation require approximation of contributions of excited-state transitions.

- Møller-Plesset methods provide perturbative corrections
- Coupled-cluster methods (CCSD, CCSDT, CCSDTQ) iteratively solve (2nd, 3rd, 4th) order equations in the state space



- tensor expressions naturally express high-order transitions
- tensor structure admits symmetries and sparsity
  - permutational index antisymmetry due to antisymmetry of wavefunction
  - sparsity due to strength of interactions diminishing with growing distance in the molecular orbital basis

CCSD using CTF

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

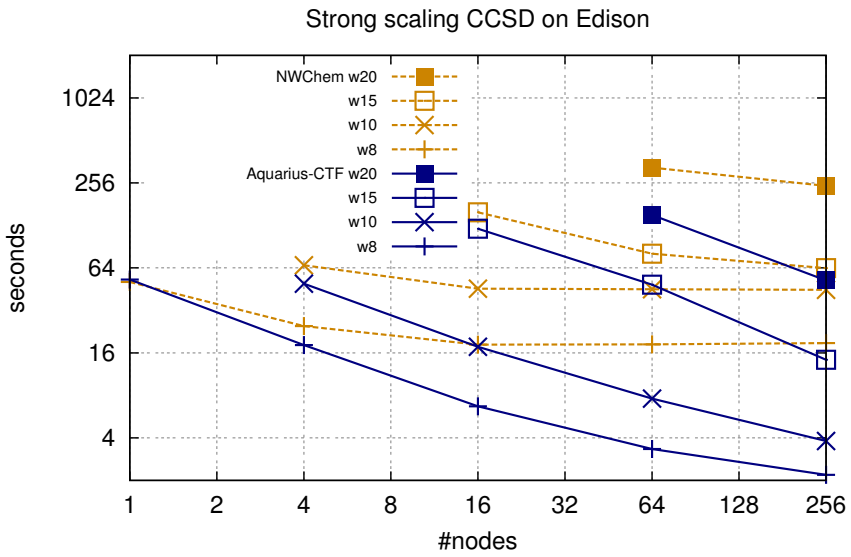
```
FMI["mi"]     += 0.5*WMNEF["mnef"]*T(2)["efin"];
WMNIJ["mnij"] += 0.5*WMNEF["mnef"]*T(2)["efij"];
FAE["ae"]     -= 0.5*WMNEF["mnef"]*T(2)["afmn"];
WAMEI["amei"] -= 0.5*WMNEF["mnef"]*T(2)["afin"];

Z(2)["abij"]  = WMNEF["ijab"];
Z(2)["abij"] += FAE["af"]*T(2)["fbij"];
Z(2)["abij"] -= FMI["ni"]*T(2)["abnj"];
Z(2)["abij"] += 0.5*WABEF["abef"]*T(2)["efij"];
Z(2)["abij"] += 0.5*WMNIJ["mnij"]*T(2)["abmn"];
Z(2)["abij"] -= WAMEI["amei"]*T(2)["ebmj"];
```

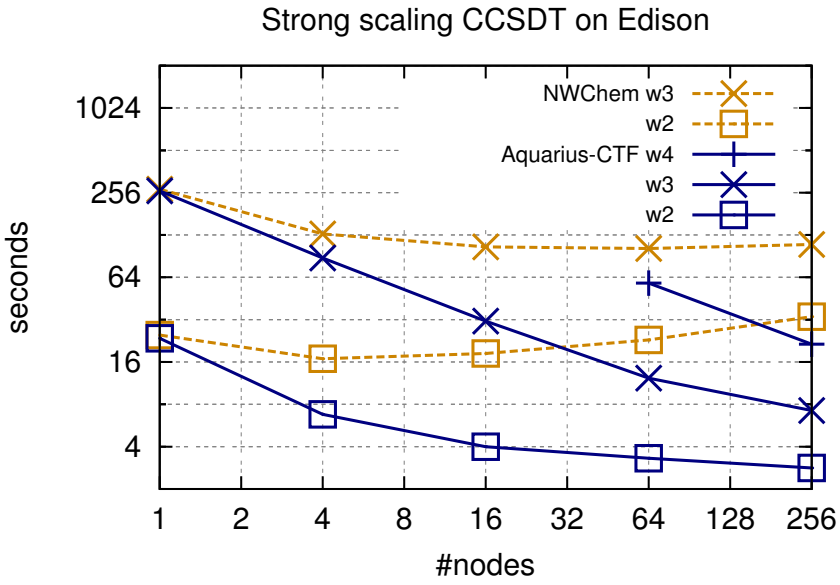
Other electronic structure codes using CTF include QChem (via Libtensor) and VASP

Comparison with NWChem

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

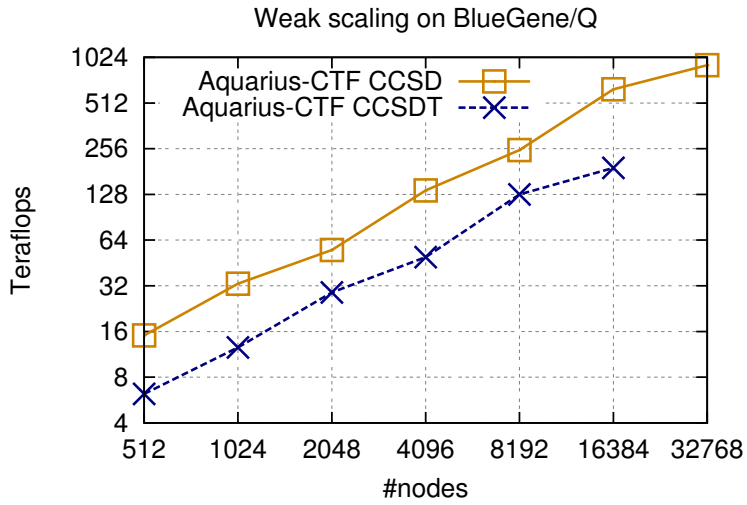
- provides CCSD and CCSDT
- uses Global Arrays a Partitioned Global Address Space (PGAS) backend for tensor contractions
- derives equations via Tensor Contraction Engine (TCE)

