Algorithms as Multilinear Tensor Equations

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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
- relations lead to solution directly or as an iterative criterion
- **algebraic descriptions of datasets and relations**

Pervasive paradigms in scientific computing

What abstractions are needed in high performance computing?

- data abstractions reflecting native dimensionality and structure
- functions orchestrating **communication** and **synchronization**
- **provably efficient building-block algorithms**

Outline

Matrix computations $\subset$ tensor computations

Tensors 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

Tensor computations naturally extend numerical linear algebra

- $=$ 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, ...)

Applications of high-order tensor representations

Numerical solution to differential equations

- nonlinear terms and differential operators
- truncated Taylor series expansions

Computer vision and graphics

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

Machine learning

- sparse multi-feature discrete datasets
- reduced-order models (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

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]

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

- rank-2 vector outer product[1]

$$C_{ij} = a_ib_j + a_jb_i = (a_i + a_j)(b_i + b_j) - a_ib_i - a_jb_j$$

- 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 multiplies [1]

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

Symmetry preserving algorithms

By exploiting symmetry, reduce multiplies (but increase adds)[2]

- partially symmetric contractions
  - *symmetry preserving algorithm can be nested over each index group*
  - reduction in multiplies $\rightarrow$ reduction in nested calls
  - cost reductions in coupled cluster:
    2X-9X for select contractions, 1.3X-2.1X for methods
- algorithms generalize to most antisymmetric tensor contractions
- for Hermitian tensors, multiplies cost 3X more than adds
  - Hermitian matrix multiplication and tridiagonal reduction (BLAS and LAPACK routines) with 25% fewer ops
- $(2/3)n^3$ bilinear rank for squaring a *nonsymmetric* matrix
- allows blocking of symmetric contractions into smaller symmetric contractions

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

Beyond computation cost

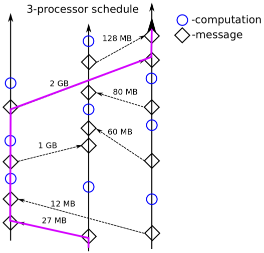
Algorithms should minimize communication, not just computation

- 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[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, hope to obtain communication cost

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

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

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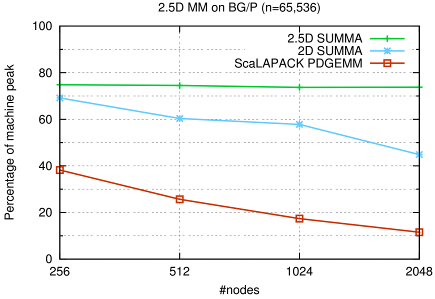
[3] Aggarwal, Chandra, Snir, TCS, 1990

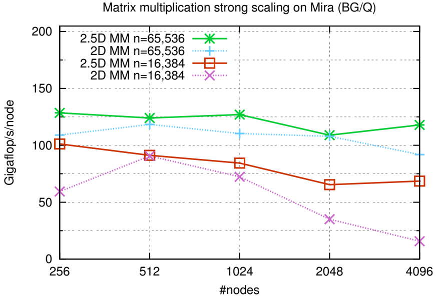
[4] Irony, Toledo, Tiskin, JPDC, 2004

Communication-efficient matrix multiplication

Communication-avoiding 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 (contain a long dependency path)

- matrix multiplication synchronization cost bound[7]

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

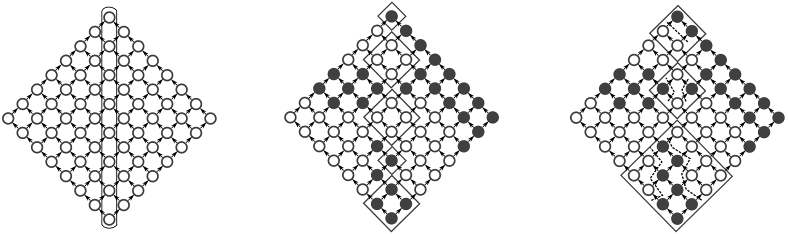
- algorithms for Cholesky, LU, QR, SVD do not attain this bound
- low granularity computation increases synchronization cost

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

Tradeoffs in the diamond DAG

Computation vs synchronization tradeoff for the $n \times n$ diamond DAG,[8]

