A parallel library for multidimensional array computations with runtime tuning

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At the crossroads of parallel libraries and languages

Parallel programming frameworks with multidimensional arrays

- HTA, Charm++ (MSA), Global Arrays, UPC, Titanium, HPF...
- flexible layouts, efficient data transformations and scheduling
- limited API, basic primitives
- rudimentary support for higher dimensional arrays (tensors)

Parallel libraries for matrix computations and numerical methods

- ScaLAPACK, Elemental, DPLASMA, PETSC, Trillinos, ...
- restrictive data distribution assumptions, variable performance
- broad API, powerful functionality
- no support for multidimensional matrices (higher order tensors)

Goal: efficient parallel library with a concise and yet general tensor API

Tensor contractions

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

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

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

Matrix/vector examples:

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

Applications of higher-order tensor contractions

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

- tensor factorization algorithms, e.g. alternating least squares
- high-order numerical solvers for differential equations
- computer vision, graphics, image/video analysis
- deep learning convolutional neural networks
- density matrix renormalization group (DMRG)
- **electronic structure calculations, e.g. coupled cluster**

Coupled cluster methods

Coupled cluster provides a systematically improvable approximation to the manybody time-independent Schrödinger equation

- considers transitions of 'doubles', 'triples', or 'quadruples' of electrons to 2, 3, 4 unoccupied orbitals (CCSD, CCSDT, CCSDTQ)
- encodes their contribution to energy via order 4, 6, 8 tensor T
- iteratively solves for T, consistent with the mean field Hamiltonian with components F, V

$$0 = V_{ij}^{ab} + P_b^a \sum_e T_{ij}^{ae} F_e^b - \frac{1}{2} P_j^i \sum_{mnef} T_{im}^{ab} V_{ef}^{mn} T_{jn}^{ef} + \dots$$

where $P_y^x f(x,y) := f(x,y) - f(y,x)$

- CCSD has 45 such multilinear terms, CCSDT 100s, CCSDTQ 1000s

Contractions in Coupled Cluster (CCSD method)

$$W_{ei}^{mn} = V_{ei}^{mn} + \sum_f V_{ef}^{mn} t_i^f,$$

$$X_{ij}^{mn} = V_{ij}^{mn} + P_j^i \sum_e V_{ie}^{mn} t_j^e + \frac{1}{2} \sum_{ef} V_{ef}^{mn} \tau_{ij}^{ef},$$

$$U_{ie}^{am} = V_{ie}^{am} - \sum_n W_{ei}^{mn} t_n^a + \sum_f V_{ef}^{ma} t_i^f + \frac{1}{2} \sum_{nf} V_{ef}^{mn} T_{in}^{af},$$

$$Q_{ij}^{am} = V_{ij}^{am} + P_j^i \sum_e V_{ie}^{am} t_j^e + \frac{1}{2} \sum_{ef} V_{ef}^{am} \tau_{ij}^{ef},$$

$$z_i^a = f_i^a - \sum_m F_i^m t_m^a + \sum_e f_e^a t_i^e + \sum_{em} V_{ei}^{ma} t_m^e + \sum_{em} V_{im}^{ae} F_e^m + \frac{1}{2} \sum_{efm} V_{ef}^{am} \tau_{im}^{ef} - \frac{1}{2} \sum_{emn} W_{ei}^{mn} T_{mn}^{ea},$$

$$Z_{ij}^{ab} = V_{ij}^{ab} + P_j^i \sum_e V_{ie}^{ab} t_j^e + P_b^a P_j^i \sum_{me} U_{ie}^{am} T_{mj}^{eb} - P_b^a \sum_m Q_{ij}^{am} t_m^b + P_b^a \sum_e F_e^a T_{ij}^{eb} - P_j^i \sum_m F_i^m T_{mj}^{ab} + \frac{1}{2} \sum_{ef} V_{ef}^{ab} \tau_{ij}^{ef} + \frac{1}{2} \sum_{mn} X_{ij}^{mn} \tau_{mn}^{ab},$$

A library for tensor computations

Cyclops Tensor Framework (MPI+OpenMP+CUDA)

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

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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 {
    //parallel for i = 1 to n
      //parallel for j = 1 to n
          x["i"] = d["i"]*(b["i"]-R["ij"]*x["j"]);
    //parallel for i = 1 to n
      //parallel for j = 1 to n
          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