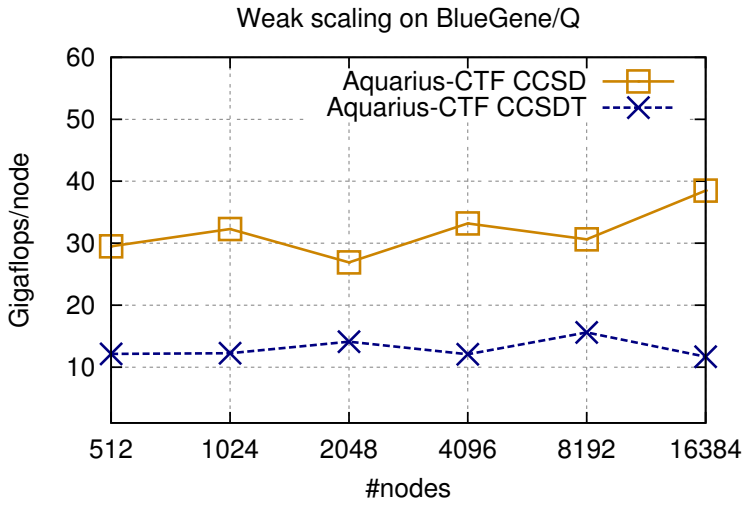


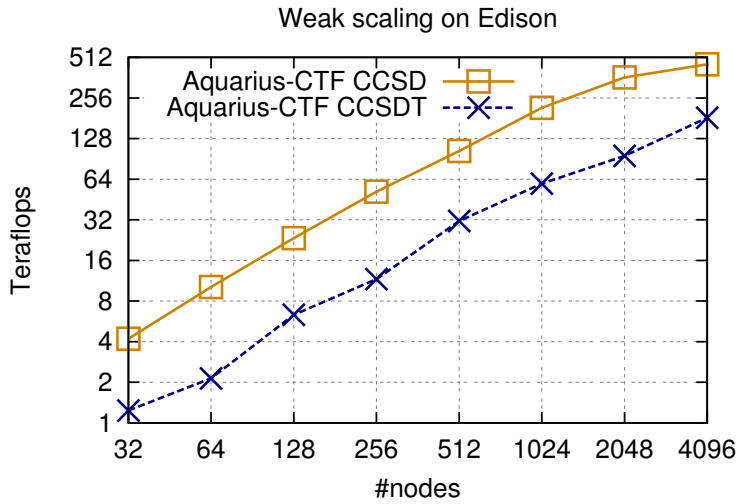


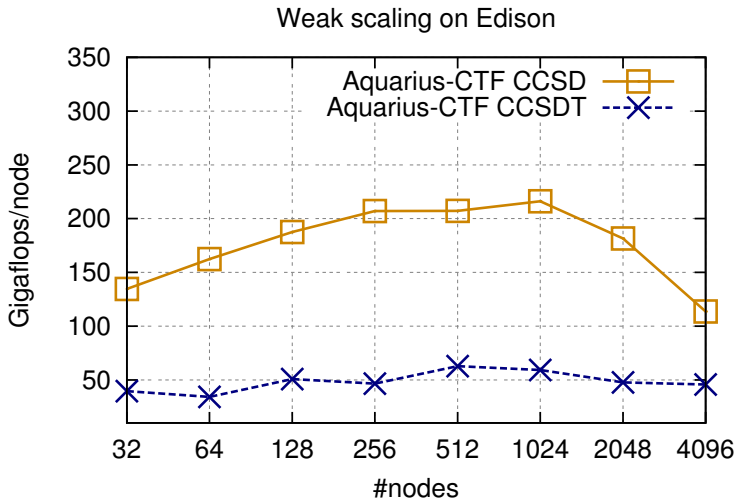
Coupled cluster on IBM BlueGene/Q and Cray XC30

CCSD up to 55 (50) water molecules with cc-pVDZ
CCSDT up to 10 water molecules with cc-pVDZ[a]