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



Dependency chain P — Monochrome dependency intervals — Multicolored dependency intervals

We generalize this idea[9]

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

[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,

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

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

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

Proof employs classical Loomis-Whitney inequality:

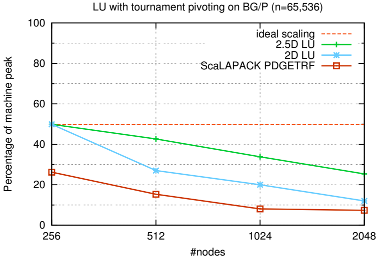
for any $R \subset \mathbb{N} \times \mathbb{N} \times \mathbb{N}$, three projections of R onto $\mathbb{N} \times \mathbb{N}$ have total size at least $|R|^{2/3}$

[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

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



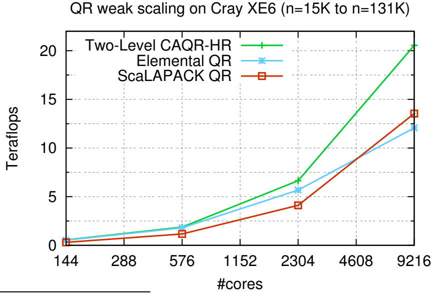
- LU with pairwise pivoting[10] extended to tournament pivoting[11]
- first implementation of a communication-optimal LU algorithm[11]

[10] Tiskin, FGCS, 2007

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

Communication-efficient QR factorization

- $W_{QR} = O(n^2/\sqrt{cp}), S_{QR} = O(\sqrt{cp})$ 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, S., IPDPS, 2014

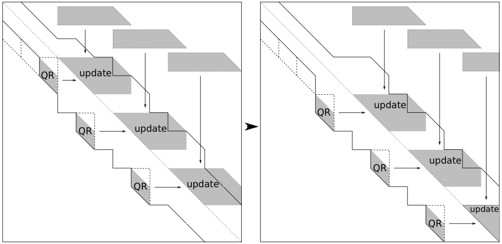
[14] S., UCB, 2014

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



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

Synchronization tradeoffs in stencils

Our lower bound analysis extends to sparse iterative methods:[15]
For computing s applications of a $(2m+1)^d$-point stencil

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

- 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

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

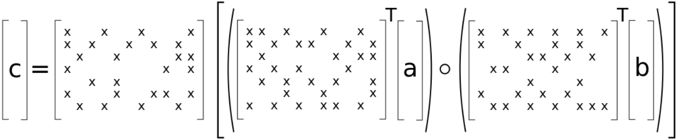
Beyond the Loomis-Whitney inequalities

Loomis-Whitney inequalities are not sufficient for all computations

- symmetry preserving tensor contraction algorithms have arbitrary order projections from order d set
- bilinear algorithms[16] 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 derived based on matrix rank[17]

[16] Pan, Springer, 1984

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

Communication cost of symmetry preserving algorithms

For contraction of order $s+v$ tensor with order $v+t$ tensor[18]

- 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 $s \neq v \neq t$

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

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

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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;
}
```

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"];
```

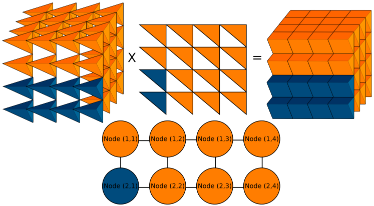
Betweenness centrality

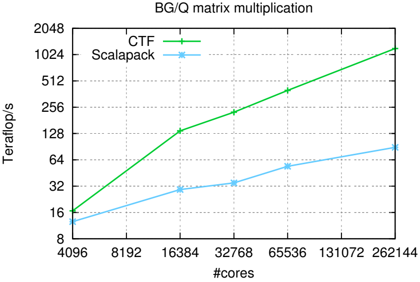
Betweenness centrality code snippet, for k of n nodes

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

CTF is highly tuned for massively-parallel machines

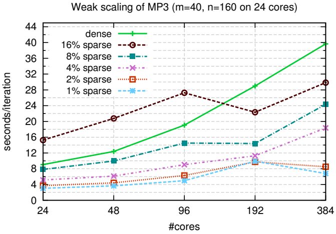
- virtualized multidimensional processor grids
- topology-aware mapping and collective communication
- performance-model-driven decomposition done at runtime
- optimized redistribution kernels for tensor transposition

