Algorithms as multilinear tensor equations

Edgar Solomonik

Department of Computer Science
ETH Zurich

Technische Universität München

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Tensors and algebraic structures

We consider the expression of data as indexable collections of elements and algorithms as applications of algebraic operators.

Definition (Algebraic structure)

A set of elements (type), potentially equipped with operators and identities

Examples: set, monoid, group, semiring, ring

Definition (Tensor)

A collection of elements of a single type, $\mathbf{T}$, with some order k and dimensions $(n_1, \ldots, n_k)$, with elements $T_{i_1 \ldots i_k}$

Examples: scalar, vector, matrix

An algebraic structure defines summation and contraction of tensors.

Numerical tensor computations

Classical matrix-based computations over the $(+, \cdot)$ ring

- stencil computations (iterative methods for sparse linear systems)

$$\mathbf{x}^{(l)} := \mathbf{A}\mathbf{x}^{(l-1)}$$

- dense matrix factorizations (direct solvers for dense linear systems)

$$\mathbf{A} \approx \mathbf{LU} \qquad \mathbf{A} \approx \mathbf{QR} \qquad \mathbf{A} \approx \mathbf{UDV}^{\mathsf{T}}$$

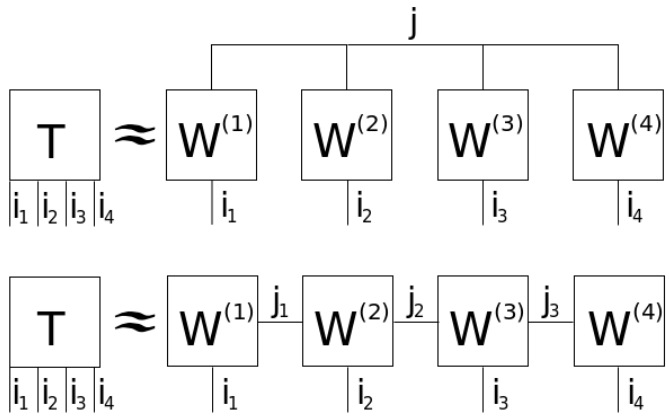
- tensor contractions (peturbation theory, solvers for nonlinear systems)

$$\sum_f F_f^a T_{ij}^{fb} - \sum_n F_i^n T_{nj}^{ab} + \frac{1}{2}\sum_{e,f} V_{ef}^{ab} T_{ij}^{ef} + \frac{1}{2}\sum_{m,n} V_{ij}^{mn} T_{mn}^{ab} - \sum_{e,m} V_{ei}^{am} T_{mj}^{eb}$$

- tensor decompositions (compression)

$$T_{i_1 \ldots i_k} \approx \sum_j W_{i_1 j}^{(1)} \cdots W_{i_k j}^{(k)}$$

$$T_{i_1 \ldots i_k} \approx \sum_{j_1 \ldots j_{k-1}} W_{i_1 j_1}^{(1)} W_{j_1 i_2 j_2}^{(2)} \cdots W_{j_{k-2} i_{k-1} j_{k-1}}^{(k-1)} W_{j_{k-1} i_k}^{(k)}$$



Discrete tensor algorithms

Alternative algebraic structures expand potential of tensor computations

- graph algorithms via tropical (geodetic) semiring $(\min, +)$
  - single-source shortest-paths via Bellman-Ford (stencil-like)
  - all-pairs shortest-paths (APSP) via Floyd-Warshall (LU-like)
  - APSP via path doubling (matrix-multiplication-like)
  - betweenness centrality
  - hypergraphs are representable by tensors
- recursion via higher order tensors
  - prefix sum, scan
  - FFT or other butterfly networks
  - bitonic sort

Cost model for parallel algorithms

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

Definition (F – computation cost)

Number of operations performed

Definition (Q – vertical communication cost)

Amount of data moved between memory and cache

Definition (W – horizontal communication cost)

Amount of data moved between processors

Definition (S – synchronization cost)