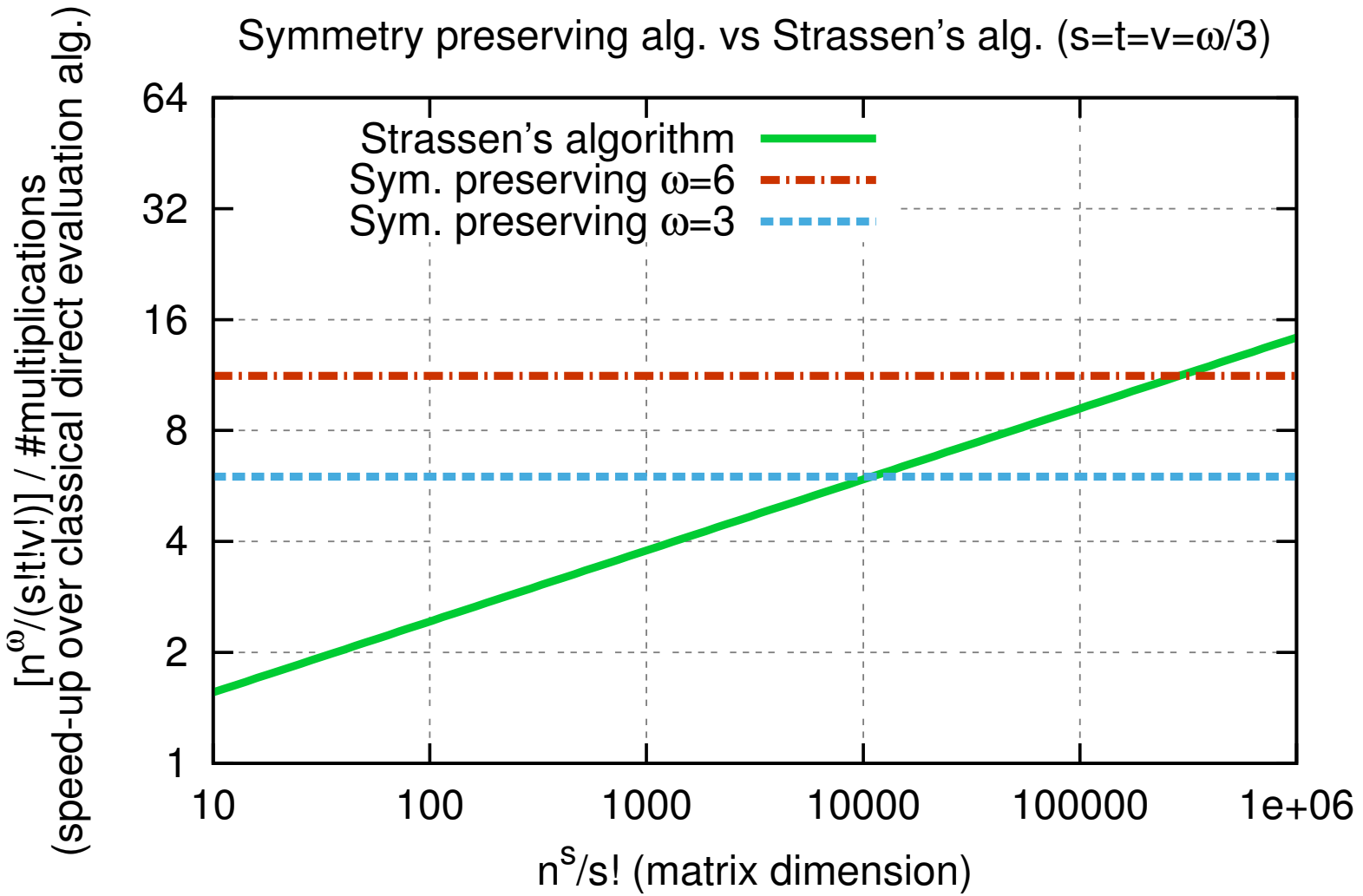


Future work

- symmetry preserving algorithms
  - high-performance implementations
  - bilinear algorithm complexity – fast matrix multiplication
- sparsity in tensor computations
  - handling multiple sparse operands and sparse output
  - worst-case lower bounds and efficient algorithms
- tensor algorithms
  - most algorithms correspond to multiple dependent tensors operations
  - scheduling, blocking, and decomposition of multiple tensor operations
  - programming abstractions for tensor factorizations
- application-driven development
  - tensor decompositions, sparsity, symmetry all motivated by electronic structure applications
  - many further applications in tensor networks (DMRG), machine learning, etc.

Backup slides

Symmetry preserving algorithm vs Strassen's algorithm



Nesting of bilinear algorithms

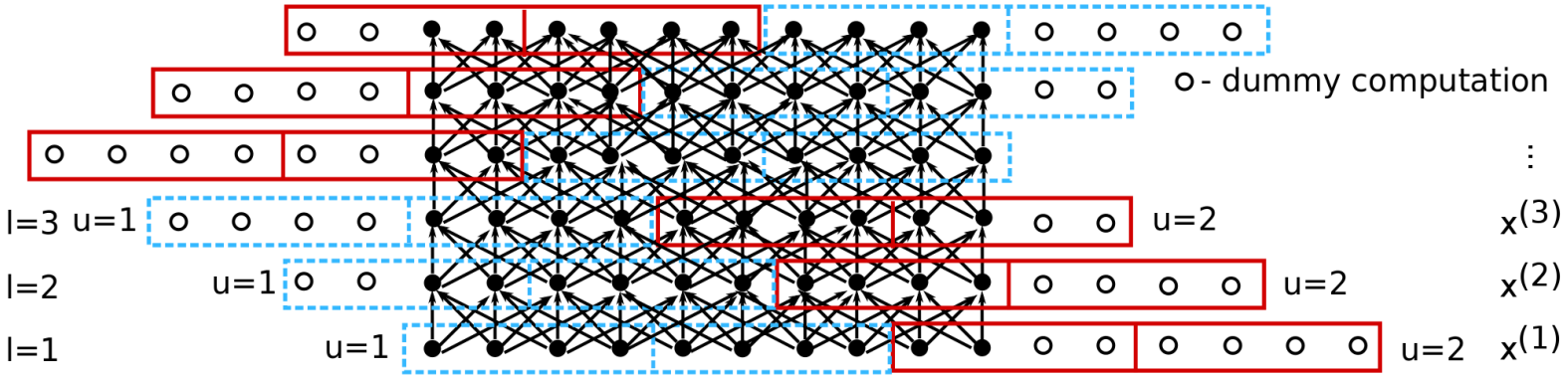
Given two bilinear algorithms:

$$\Lambda_1 = (\mathbf{F_1^{(A)}}, \mathbf{F_1^{(B)}}, \mathbf{F_1^{(C)}})$$
$$\Lambda_2 = (\mathbf{F_2^{(A)}}, \mathbf{F_2^{(B)}}, \mathbf{F_2^{(C)}})$$

We can nest them by computing their tensor product

$$\Lambda_1 \otimes \Lambda_2 := (\mathbf{F_1^{(A)}} \otimes \mathbf{F_2^{(A)}}, \mathbf{F_1^{(B)}} \otimes \mathbf{F_2^{(B)}}, \mathbf{F_1^{(C)}} \otimes \mathbf{F_2^{(C)}})$$
$$\mathsf{rank}(\Lambda_1 \otimes \Lambda_2) = \mathsf{rank}(\Lambda_1) \cdot \mathsf{rank}(\Lambda_2)$$

