Algorithms as Multilinear Tensor Equations

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March 9, 2016

Pervasive paradigms in scientific computing

What commonalities exist in simulation and data analysis applications?

- multidimensional datasets (observations, discretizations)
- higher-order relations: equations, maps, graphs, hypergraphs
- **sparsity** and **symmetry** in structure of relations
- **algebraic descriptions of datasets and relations**

Tensor computations as programming abstractions

Tensors (scalars, vectors, matrices, etc.) are convenient abstractions for multidimensional data

- one type of object for any homogeneous dataset
- enable expression of symmetries
- reveal sparsity structure of relations in multidimensional space

Matrix computations $\subset$ tensor computations

- $=$ often reduce to or employ matrix algorithms
  - can leverage high performance matrix libraries
- $+$ high-order tensors can ‘act’ as many matrix unfoldings
- $+$ symmetries lower memory footprint and cost
- $+$ tensor factorizations (CP, Tucker, tensor train, ...)

What is the power of a parallel tensor library?

The ability to **optimally** orchestrate

- *algebraic transformations*
- *data movement*
- *synchronization*

for a **universal** class of algebraic computations

Applications of high-order tensor representations

Numerical solution to differential equations

- higher-order Taylor series expansion terms
- nonlinear terms and differential operators

Computer vision and graphics

- 2D image $\otimes$ angle $\otimes$ time
- compression (tensor factorizations, sparsity)

Machine learning

- sparse multi-feature discrete datasets
- reduced-order models, recommendation systems (tensor factorizations)

Graph computations

- hypergraphs, time-dependent graphs
- clustering/partitioning/path-finding (eigenvector computations)

Divide-and-conquer algorithms representable by tensor folding

- bitonic sort, FFT, scans

Applications to quantum systems

Manybody Schrödinger equation

- "curse of dimensionality" – exponential state space

Condensed matter physics

- tensor network models (e.g. DMRG), tensor per lattice site
- highly symmetric multilinear tensor representation
- exponential state space localized $\rightarrow$ factorized tensor form

Quantum chemistry (**electronic structure calculations**)

- models of molecular structure and chemical reactions
- methods for calculating electronic correlation:
  - "Post Hartree-Fock": configuration interaction, **coupled cluster**, Møller-Plesset perturbation theory
- multi-electron states as tensors,
  e.g. electron $\otimes$ electron $\otimes$ orbital $\otimes$ orbital
- nonlinear equations of partially (anti)symmetric tensors
- interactions diminish with distance $\rightarrow$ sparsity, low rank

Outline and highlights

1. Massively-parallel electronic structure calculations
   - Cyclops Tensor Framework (CTF): first distributed-memory tensor contraction framework
   - codes using CTF for wavefunction methods: Aquarius, QChem, VASP, Psi4
   - coupled cluster faster than NWChem by > 10X, nearly 1 petaflop/s
2. Sparse and discrete tensor computations
   - CTF supports arbitrary sparse multidimensional arrays
   - sparsity used to accelerate algebraic all-pairs shortest-paths
3. Communication-optimal algorithms for linear solvers
   - novel tradeoffs: synchronization vs communication in Cholesky and stencils
   - algorithms with $p^{1/6}$ less communication on p processors for LU, QR, eigs
   - topology-aware implementations: 12X speed-up for MM, 2X for LU
4. Preserving symmetry in tensor contractions
   - contraction of order $2s$ symmetric tensors in $\frac{(3s)!}{(s!)^3}$ fewer multiplies
   - up to 9X speed-up for partially-symmetric contractions in coupled cluster

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 ϕ is a Slater determinant
- expanding $0 = \langle\phi'|H|\Psi\rangle$ yields nonlinear equations for $\{T_i\}$ in F, V

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

where $\mathcal{P}$ is an antisymmetrization operator

A library for tensor computations

Cyclops Tensor Framework[1]

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

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

A library for tensor computations

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

```
Vector<> Jacobi(Matrix<> A, Vector<> b, int n){
  ... // split A = R + diag(1./d)
  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
  return x;
}
```

A library for tensor computations

Cyclops Tensor Framework

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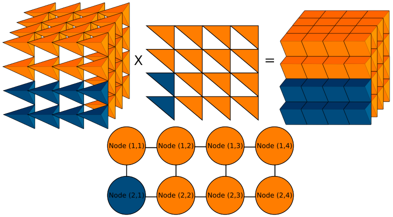
Jacobi iteration (solves $Ax = b$ iteratively) example code snippet