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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;
}
```

Coupled cluster using CTF

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

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

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

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

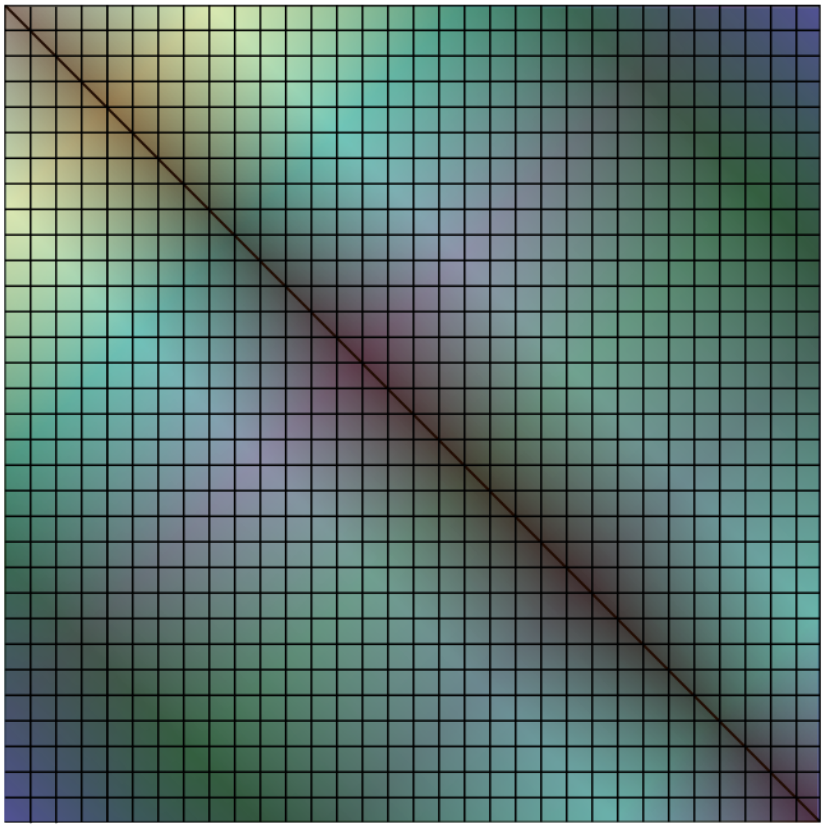
Access and write tensor data

CTF abstracts that data distribution from the user

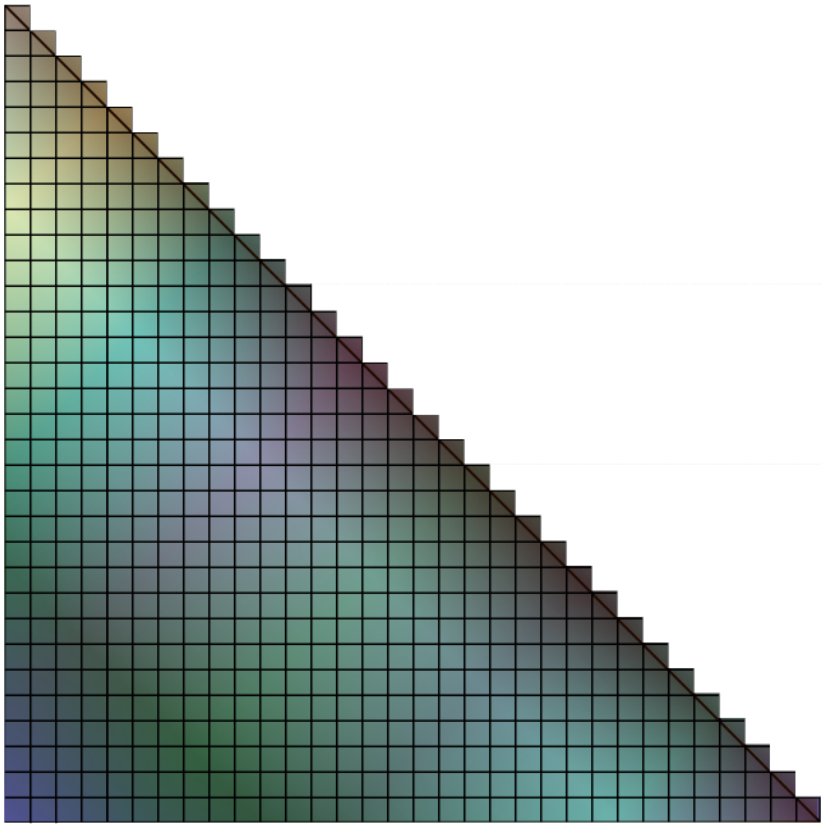
- Access arbitrary sparse subsets of the tensor by global index (coordinate format)