Block-cyclic algorithm for s-step methods

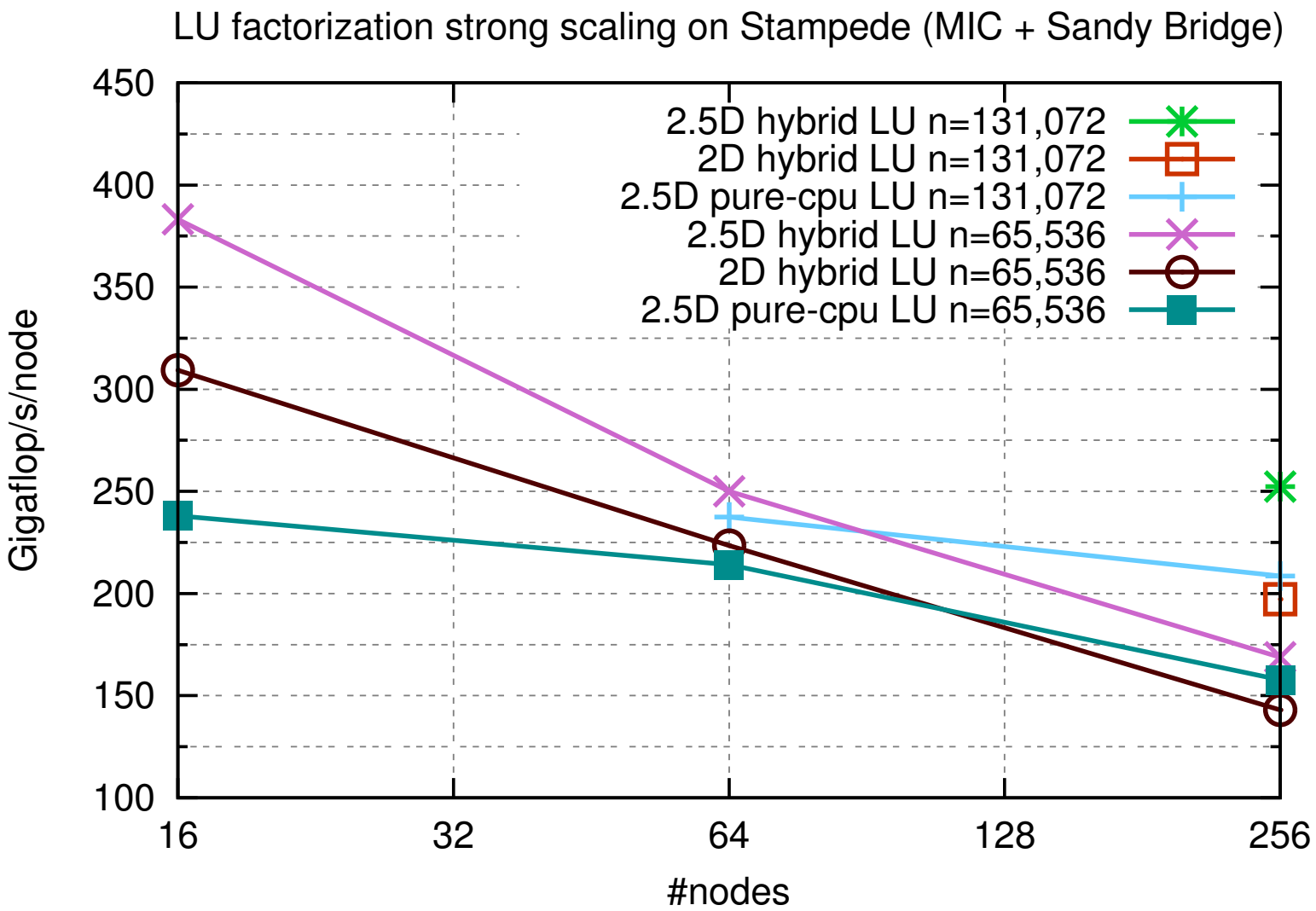


For s-steps of a $(2m+1)^d$-point stencil with block-size of $H^{1/d}/m$,

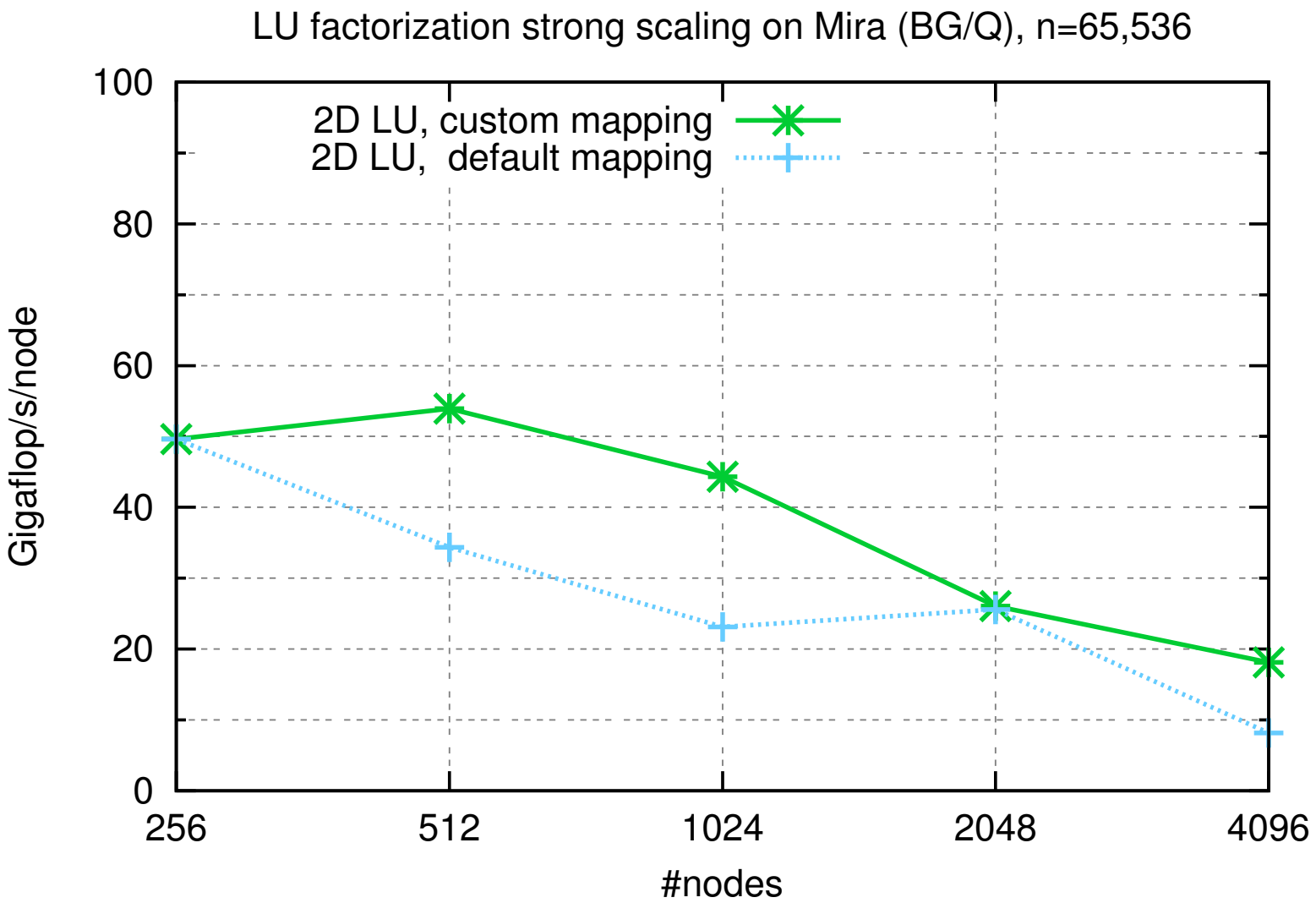
$$W_{\mathrm{Kr}} = O\left(\frac{msn^d}{H^{1/d}p}\right) \quad S_{\mathrm{Kr}} = O(sn^d/(pH)) \quad Q_{\mathrm{Kr}} = O\left(\frac{msn^d}{H^{1/d}p}\right)$$