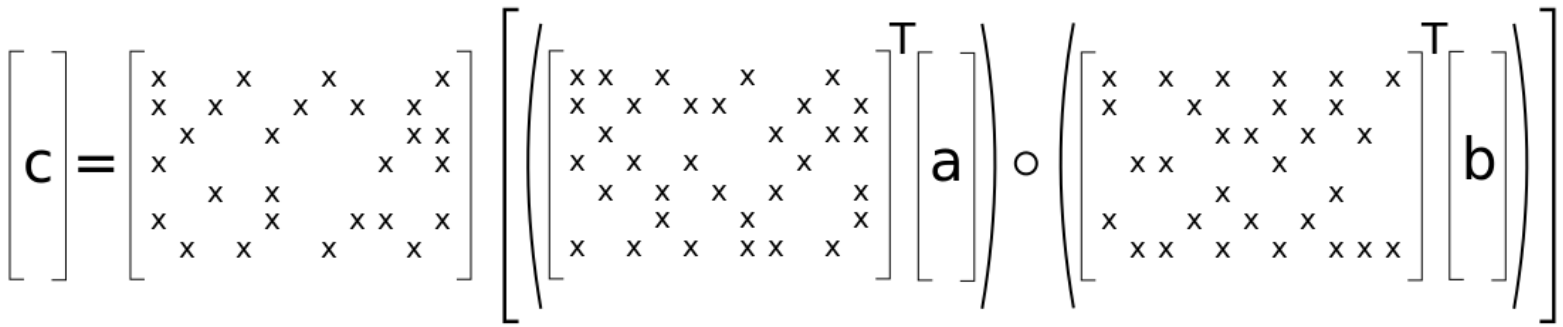
Number of distinct messages sent between processors

Bilinear algorithms

A bilinear algorithm Λ is defined by three matrices, $\Lambda = (\mathbf{F^{(A)}}, \mathbf{F^{(B)}}, \mathbf{F^{(C)}})$
Given input vectors $\mathbf{a}$ and $\mathbf{b}$, it computes vector,

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

where $\circ$ is the Hadamard (pointwise) product

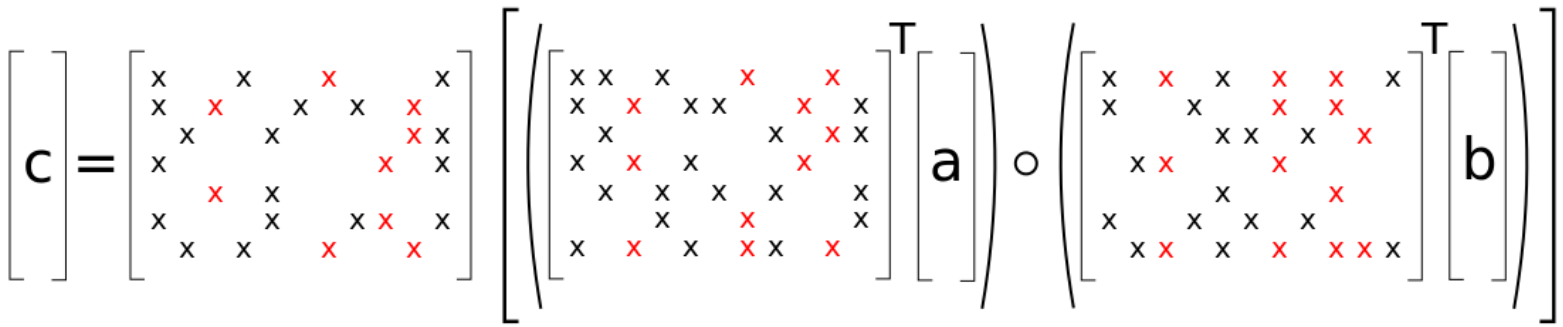


- the number of columns in the three matrices is equal and is the *bilinear algorithm rank*, denoted rank(Λ)
- the number of rows in each matrix corresponds to the number of inputs (dimensions of $\mathbf{a}$ and $\mathbf{b}$) and outputs (dimension of $\mathbf{c}$)

Bilinear algorithm expansion

A bilinear algorithm $\Lambda = (\mathbf{F}^{(\mathbf{A})}, \mathbf{F}^{(\mathbf{B})}, \mathbf{F}^{(\mathbf{C})})$ has expansion bound $\mathcal{E}_\Lambda : \mathbb{N}^3 \to \mathbb{N}$, if for all projection matrices $\mathbf{P}$,