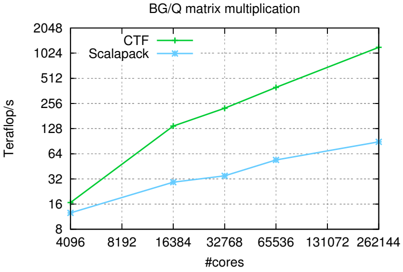
```
Vector<> Jacobi(Matrix<> A, Vector<> b, int n){
  Matrix<> R(A);
  R["ii"] = 0.0;
  Vector<> x(n), d(n), r(n);
  Function<> inv([](double & d){ return 1./d; });
  d["i"] = inv(A["ii"]); // set d to inverse of diagonal of A
  do {
    x["i"] = d["i"]*(b["i"]-R["ij"]*x["j"]);
    r["i"] = b["i"]-A["ij"]*x["j"];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

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





CCSD using CTF

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

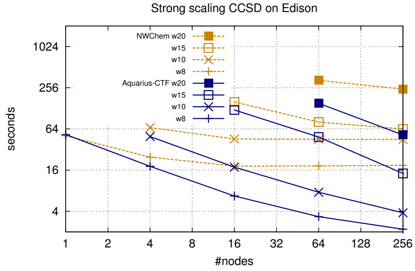
```
FMI["mi"]      += 0.5*WMNEF["mnef"]*T2["efin"];
WMNIJ["mnij"] += 0.5*WMNEF["mnef"]*T2["efij"];
FAE["ae"]      -= 0.5*WMNEF["mnef"]*T2["afmn"];
WAMEI["amei"] -= 0.5*WMNEF["mnef"]*T2["afin"];

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"];
```

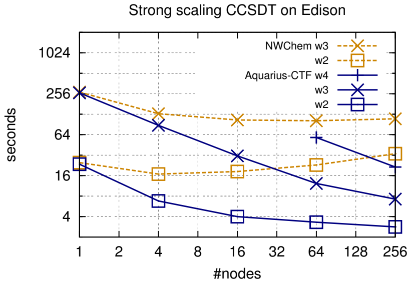
CTF is used within **Aquarius, QChem, VASP, and Psi4**

Comparison with NWChem

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

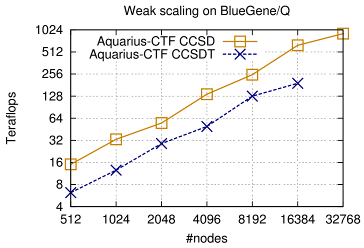
- provides CCSD and CCSDT
- derives equations via Tensor Contraction Engine (TCE)
- generates contractions as blocked loops leveraging Global Arrays

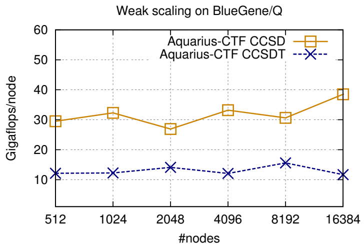


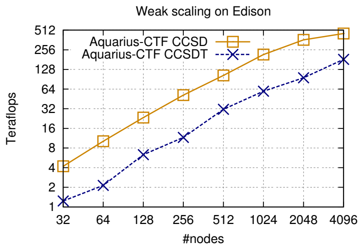


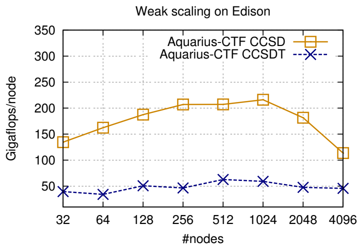
Coupled cluster on IBM BlueGene/Q and Cray XC30

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









[a] S., Matthews, Hammond, Demmel, JPDC, 2014

Sparsity in electronic structure computations

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"];
```

Consider sparse two-electron integrals: **`Vabcd`**, **`Vijkl`**, **`Vaibj`**

Algebraic shortest path computations

An n node graph can be represented by an $n \times n$ adjacency matrix

- a hypergraph with hyperedges of cardinality k, by an order k tensor

Tropical (geodetic) semiring

- additive (idempotent) operator: $a \oplus b \coloneqq \min(a, b)$, identity: ∞
- multiplicative operator: $a \otimes b \coloneqq a + b$, identity: 0
- matrix multiplication defined accordingly,

$$C = A \otimes B \quad \coloneqq \quad \forall i, j, C_{ij} = \min_k (A_{ik} + B_{kj})$$

Algebraic shortest path computations

Bellman-Ford algorithm (SSSP) for adjacency matrix A:

1. initialize $v^{(1)} = (0, \infty, \infty, \ldots)$
2. compute $v^{(n)}$ via recurrence $\qquad v^{(i+1)} = v^{(i)} \oplus (v^{(i)} \otimes A)$

All-pairs shortest-paths (APSP):