which are good when $H = \Theta(n^d/p)$, so the algorithm is useful when the cache size is a bit smaller than n^d/p

2.5D LU on MIC

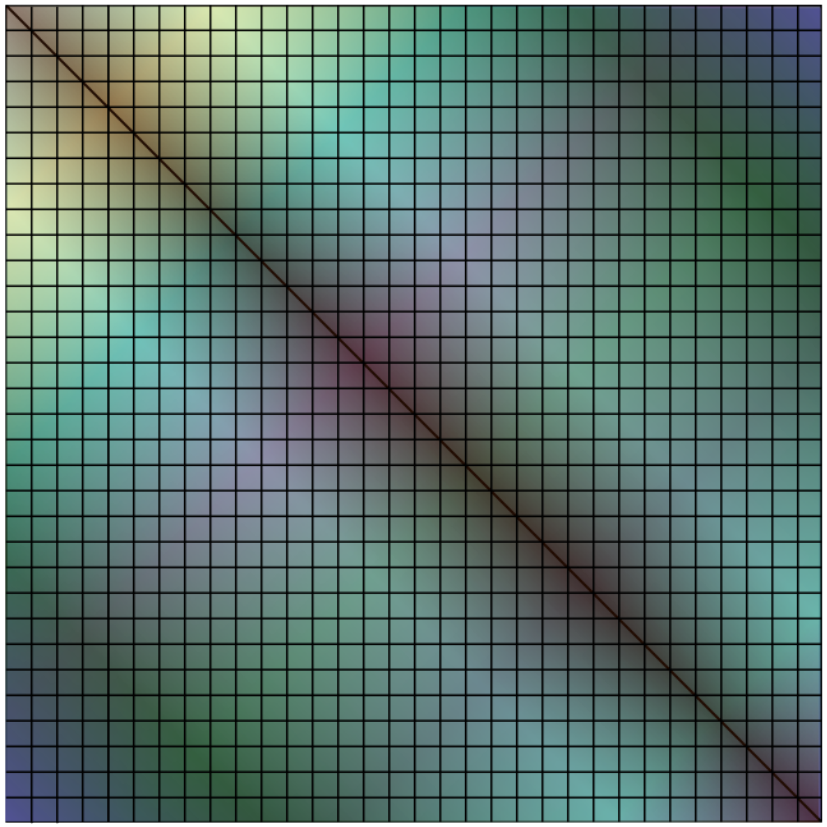

LU factorization strong scaling on Stampede (MIC + Sandy Bridge)
Gigaflop/s/node
#nodes
450
400
350
300
250
200
150
100
16
32
64
128
256
2.5D hybrid LU n=131,072
2D hybrid LU n=131,072
2.5D pure-cpu LU n=131,072
2.5D hybrid LU n=65,536
2D hybrid LU n=65,536
2.5D pure-cpu LU n=65,536