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



has rank bounded by $\mathcal{E}_\Lambda$,

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

Communication lower bounds

Consider any algorithm $\Lambda = (\mathbf{F^{(A)}}, \mathbf{F^{(B)}}, \mathbf{F^{(C)}})$ and expansion bound $\mathcal{E}_\Lambda$.
For a cache size H, Λ requires total vertical communication cost,

$$Q \geq \left\lceil 2H \frac{\text{rank}(\Lambda)}{\mathcal{E}_\Lambda^{\max}(H)} \right\rceil$$

where $\mathcal{E}_\Lambda^{\max}(H) := \max_{c^{(A)}+c^{(B)}+c^{(C)}=3H} \mathcal{E}_\Lambda(c^{(A)}, c^{(B)}, c^{(C)})$.
Given p processors, Λ requires horizontal communication cost,

$$W \geq \min_{\mathcal{E}_\Lambda\left(c^{(A)}+\frac{r^{(A)}}{p}, c^{(B)}+\frac{r^{(B)}}{p}, c^{(B)}+\frac{r^{(C)}}{p}\right) \geq \frac{\text{rank}(\Lambda)}{p}} \left[c^{(A)} + c^{(B)} + c^{(C)} \right]$$

where $r^{(A)}$, $r^{(B)}$, and $r^{(C)}$ are the number of rows in $\mathbf{F^{(A)}}$, $\mathbf{F^{(B)}}$, and $\mathbf{F^{(C)}}$, respectively.

Dependency interval expansion

Consider a bilinear algorithm that computes a set of multiplications V with a partial ordering, we denote a dependency interval between $a, b \in V$ as

$$[a, b] = \{a, b\} \cup \{c : a < c < b, c \in V\}$$

If there exists $\{v_1, \ldots, v_n\} \in V$ with $v_i < v_{i+1}$ and $\left|[v_{i+1}, v_{i+k}]\right| = \Theta(k^d)$ for all $k \in \mathbb{N}$, then

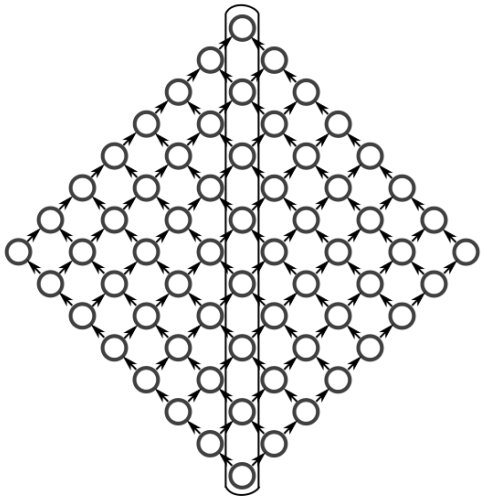
$$F \cdot S^{d-1} = \Omega(n^d)$$

where F is the computation cost and S is the synchronization cost

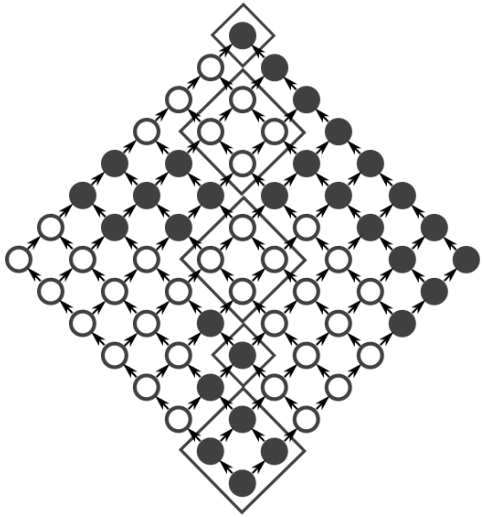
Further, if the algorithm has bilinear expansion $\mathcal{E}$, satisfying $\mathcal{E}^{\max}(H) = \Omega(H^{\frac{d}{d-1}})$, then