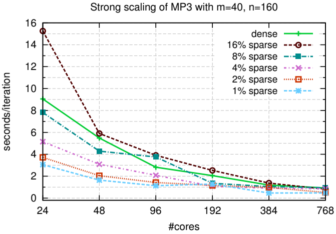




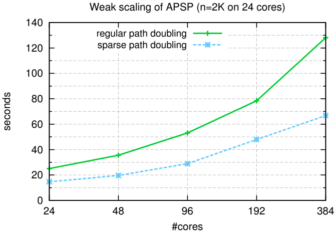
Performance of CTF for sparse computations

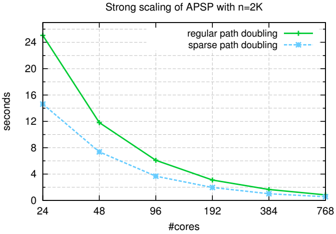
MP3 leveraging sparse-dense tensor contractions[a]





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





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

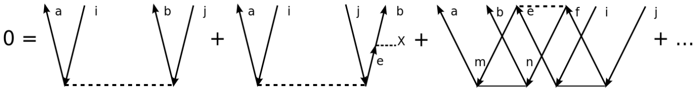
Coupled cluster methods

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

- 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 tensors T_1, T_2, T_3, T_4
- they use an exponential ansatz for the wavefunction,

$$\Psi = e^{T_1+T_2+T_3+T_4}\phi$$

  where ϕ is a fully-antisymmetric simple Slater determinant
- expanding Ψ as a Taylor series $\rightarrow$ nonlinear equations in T, F, V



CCSD using CTF

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

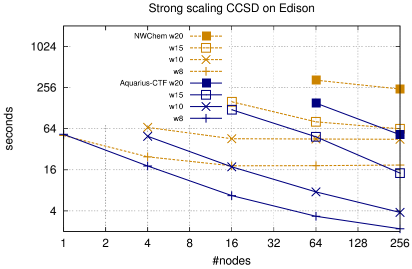
```
FMI["mi"]      += 0.5*WMNEF["mnef"]*T2["efin"];
WMNIJ["mnij"] += 0.5*WMNEF["mnef"]*T2["efij"];
FAE["ae"]      -= 0.5*WMNEF["mnef"]*T2["afmn"];
WAMEI["amei"] -= 0.5*WMNEF["mnef"]*T2["afin"];

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"];
```

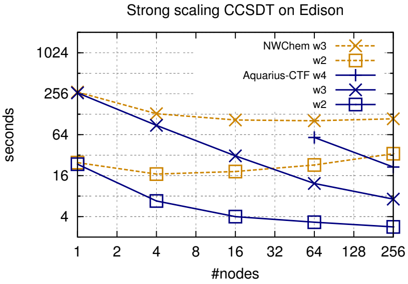
CTF-based CCSD codes exist in Aquarius, QChem, VASP, and Psi4

Comparison with NWChem

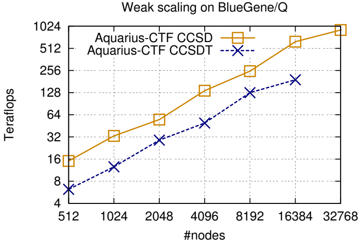
NWChem is the most commonly-used distributed-memory quantum chemistry method suite

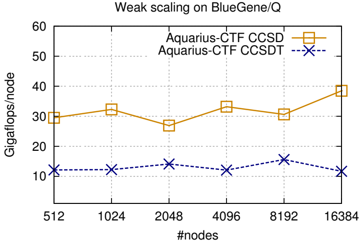
- provides CCSD and CCSDT
- derives equations via Tensor Contraction Engine (TCE)
- generates contractions as blocked loops leveraging Global Arrays