Topology-aware mapping on BG/Q

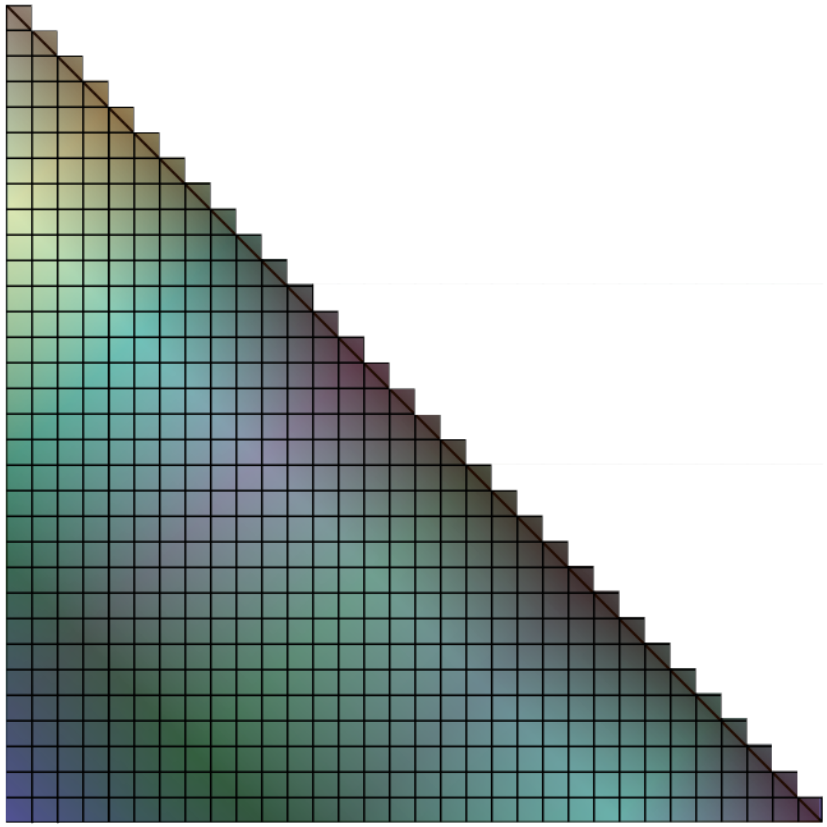


Symmetric matrix representation

Symmetric matrix

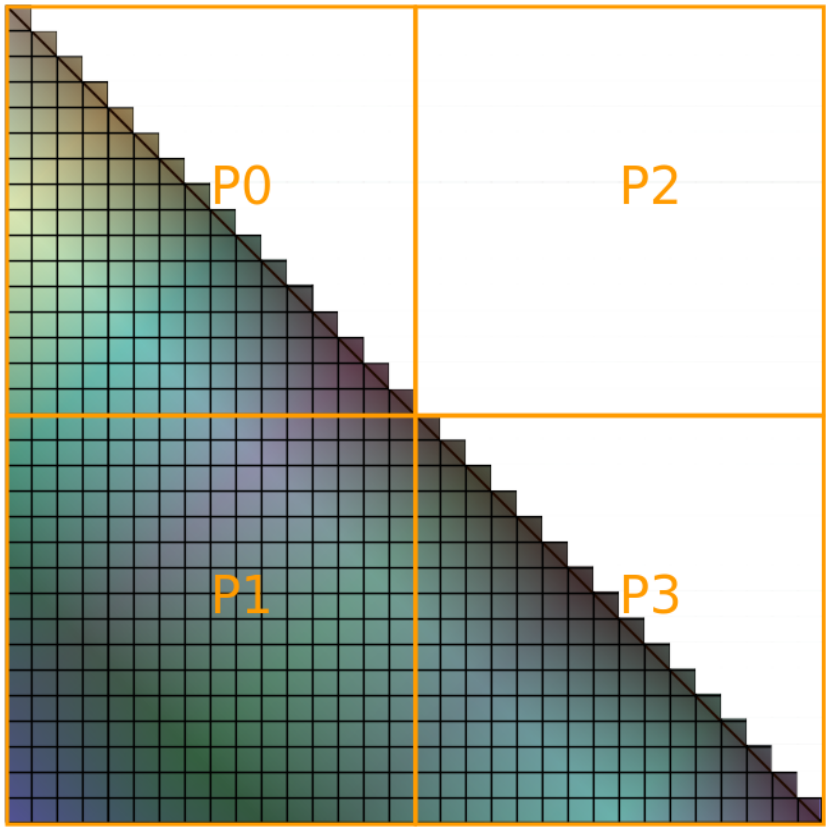


Unique part of symmetric matrix

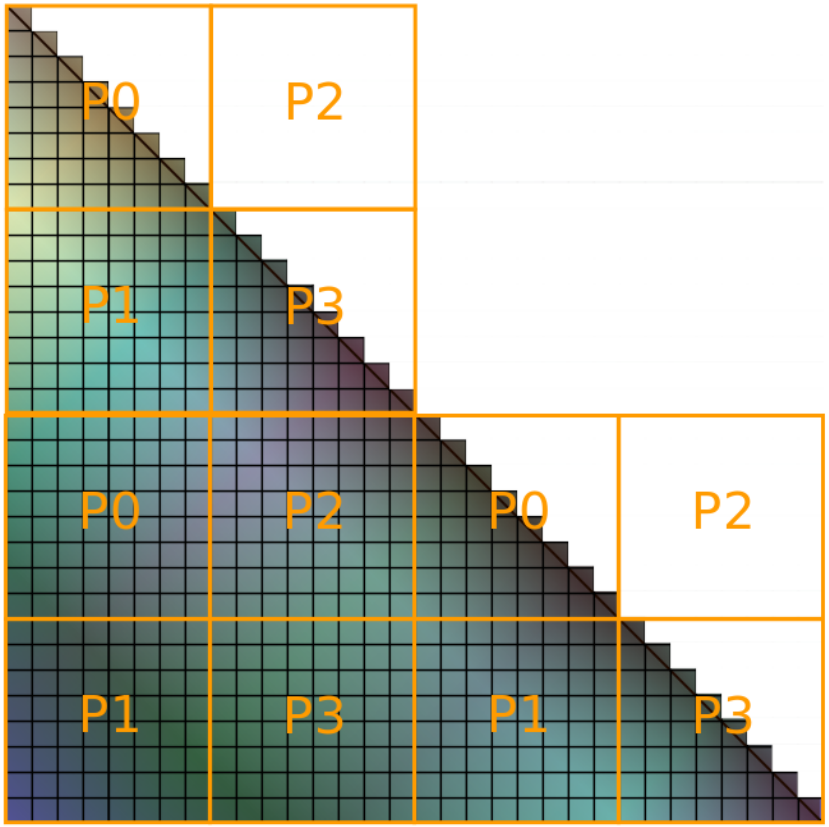