$$W \cdot S^{d-2} = \Omega(n^{d-1})$$

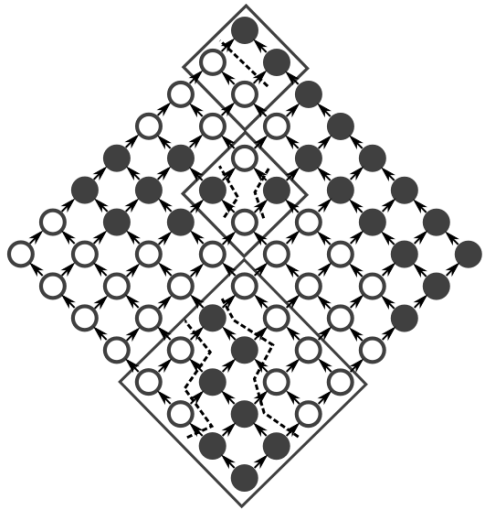
Example: diamond DAG



Dependency chain P



Monochrome dependency intervals



Multicolored dependency intervals

For the $n \times n$ diamond DAG ($d = 2$),

$$F \cdot S^{2-1} = F \cdot S = \Omega((n/b)b^2) \cdot \Omega(n/b) = \Omega(n^2)$$
$$W \cdot S^{2-2} = W \quad = \Omega((n/b)b) \qquad\qquad = \Omega(n)$$

idea goes back to Papadimitriou and Ullman, 1987

Tradeoffs involving synchronization

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

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

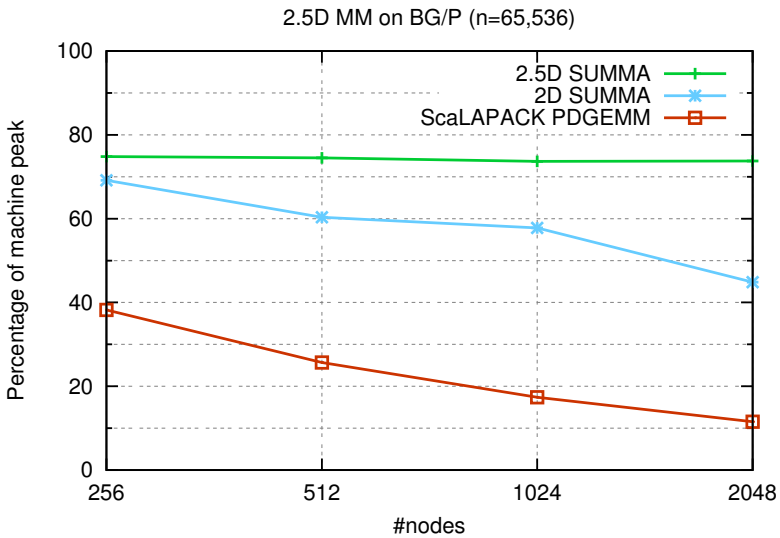
For computing s applications of a $(2m+1)^d$-point stencil

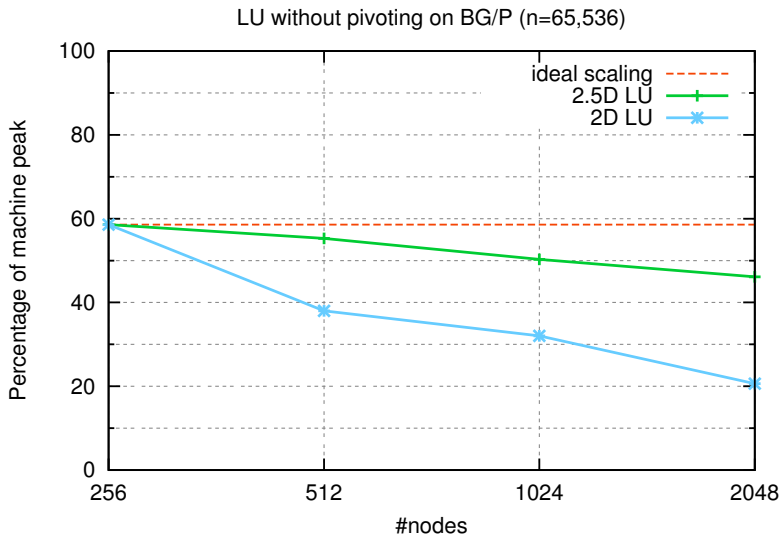
$$F_{\mathrm{St}} \cdot S_{\mathrm{St}}^d = \Omega\left(m^{2d} \cdot s^{d+1}\right) \qquad W_{\mathrm{St}} \cdot S_{\mathrm{St}}^{d-1} = \Omega\left(m^d \cdot s^d\right)$$