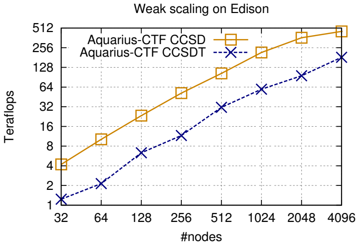


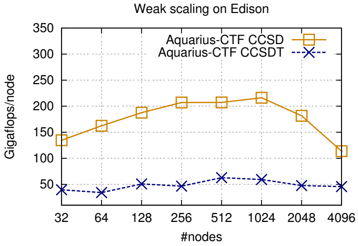


CCSD up to 55 (50) water molecules with cc-pVDZ
CCSDT up to 10 water molecules with cc-pVDZ[a]









Summary of contributions

Novel results described in this talk:

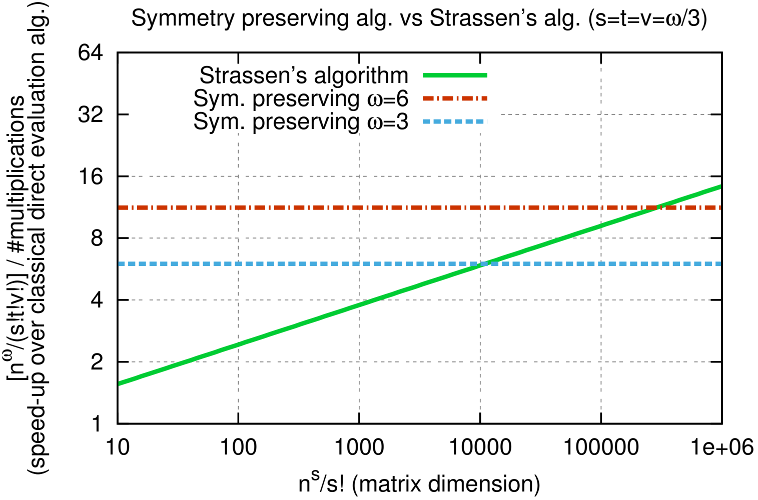
- symmetry preserving algorithms
  - reduce number of multiplications in symmetric contractions by $\omega!$
  - reduce cost of basic Hermitian matrix operations by 25%
  - reduce cost of some contractions in coupled cluster by 2X in CCSD (1.3X overall), 4X in CCSDT (2.1X overall), 9X in CCSDTQ
- communication and synchronization lower bounds
  - tradeoffs: synchronization vs computation or communication in TRSV, Cholesky, and stencils
  - rank-based lower bounds to analyze symmetric contractions
- communication avoiding dense matrix factorizations
  - 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
- 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

Future work

- open theoretical problems
  - relation of symmetry preserving algorithms to displacement rank and bilinear algorithm complexity
  - exploiting symmetry across tensors (e.g. in tensor networks)
  - synchronization lower bounds for QR and SVD
  - tight communication lower bounds for sparse–dense multiply
  - communication-avoiding algorithms for tensor factorizations
- high performance implementations
  - nested symmetry preserving algorithms
  - communication-optimal QR, improvements to symmetric eigensolver
  - tensor factorizations as part of CTF
  - optimized evaluation and scheduling of tensor expressions
  - extensions to sparsity and algebraic structure support in CTF
- programming abstractions for applications
  - representations for factorized tensors (tensor networks)
  - block-sparsity and block-factorization of tensors
  - expansion of application-based feedback loop

Backup slides

Symmetry preserving algorithm vs Strassen's algorithm



Nesting of bilinear algorithms

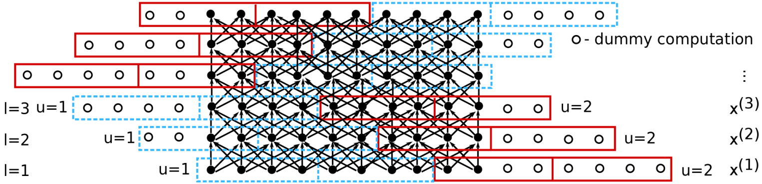
Given two bilinear algorithms:

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

We can nest them by computing their tensor product

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

Block-cyclic algorithm for s-step methods

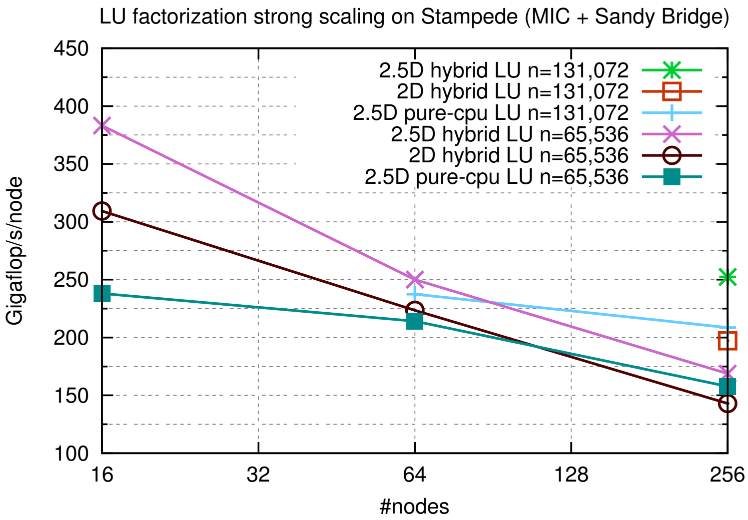


For s-steps of a $(2m+1)^d$-point stencil with block-size of $H^{1/d}/m$,

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

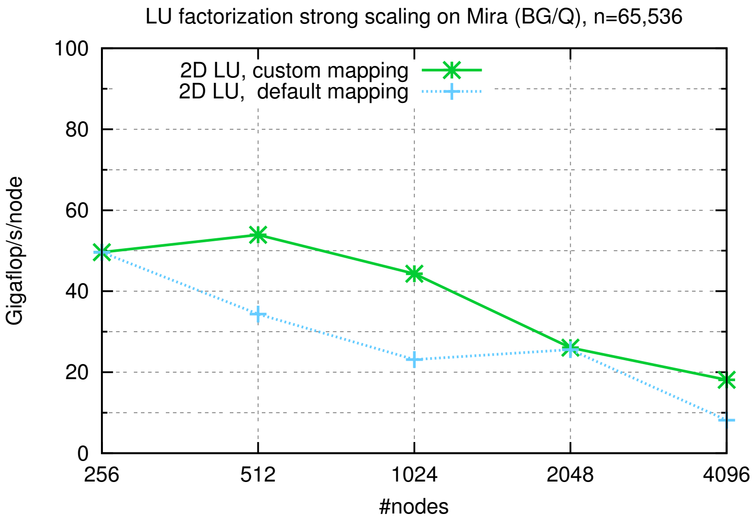
which are good when $H = \Theta(n^d/p)$, so the algorithm is useful when the cache size is a bit smaller than n^d/p

2.5D LU on MIC

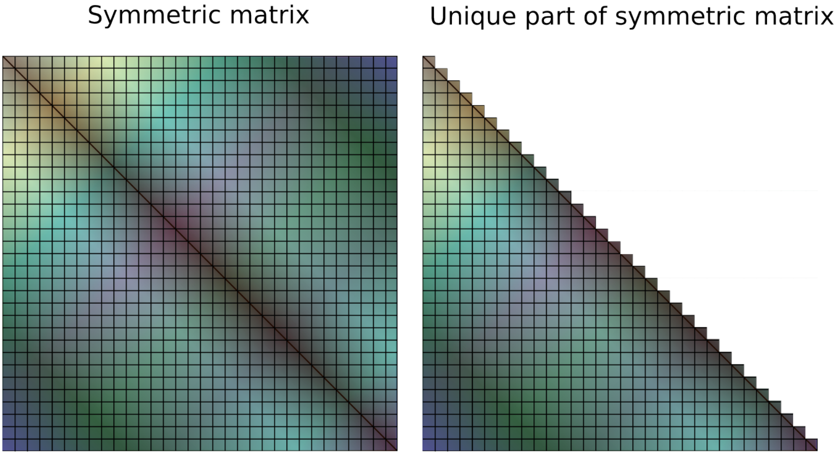


LU factorization strong scaling on Stampede (MIC + Sandy Bridge)
Gigaflop/s/node
#nodes
450
400
350
300
250
200
150
100
16
32
64
128
256
2.5D hybrid LU n=131,072
2D hybrid LU n=131,072
2.5D pure-cpu LU n=131,072
2.5D hybrid LU n=65,536
2D hybrid LU n=65,536
2.5D pure-cpu LU n=65,536