Blocked distributions of a symmetric matrix

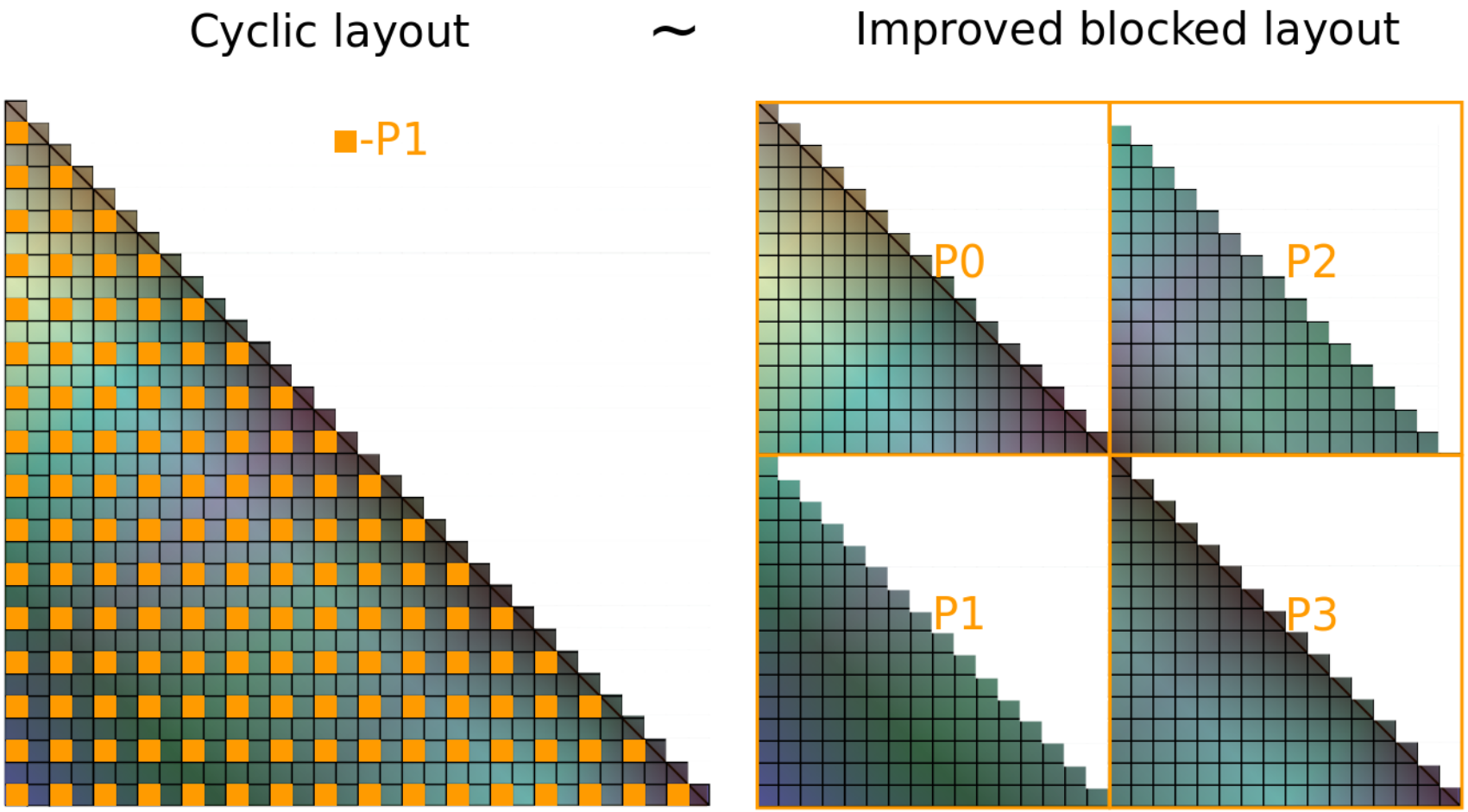
Naive blocked layout



Block-cyclic layout



Cyclic distribution of a symmetric matrix



Our CCSD factorization

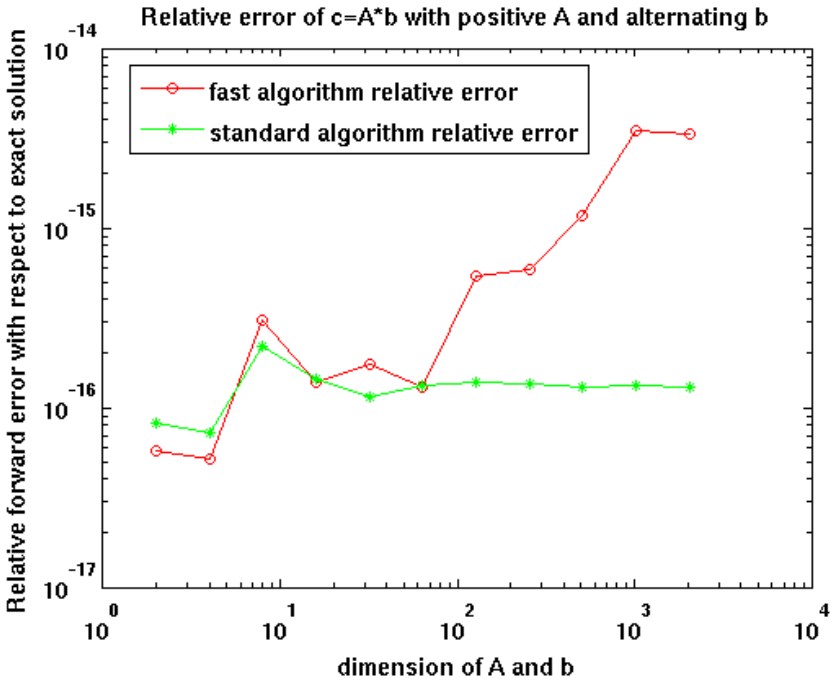
Credit to John F. Stanton and Jurgen Gauss