- distance matrix is the closure of A, $\qquad A^* = I \oplus A \oplus A^2 \oplus \ldots A^n$
- Floyd–Warshall = Gauss–Jordan elimination $\approx$ Gaussian elimination
  - $O(n^3)$ cost, but contains length $n \log n$ dependency path
- path doubling: $\log n$ steps, $O(n^3 \log n)$ cost:

$$B = I \oplus A, \qquad B^{2k} = B^k \otimes B^k, \qquad B^n = A^*$$

- sparse path doubling[a]:
  1. let C be subset of B^k corresponding to paths containing *exactly* k edges
  2. $B^{2k} = B^k \oplus (C \otimes B^k)$
  3. $O(n^3)$ cost, dependency paths length $O(\log^2 n)$

[a] Tiskin, Springer LNCS, 2001

Bellman–Ford Algorithm using CTF

CTF code for n node single-source shortest-paths (SSSP) calculation:

```
World w(MPI_COMM_WORLD);
Semiring<int> s(INT_MAX/2,
                []( int a, int b){ return min(a,b); },
                MPI_MIN,
                0,
                []( int a, int b){ return a+b; });

Matrix<int> A(n,n,SP,w,s); // Adjacency matrix
Vector<int> v(n,w,s); // Distances from starting vertex

... // Initialize A and v

//Bellman-Ford SSSP algorithm
for (int t=0; t<n; t++){
  v["i"] += v["j"]*A["ji"];
}
```

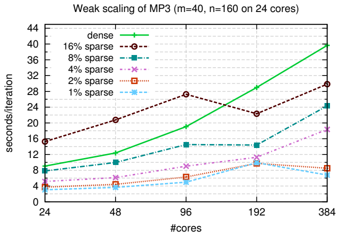
Betweenness centrality

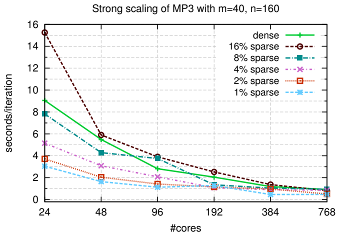
Betweenness centrality code snippet, for *k* of *n* nodes

```
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"]);
  ...
}
```

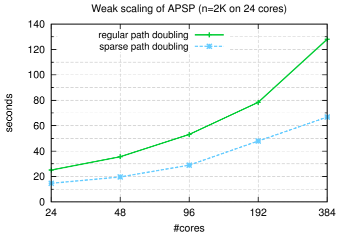
Performance of CTF for sparse computations

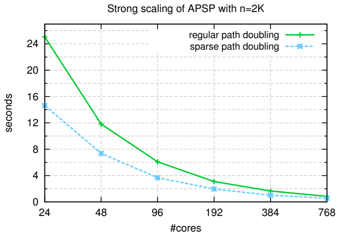
MP3 leveraging sparse-dense tensor contractions[a]





All-pairs shortest-paths based on path doubling with sparsification[a]





[a] S., Hoefler, Demmel, arXiv, 2015

Beyond computation cost

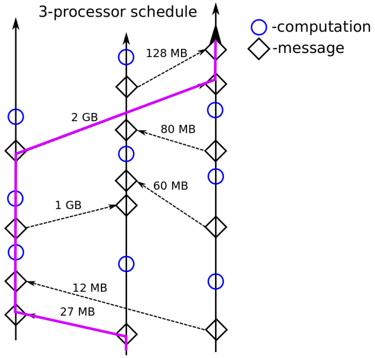
Algorithms should minimize communication, not just computation

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

Cost model for parallel algorithms

Given a schedule of work and communication tasks on p processors, 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[2]

$$W_{\text{MM}} = \Omega\left(\frac{n^2}{p^{2/3}}\right)$$

- memory-dependent horizontal communication lower bound[3]

$$W_{\text{MM}} = \Omega\left(\frac{n^3}{p\sqrt{M}}\right)$$

- with $M = cn^2/p$ memory, hope to obtain communication cost

$$W = O(n^2/\sqrt{cp})$$

- libraries like ScaLAPACK, Elemental optimal only for $c = 1$

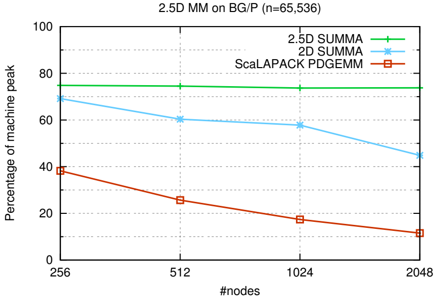
[2] Aggarwal, Chandra, Snir, TCS, 1990

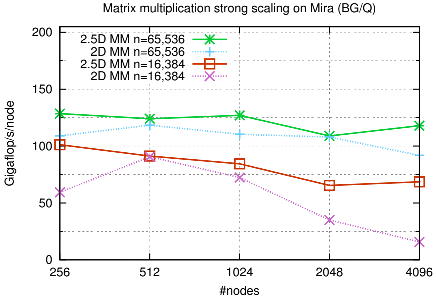
[3] Irony, Toledo, Tiskin, JPDC, 2004

Communication-efficient matrix multiplication

Communication-avoiding algorithms for matrix multiplication have been studied extensively[4]