Communication-optimal dense matrix algorithms

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

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





- LU with pairwise pivoting extended to tournament pivoting
- QR with Givens rotations extended to Householder transformations
- full-to-banded reduction for symmetric eigenvalue problem
- successive band reduction for symmetric eigenvalue problem

Communication-efficient sparse matrix computations

Iterative stencil computations

- previous work: in-time blocking
  - lowers synchronization cost
  - lowers vertical communication cost
  - increases horizontal communication cost when mesh at least 2D
- new 'cyclic' algorithm, in-time blocks executed bulk synchronously
  - lowers vertical communication cost
  - maintains minimal horizontal communication cost
  - increases synchronization cost
- alternatives are both optimal in different lower bound regimes

Multiplication of a sparse matrix by a dense matrix

- key primitive with many applications
  - iterative solvers
  - tensor computations (MP3 or coupled cluster with localized orbitals)
  - graph algorithms (Bellman-Ford, APSP, betweenness centrality)
- communication-efficient 3D algorithms and lower bound analysis

Exploiting symmetry in tensors

Coupled cluster methods for electronic structure calculations

- approximates electronic wavefunction using $2r$-order tensor representing r-electron correlation
- systematically improvable, CCSD, CCSDT, CCSDTQ ($r = 1, 2, 3$)
- cost dominated by contractions of partially antisymmetric tensors

Exploiting tensor (anti)symmetry

- saves storage and provides easy reduction in cost if set of contraction multiplications is symmetric
- new symmetry-preserving algorithm uses algebraic reorganization to reduce cost (lowers bilinear algorithm rank) when set of contraction multiplications breaks tensor symmetry

$$W_{ikj} = A_{ik} \cdot B_{kj} \quad \rightarrow \quad Z_{ikj} = (A_{ik} + A_{kj} + A_{ji}) \cdot (B_{ik} + B_{kj} + B_{ji})$$

- nested use reduces cost of CCSD by about 1.3, CCSDT by about 2.1

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)

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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
}
```

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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"];
```