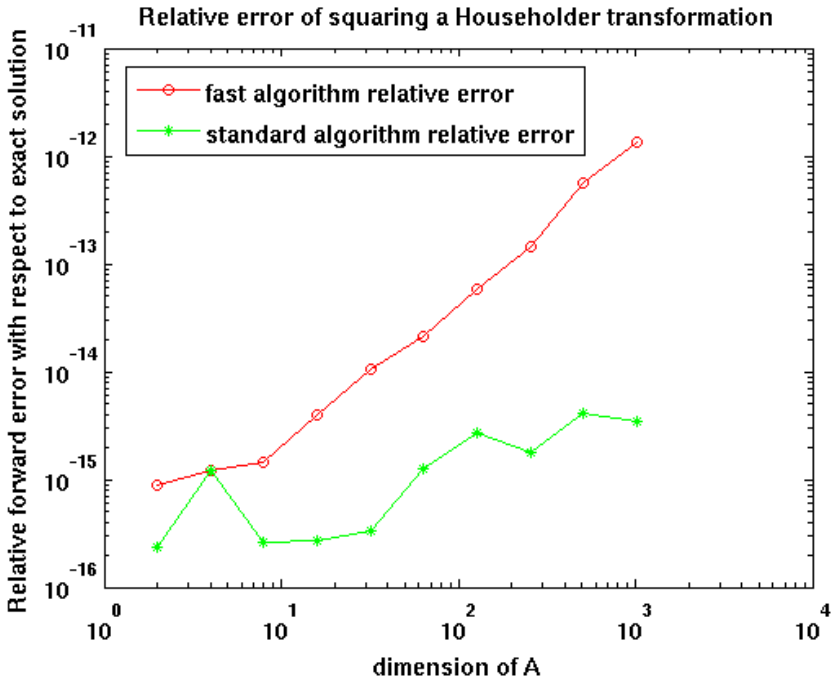
$$
\begin{aligned}
\tau_{ij}^{ab} &= t_{ij}^{ab} + \frac{1}{2} P_b^a P_j^i t_i^a t_j^b, \\
\tilde{F}_e^m &= f_e^m + \sum_{fn} v_{ef}^{mn} t_n^f, \\
\tilde{F}_e^a &= (1 - \delta_{ae}) f_e^a - \sum_m \tilde{F}_e^m t_m^a - \frac{1}{2} \sum_{mnf} v_{ef}^{mn} t_{mn}^{af} + \sum_{fn} v_{ef}^{an} t_n^f, \\
\tilde{F}_i^m &= (1 - \delta_{mi}) f_i^m + \sum_e \tilde{F}_e^m t_i^e + \frac{1}{2} \sum_{nef} v_{ef}^{mn} t_{in}^{ef} + \sum_{fn} v_{if}^{mn} t_n^f,
\end{aligned}
$$

Our CCSD factorization

$$
\begin{aligned}
\tilde{W}_{ei}^{mn} &= v_{ei}^{mn} + \sum_{f} v_{ef}^{mn} t_i^f, \\
\tilde{W}_{ij}^{mn} &= v_{ij}^{mn} + P_j^i \sum_{e} v_{ie}^{mn} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{mn} \tau_{ij}^{ef}, \\
\tilde{W}_{ie}^{am} &= v_{ie}^{am} - \sum_{n} \tilde{W}_{ei}^{mn} t_n^a + \sum_{f} v_{ef}^{ma} t_i^f + \frac{1}{2} \sum_{nf} v_{ef}^{mn} t_{in}^{af}, \\
\tilde{W}_{ij}^{am} &= v_{ij}^{am} + P_j^i \sum_{e} v_{ie}^{am} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{am} \tau_{ij}^{ef}, \\
z_i^a &= f_i^a - \sum_{m} \tilde{F}_i^m t_m^a + \sum_{e} f_e^a t_i^e + \sum_{em} v_{ei}^{ma} t_m^e + \sum_{em} v_{im}^{ae} \tilde{F}_e^m + \frac{1}{2} \sum_{efm} v_{ef}^{am} \tau_{im}^{ef} \\
&- \frac{1}{2} \sum_{emn} \tilde{W}_{ei}^{mn} t_{mn}^{ea}, \\
z_{ij}^{ab} &= v_{ij}^{ab} + P_j^i \sum_{e} v_{ie}^{ab} t_j^e + P_b^a P_j^i \sum_{me} \tilde{W}_{ie}^{am} t_{mj}^{eb} - P_b^a \sum_{m} \tilde{W}_{ij}^{am} t_m^b \\
&+ P_b^a \sum_{e} \tilde{F}_e^a t_{ij}^{eb} - P_j^i \sum_{m} \tilde{F}_i^m t_{mj}^{ab} + \frac{1}{2} \sum_{ef} v_{ef}^{ab} \tau_{ij}^{ef} + \frac{1}{2} \sum_{mn} \tilde{W}_{ij}^{mn} \tau_{mn}^{ab},
\end{aligned}
$$

Stability of symmetry preserving algorithms





Performance breakdown on BG/Q

Performance data for a CCSD iteration with 200 electrons and 1000 orbitals on 4096 nodes of Mira
4 processes per node, 16 threads per process
Total time: 18 mins
v-orbitals, o-electrons

kernel	% of time	complexity	architectural bounds
DGEMM	45%	$O(v^4o^2/p)$	flops/mem bandwidth
broadcasts	20%	$O(v^4o^2/p\sqrt{M})$	multicast bandwidth
prefix sum	10%	$O(p)$	allreduce bandwidth
data packing	7%	$O(v^2o^2/p)$	integer ops
all-to-all-v	7%	$O(v^2o^2/p)$	bisection bandwidth
tensor folding	4%	$O(v^2o^2/p)$	memory bandwidth

Tiskin's path doubling algorithm

Tiskin gives a way to do path-doubling in $F = O(n^3/p)$ operations.
We can partition each $\mathbf{A}^k$ by path size (number of edges)

$$\mathbf{A}^k = \mathbf{I} \oplus \mathbf{A}^k(1) \oplus \mathbf{A}^k(2) \oplus \ldots \oplus \mathbf{A}^k(k)$$

where each $\mathbf{A}^k(l)$ contains the shortest paths of up to $k \geq l$ edges, which have exactly l edges. We can see that

$$\mathbf{A}^l(l) \leq \mathbf{A}^{l+1}(l) \leq \ldots \leq \mathbf{A}^n(l) = \mathbf{A}^*(l),$$

in particular $\mathbf{A}^*(l)$ corresponds to a sparse subset of $\mathbf{A}^l(l)$.
The algorithm works by picking $l \in [k/2, k]$ and computing

$$(\mathbf{I} \oplus \mathbf{A})^{3k/2} \leq (\mathbf{I} \oplus \mathbf{A}^k(l)) \otimes \mathbf{A}^k,$$

which finds all paths of size up to $3k/2$ by taking all paths of size exactly $l \geq k/2$ followed by all paths of size up to k.