They continue to be attractive on modern architectures[5]





12X speed-up, 95% reduction in comm. for $n = 8\text{K}$ on 16K nodes of BG/P

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

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

Synchronization cost lower bounds

Unlike matrix multiplication, many algorithms in numerical linear algebra have polynomial depth (contain a long dependency path)

- matrix multiplication synchronization cost bound[6]

$$S_{\mathrm{MM}} = \Theta\left(\frac{n^3}{pM^{3/2}}\right)$$

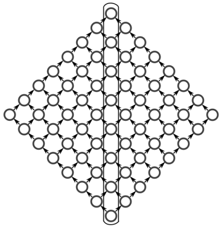
- algorithms for Cholesky, LU, QR, SVD do not attain this bound
- low granularity computation increases synchronization cost

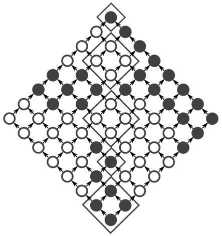
[6] Ballard, Demmel, Holtz, Schwartz, SIAM JMAA, 2011

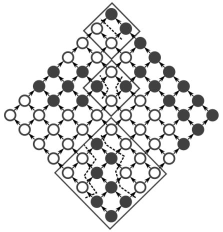
Tradeoffs in the diamond DAG

Computation vs synchronization tradeoff for the $n \times n$ diamond DAG,[7]

$$F \cdot S = \Omega(n^2)$$


Dependency chain P


Monochrome dependency intervals


Multicolored dependency intervals

We generalize this idea[8]

- additionally consider horizontal communication
- allow arbitrary (polynomial or exponential) interval expansion

[7] Papadimitriou, Ullman, SIAM JC, 1987

[8] 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,

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

For Cholesky of an $n \times n$ matrix,

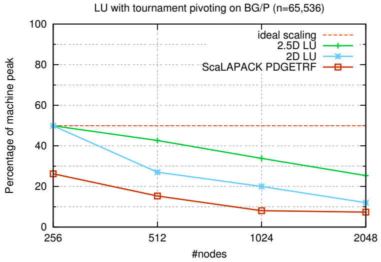
$$F_{\mathrm{CHOL}} \cdot S_{\mathrm{CHOL}}^2 = \Omega\left(n^3\right) \qquad W_{\mathrm{CHOL}} \cdot S_{\mathrm{CHOL}} = \Omega\left(n^2\right)$$

[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

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



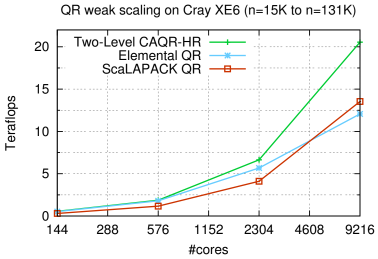
- LU with pairwise pivoting[9] extended to tournament pivoting[10]
- first implementation of a communication-optimal LU algorithm[10]

[9] Tiskin, FGCS, 2007

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

Communication-efficient QR factorization

- $W_{\text{QR}} = O(n^2/\sqrt{cp}), S_{\text{QR}} = O(\sqrt{cp})$ using Givens rotations[a]
- Householder form can be reconstructed quickly from TSQR[b]
  $$Q = I - YTY^T \qquad \Rightarrow \qquad \text{LU}(I - Q) \rightarrow (Y, TY^T)$$
- enables communication-optimal Householder QR[c]
- Householder aggregation yields performance improvements



Further directions: 2.5D QR implementation, lower bounds, pivoting

[a] Tiskin, FGCS, 2007

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

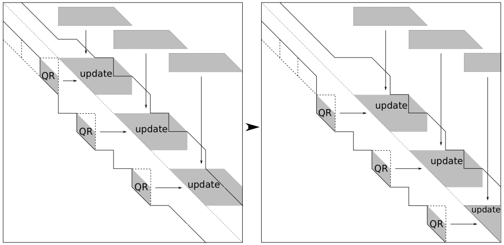
[c] S., UCB, 2014

Communication-efficient eigenvalue computation

For the dense symmetric matrix eigenvalue problem[a]

$$W_{\mathrm{SE}} = O(n^2/\sqrt{cp}), S_{\mathrm{QR}} = O(\sqrt{cp}\log^2 p)$$

- above costs obtained by left-looking algorithm with Householder aggregation, however, with increased vertical communication
- successive band reduction minimizes both communication costs