Topology-aware mapping on BG/Q

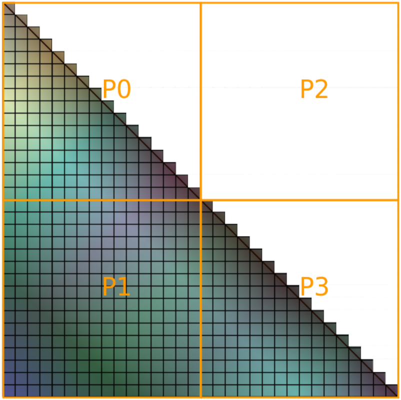


Symmetric matrix representation

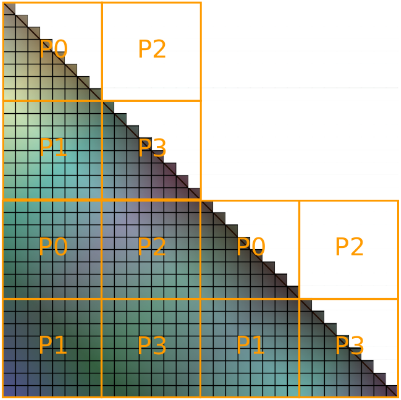


Blocked distributions of a symmetric matrix

Naive blocked layout

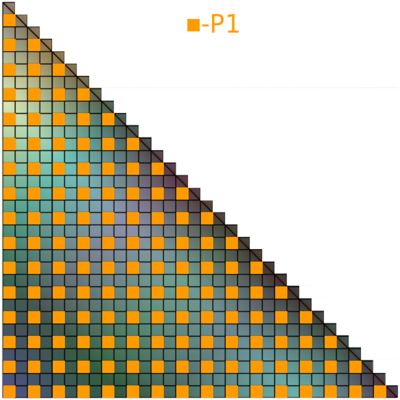


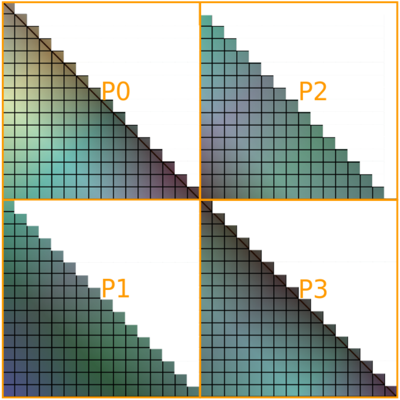
Block-cyclic layout



Cyclic distribution of a symmetric matrix

Cyclic layout $\sim$ Improved blocked layout





Our CCSD factorization

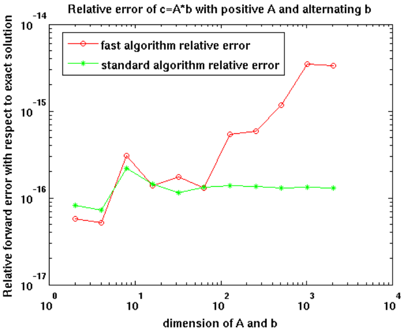
Credit to John F. Stanton and Jurgen Gauss

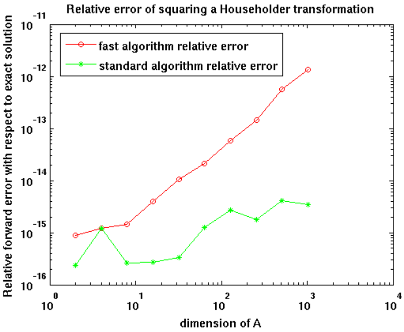
$$
\begin{aligned}
\tau_{ij}^{ab} &= t_{ij}^{ab} + \frac{1}{2} P_b^a P_j^i t_i^a t_j^b, \\
\tilde{F}_e^m &= f_e^m + \sum_{fn} v_{ef}^{mn} t_n^f, \\
\tilde{F}_e^a &= (1-\delta_{ae}) f_e^a - \sum_m \tilde{F}_e^m t_m^a - \frac{1}{2} \sum_{mnf} v_{ef}^{mn} t_{mn}^{af} + \sum_{fn} v_{ef}^{an} t_n^f, \\
\tilde{F}_i^m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

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.