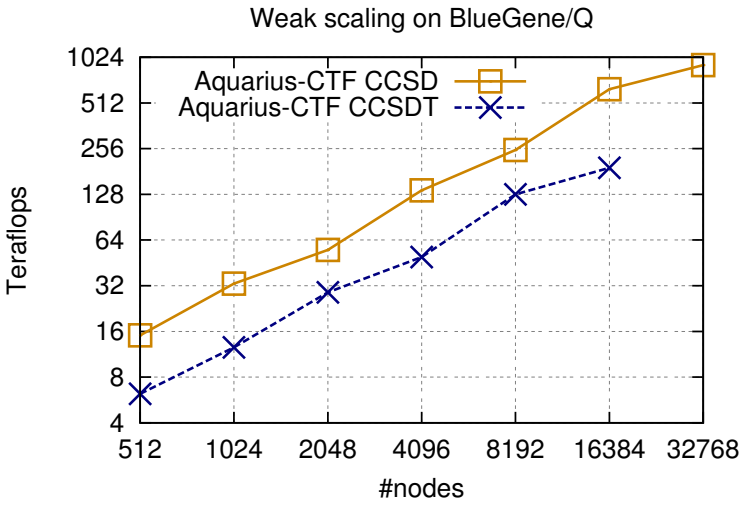
Betweenness centrality

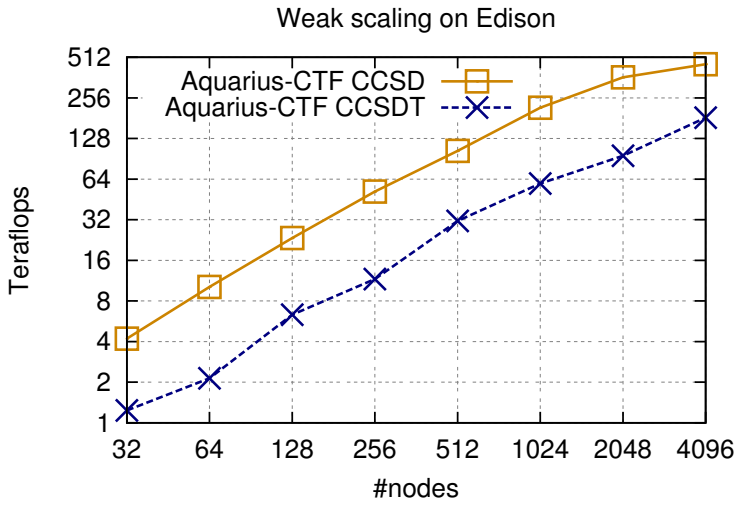
Betweenness centrality code snippet, for k of n nodes

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

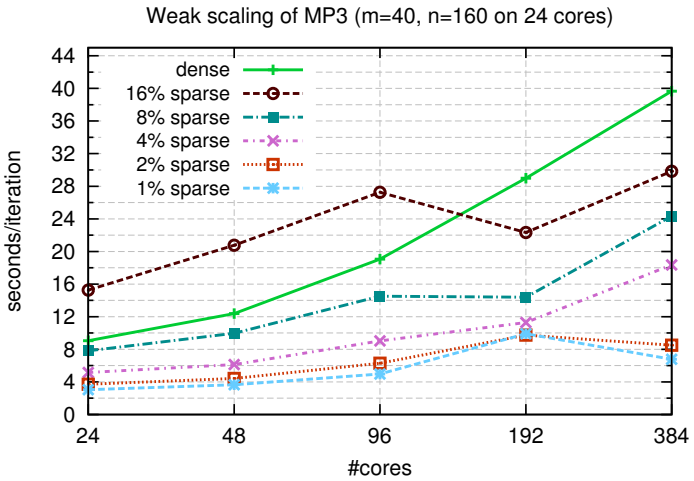
Performance highlights

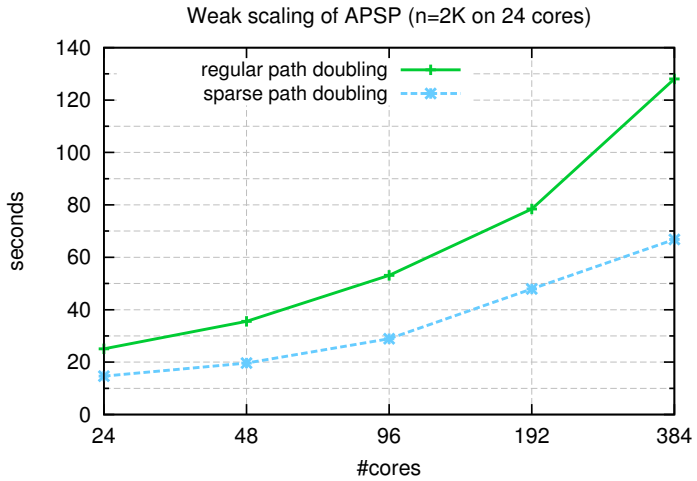
Coupled cluster calculations using dense tensors