Further directions: implementations (ongoing), eigenvector computation, SVD

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

Synchronization tradeoffs in stencils

Our lower bound analysis extends to sparse iterative methods:[11]
For computing s applications of a $(2m+1)^d$-point stencil,

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

- 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
- further directions:
  - implementation of proposed algorithm
  - lower bounds for graph traversals

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

Exploiting symmetry in tensors

Tensor symmetry (e.g. $A_{ij} = A_{ji}$) reduces memory and cost[12]

- 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 $(A_{ij} = A_{ji})^1$

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

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

$$c^{kl}_i = \sum_{j,m} A^{km}_{ij} b^{ml}_j = \quad \sum_j \left(\sum_m A^{km}_{ij}(b^{ml}_i + b^{ml}_j) \right) - \sum_m \left(\sum_j A^{km}_{ij} \right) b^{ml}_i$$

- let $Z^{kl}_{ij} = \sum_m A^{km}_{ij}(b^{ml}_i + b^{ml}_j)$ and observe $Z^{kl}_{ij} = Z^{kl}_{ji}$
- Z^{kl}_{ij} can be computed using $(1/2)n^5$ multiplies and $(1/2)n^5$ adds

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

Symmetry preserving algorithms

By exploiting symmetry, reduce multiplies (but increase adds)[13]

- rank-2 vector outer product

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

- squaring a symmetric matrix A (or $AB + BA$)

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

- for symmetrized contraction of symmetric order $s + v$ and $v + t$ tensors

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

e.g. cases above are

- $s = 1, t = 1, v = 0 \rightarrow$ reduction by 2X
- $s = 1, t = 1, v = 1 \rightarrow$ reduction by 6X

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

Applications of symmetry preserving algorithms

Extensions and applications:

- algorithms generalize to antisymmetric and Hermitian tensors
- cost reductions in partially-symmetric coupled cluster contractions: 2X-9X for select contractions, 1.3X-2.1X for methods
- for Hermitian tensors, multiplies cost 3X more than adds
  - Hermitian matrix multiplication and tridiagonal reduction (BLAS and LAPACK routines) with 25% fewer operations
- $(2/3)n^3$ bilinear rank for squaring a *nonsymmetric* matrix
- decompose symmetric contractions into smaller symmetric contractions

Further directions:

- high performance implementation
- symmetry in tensor equations (e.g. Cholesky factors)
- generalization to other group actions
- relationships to fast matrix multiplication and structured matrices

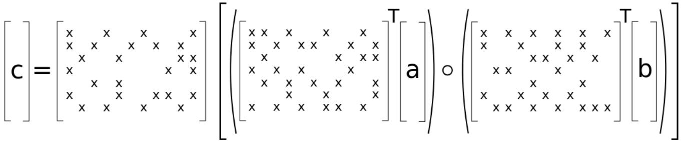
Lower bounds for symmetry preserving algorithms

Bilinear algorithms[14] enable robust communication lower bounds

- 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 derived based on matrix rank[15]

[14] Pan, Springer, 1984

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

Communication cost of symmetry preserving algorithms

For contraction of order $s + v$ tensor with order $v + t$ tensor[16]

- symmetry preserving algorithm requires $\frac{(s+v+t)!}{s!v!t!}$ fewer multiplies
- matrix-vector-like algorithms ($\min(s, v, t) = 0$)
    - vertical communication dominated by largest tensor
    - horizontal communication asymptotically greater if only unique elements are stored and $s \neq v \neq t$
- matrix-matrix-like algorithms ($\min(s, v, t) > 0$)
    - vertical and horizontal communication costs asymptotically greater for symmetry preserving algorithm when $s \neq v \neq t$
- further work: bounds for nested and iterative bilinear algorithms

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

Summary of contributions

Novel results described in this talk:

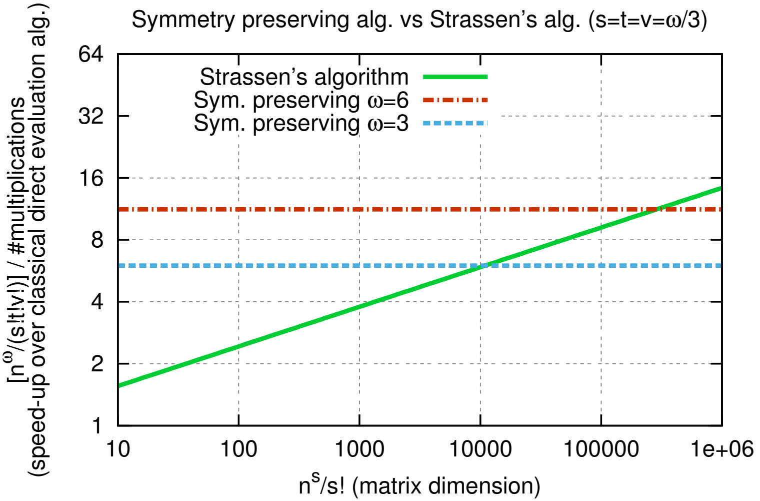
- Cyclops Tensor Framework
  - first fully robust distributed-memory tensor contraction library
  - supports symmetry, sparsity, general algebraic structures
  - coupled cluster performance more than 10X faster than state-of-the-art, reaching 1 petaflop/s performance
- communication-avoiding linear solvers
  - tradeoffs: synchronization vs computation or communication in TRSV, Cholesky, and stencils
  - new algorithms and implementations with up to $p^{1/6}$ less communication for LU, QR, symmetric eigenvalue problem
  - speed-ups of up to 2X for LU and QR over vendor-optimized libraries
- symmetry preserving algorithms
  - reduce number of multiplications in symmetric contractions by $\frac{(s+t+v)!}{s!t!v!}$
  - reduce cost of basic Hermitian matrix operations by 25%
  - reduce cost of some contractions in coupled cluster by 2X in CCSD (1.3X overall), 4X in CCSDT (2.1X overall), 9X in CCSDTQ
  - new algebraic formulation of communication lower bounds

Impact and future work

- Cyclops Tensor Framework
  - already widely-adapted in quantum chemistry, many requests for features
  - study algorithms for tensor expressions $\rightarrow$ factorization, scheduling, ...
  - engage new application domains (via sparsity and algebraic structures)
    - tensor networks for condensed matter-physics, particle methods
    - graph algorithms, discrete data analysis
    - graphics, computer vision, machine learning
- communication-avoiding algorithms
  - existing fast implementations already used by applications (e.g. QBox)
  - find efficient methods of searching larger tuning spaces
  - algorithms for computing eigenvectors, SVD, tensor factorizations
  - study (randomized) algorithms for sparse matrix factorization
- symmetry in tensor computations
  - cost improvements $\rightarrow$ fast library implementations $\rightarrow$ application speed-ups
  - study symmetries in tensor equations and factorizations
  - consider other symmetries and relation to fast matrix multiplication

Backup slides

Symmetry preserving algorithm vs Strassen's algorithm



Nesting of bilinear algorithms

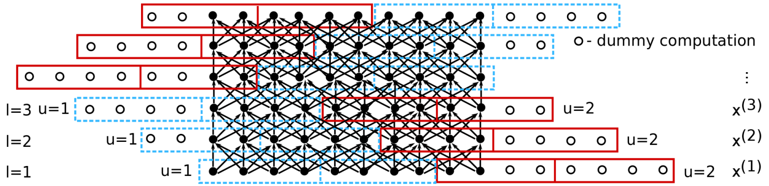
Given two bilinear algorithms:

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

We can nest them by computing their tensor product

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

Block-cyclic algorithm for s-step methods

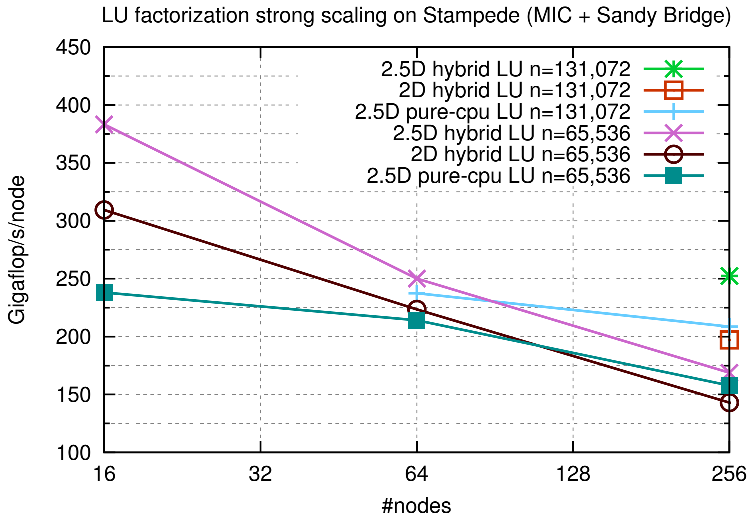


For s-steps of a $(2m+1)^d$-point stencil with block-size of $H^{1/d}/m$,

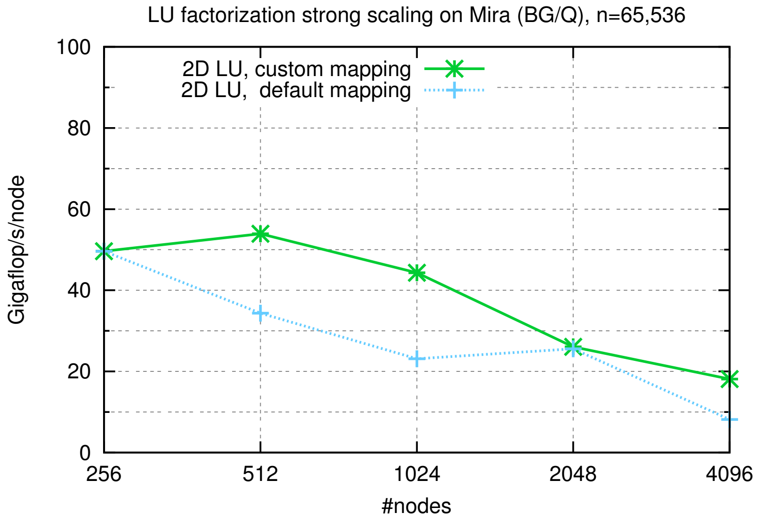
$$W_{\mathrm{Kr}} = O\left(\frac{msn^d}{H^{1/d}p}\right) \quad S_{\mathrm{Kr}} = O(sn^d/(pH)) \quad Q_{\mathrm{Kr}} = O\left(\frac{msn^d}{H^{1/d}p}\right)$$

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

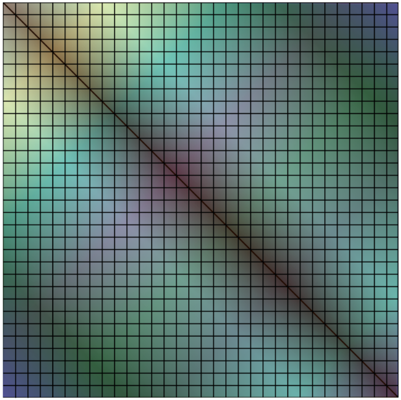

LU factorization strong scaling on Stampede (MIC + Sandy Bridge)
2.5D hybrid LU n=131,072
2D hybrid LU n=131,072
2.5D pure-cpu LU n=131,072
2.5D hybrid LU n=65,536
2D hybrid LU n=65,536
2.5D pure-cpu LU n=65,536
Gigaflop/s/node
450
400
350
300
250
200
150
100
16
32
64
128
256
#nodes

Topology-aware mapping on BG/Q

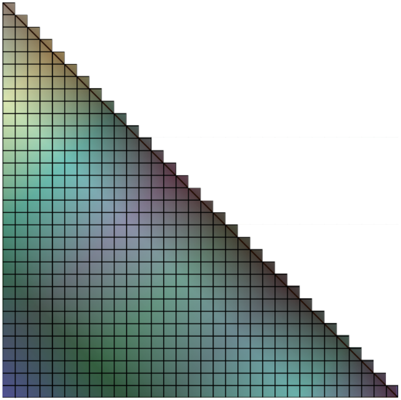


Symmetric matrix representation

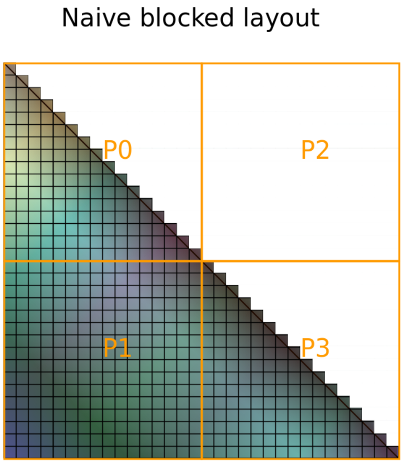
Symmetric matrix

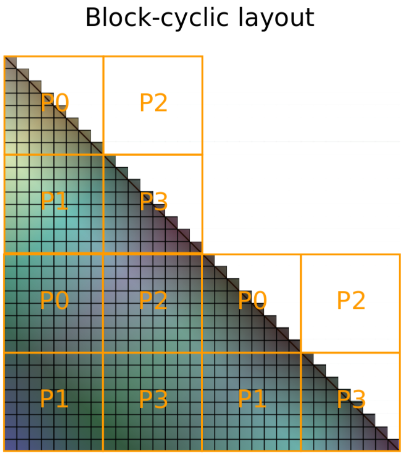


Unique part of symmetric matrix



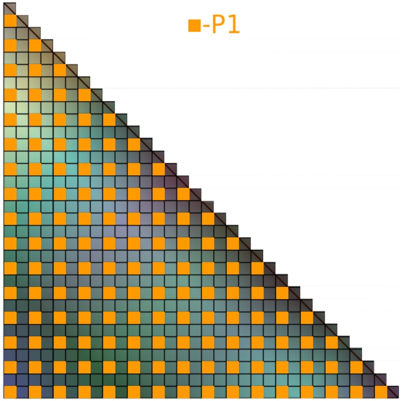
Blocked distributions of a symmetric matrix