MP3 and all-pairs shortest-paths using sparse tensors



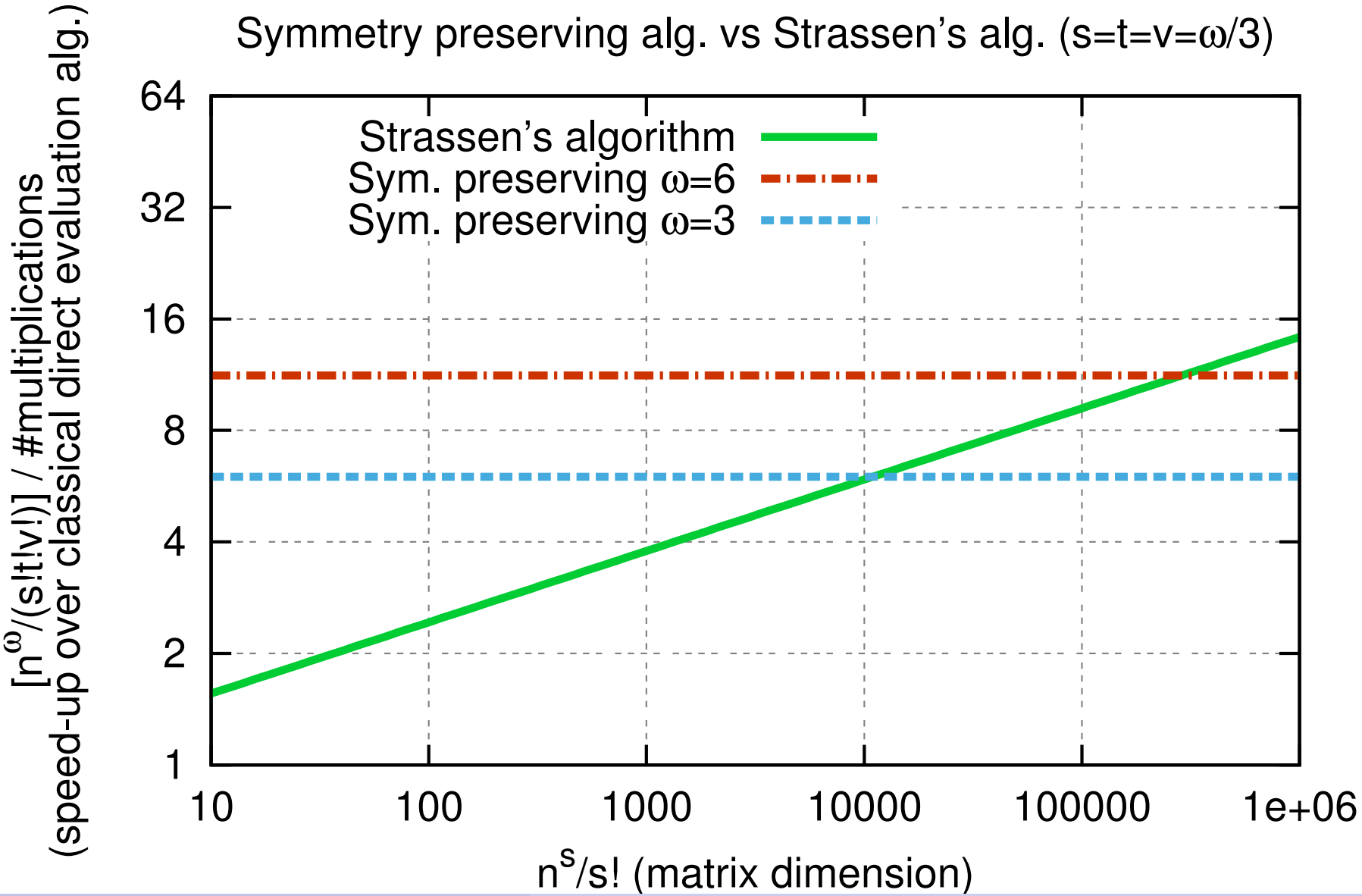


Future work

- further work sparse and symmetric tensor computations
  - bridging the gap between abstractions and application performance
  - bilinear algorithm complexity – fast matrix multiplication
- tensor decompositions
  - communication-efficient parallel algorithms and lower bounds
  - symmetry-preserving tensor decomposition algorithms
  - programming abstractions for dense and sparse tensors
- sets of tensor operations
  - most algorithms correspond to multiple dependent tensors operations
  - communication cost analysis for sets of contractions
  - scheduling, blocking, and decomposition of multiple tensor operations
  - higher-level programming abstractions
- application-driven development
  - tensor decompositions, sparsity, symmetry all motivated by electronic structure applications
  - optimization of primitives serves as feedback loop for development of new electronic structure methods

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

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

Comparison with NWChem

NWChem is a commonly-used distributed-memory quantum chemistry method suite

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