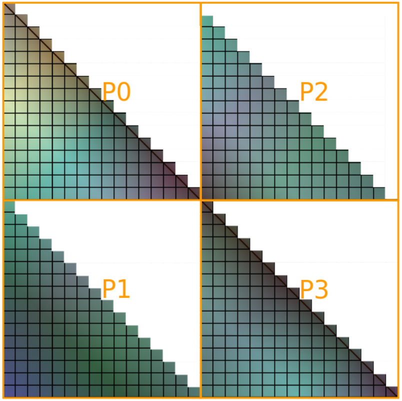




Cyclic distribution of a symmetric matrix

Cyclic layout ~ Improved blocked layout





Our CCSD factorization

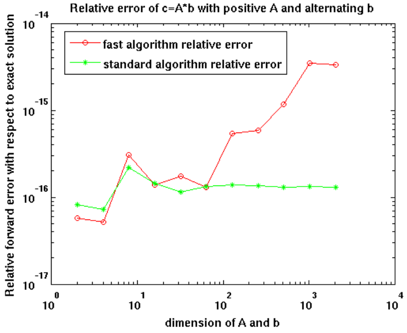
Credit to John F. Stanton and Jurgen Gauss

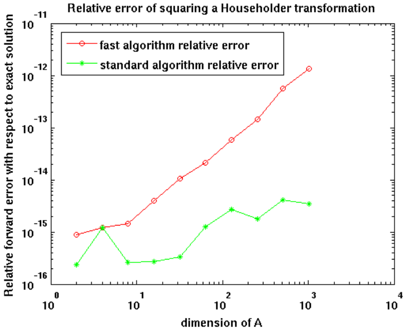
$$
\begin{aligned}
\tau_{ij}^{ab} &= t_{ij}^{ab} + \frac{1}{2} P_b^a P_j^i t_i^a t_j^b, \\
\tilde{F}_e^m &= f_e^m + \sum_{fn} v_{ef}^{mn} t_n^f, \\
\tilde{F}_e^a &= (1 - \delta_{ae}) f_e^a - \sum_m \tilde{F}_e^m t_m^a - \frac{1}{2} \sum_{mnf} v_{ef}^{mn} t_{mn}^{af} + \sum_{fn} v_{ef}^{an} t_n^f, \\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

Our CCSD factorization

$$
\begin{aligned}
\tilde{W}^{mn}_{ei} &= v^{mn}_{ei} + \sum_f v^{mn}_{ef} t^f_i , \\
\tilde{W}^{mn}_{ij} &= v^{mn}_{ij} + P^i_j \sum_e v^{mn}_{ie} t^e_j + \frac{1}{2} \sum_{ef} v^{mn}_{ef} \tau^{ef}_{ij} , \\
\tilde{W}^{am}_{ie} &= v^{am}_{ie} - \sum_n \tilde{W}^{mn}_{ei} t^a_n + \sum_f v^{ma}_{ef} t^f_i + \frac{1}{2} \sum_{nf} v^{mn}_{ef} t^{af}_{in} , \\
\tilde{W}^{am}_{ij} &= v^{am}_{ij} + P^i_j \sum_e v^{am}_{ie} t^e_j + \frac{1}{2} \sum_{ef} v^{am}_{ef} \tau^{ef}_{ij} , \\
z^a_i &= f^a_i - \sum_m \tilde{F}^m_i t^a_m + \sum_e f^a_e t^e_i + \sum_{em} v^{ma}_{ei} t^e_m + \sum_{em} v^{ae}_{im} \tilde{F}^m_e + \frac{1}{2} \sum_{efm} v^{am}_{ef} \tau^{ef}_{im} \\
&- \frac{1}{2} \sum_{emn} \tilde{W}^{mn}_{ei} t^{ea}_{mn} , \\
z^{ab}_{ij} &= v^{ab}_{ij} + P^i_j \sum_e v^{ab}_{ie} t^e_j + P^a_b P^i_j \sum_{me} \tilde{W}^{am}_{ie} t^{eb}_{mj} - P^a_b \sum_m \tilde{W}^{am}_{ij} t^b_m \\
&+ P^a_b \sum_e \tilde{F}^a_e t^{eb}_{ij} - P^i_j \sum_m \tilde{F}^m_i t^{ab}_{mj} + \frac{1}{2} \sum_{ef} v^{ab}_{ef} \tau^{ef}_{ij} + \frac{1}{2} \sum_{mn} \tilde{W}^{mn}_{ij} \tau^{ab}_{mn} ,
\end{aligned}
$$

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.