  - `T.write(int * indices, double * data)` (can also accumulate)
  - `T.read(int * indices, double * data)` (can also accumulate)
- Matlab submatrix notation: $A[j:k, l:m]$
  - `T.slice(int * offsets, int * ends)` returns the subtensor
  - `T.slice(int corner_off, int corner_end)` does the same
  - can also sum subtensors
  - different subworlds can read different subtensors simultaneously
- Extract a subtensor of any permutation of the tensor
  - given mappings P, Q, does $B[i,j] = A[P[i], Q[j]]$ via `permute()`
  - P and Q may access only subsets of **A** (if **B** is smaller)
  - **B** may be defined on subworlds on the world on which **A** is defined and each subworld may specify different P and Q

Symmetric matrix representation

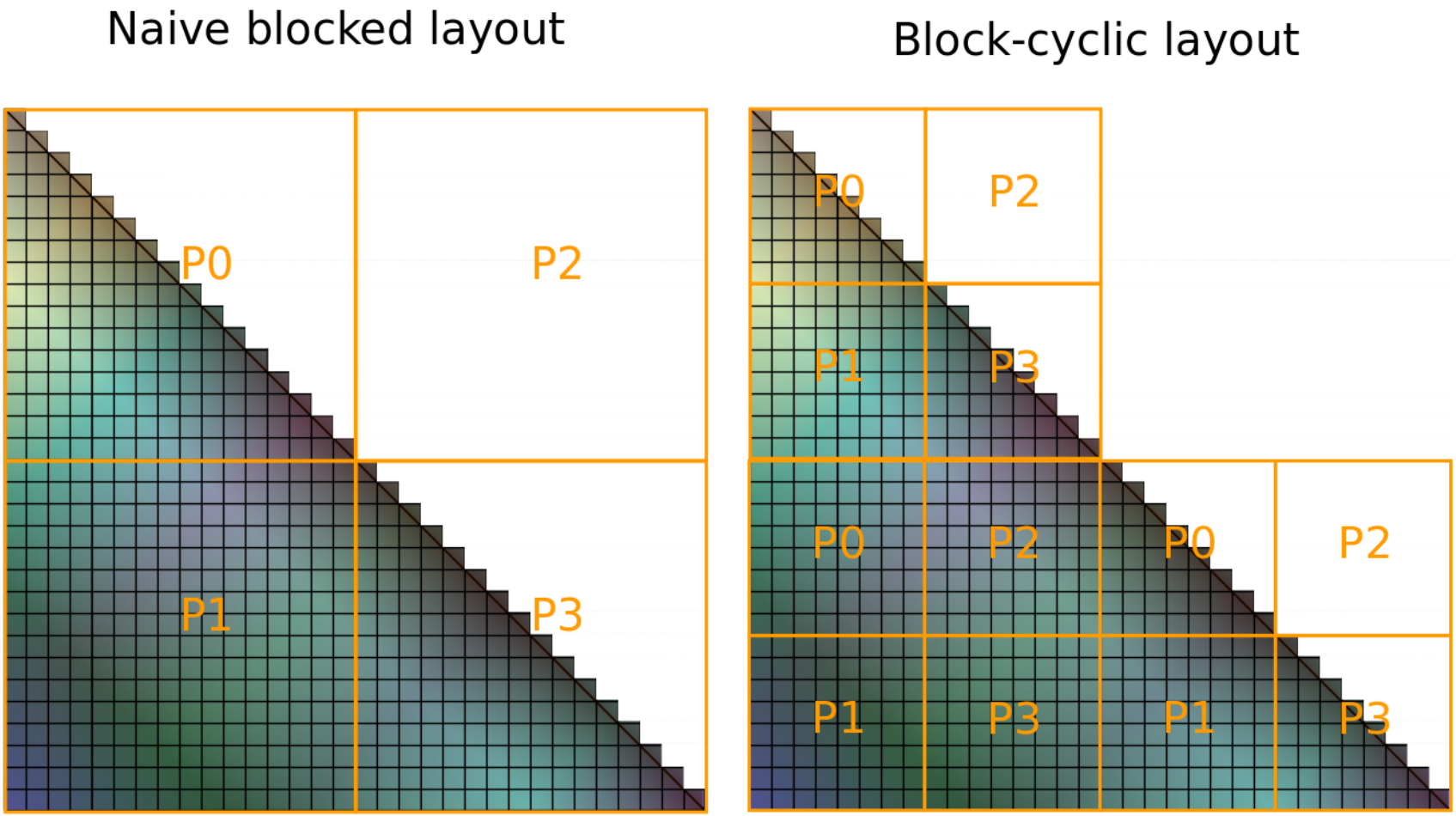
Symmetric matrix



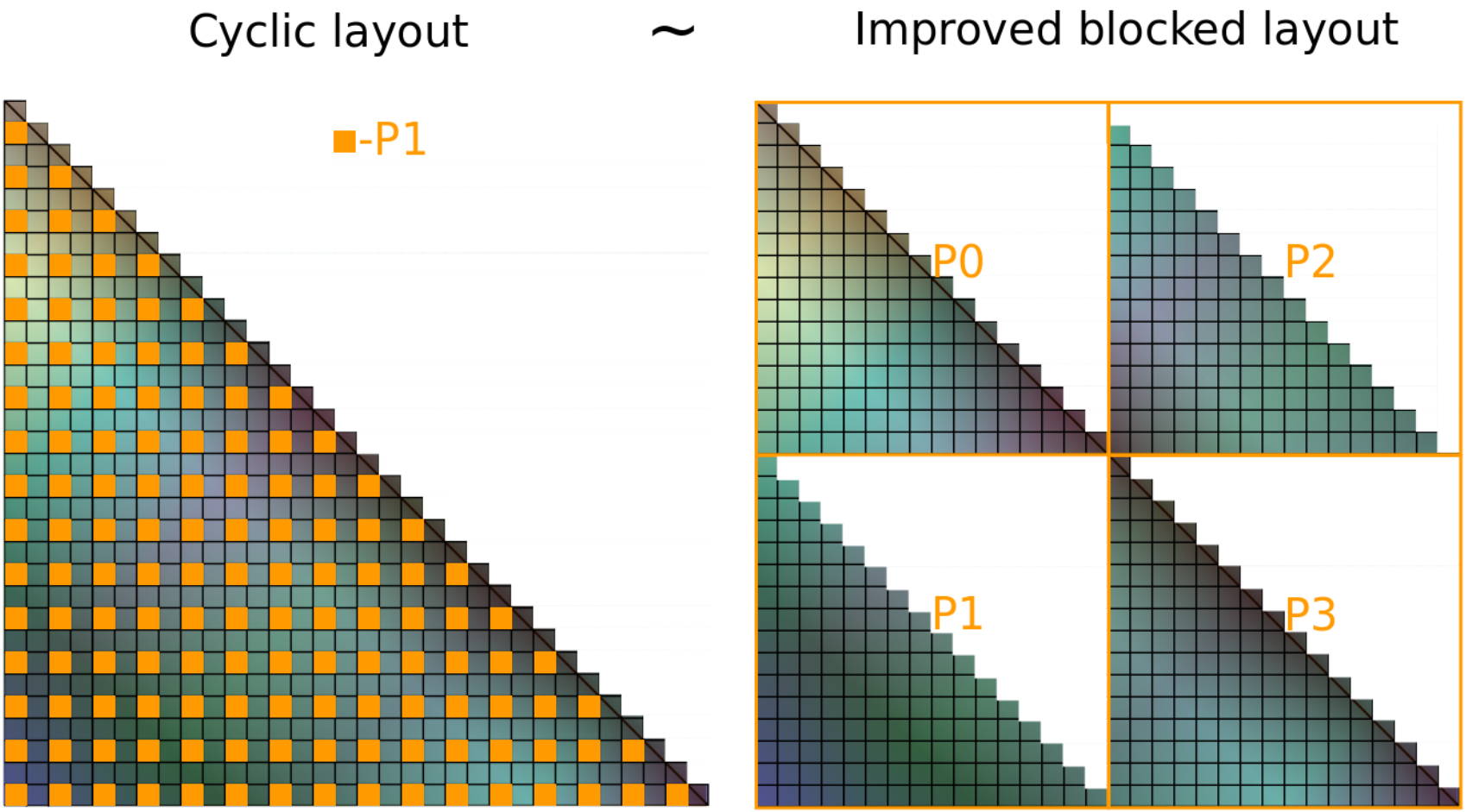
Unique part of symmetric matrix



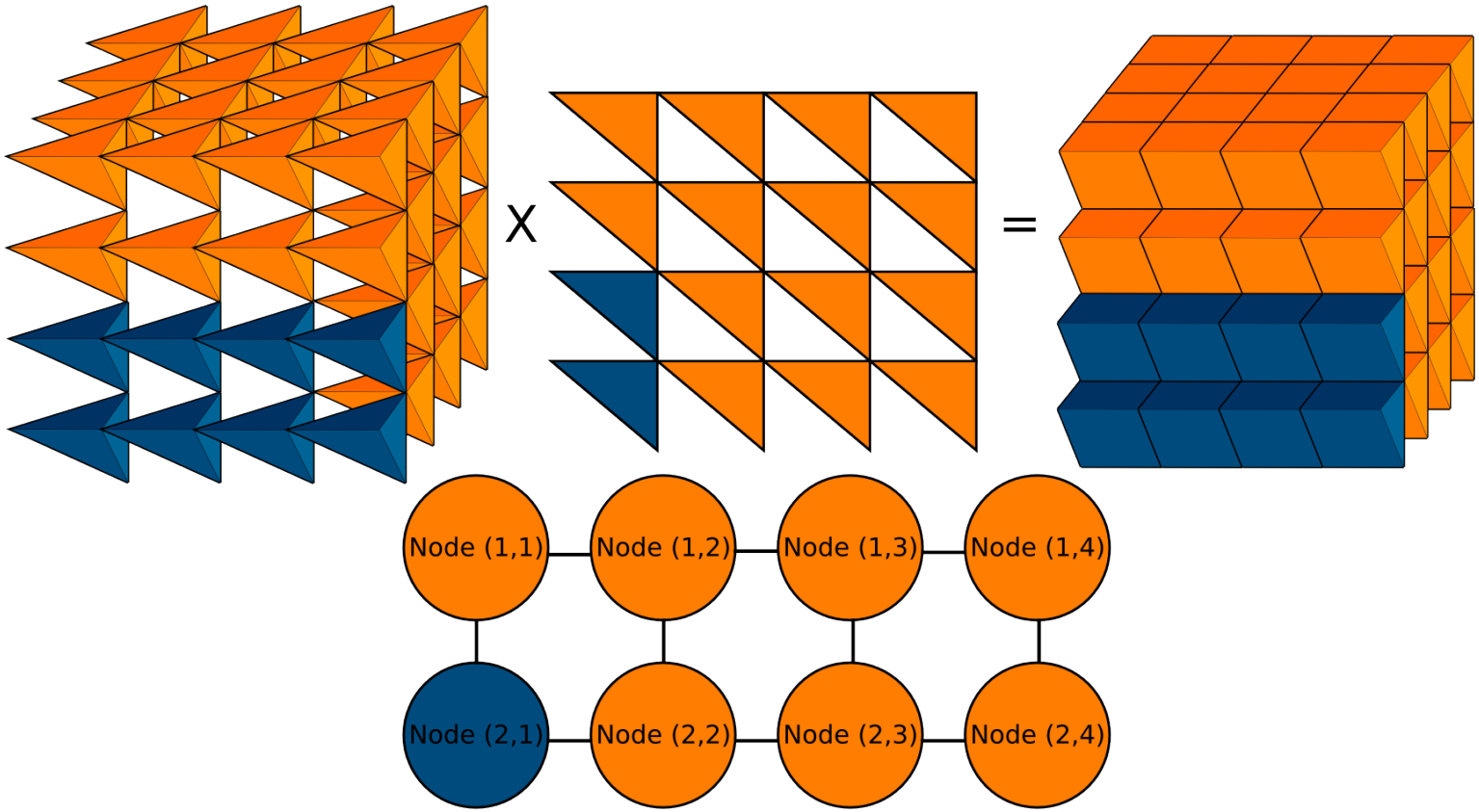
Blocked distributions of a symmetric matrix



Cyclic distribution of a symmetric matrix



3D tensor mapping



Tensor decomposition and mapping

CTF tensor decomposition

- cyclic layout used to preserve packed symmetric structure
- overdecomposition (virtualization) employed to decouple the decomposition from the physical processor grid

CTF mapping logic

- arrange physical topology into all possible processor grids
  - assumes a torus topology
  - by default, factorize number of processors to produce torus
- dynamically (in parallel) autotune over all topologies and mappings
  - topologies: all foldings of physical (default) topology
  - mappings: assignments of tensor modes (indices) to torus modes
- select best mapping based on model-based performance prediction
  - performance models for communication, memory-bandwidth, synchronization, and work for contractions and redistributions
  - for sparse tensors, estimate load imbalance

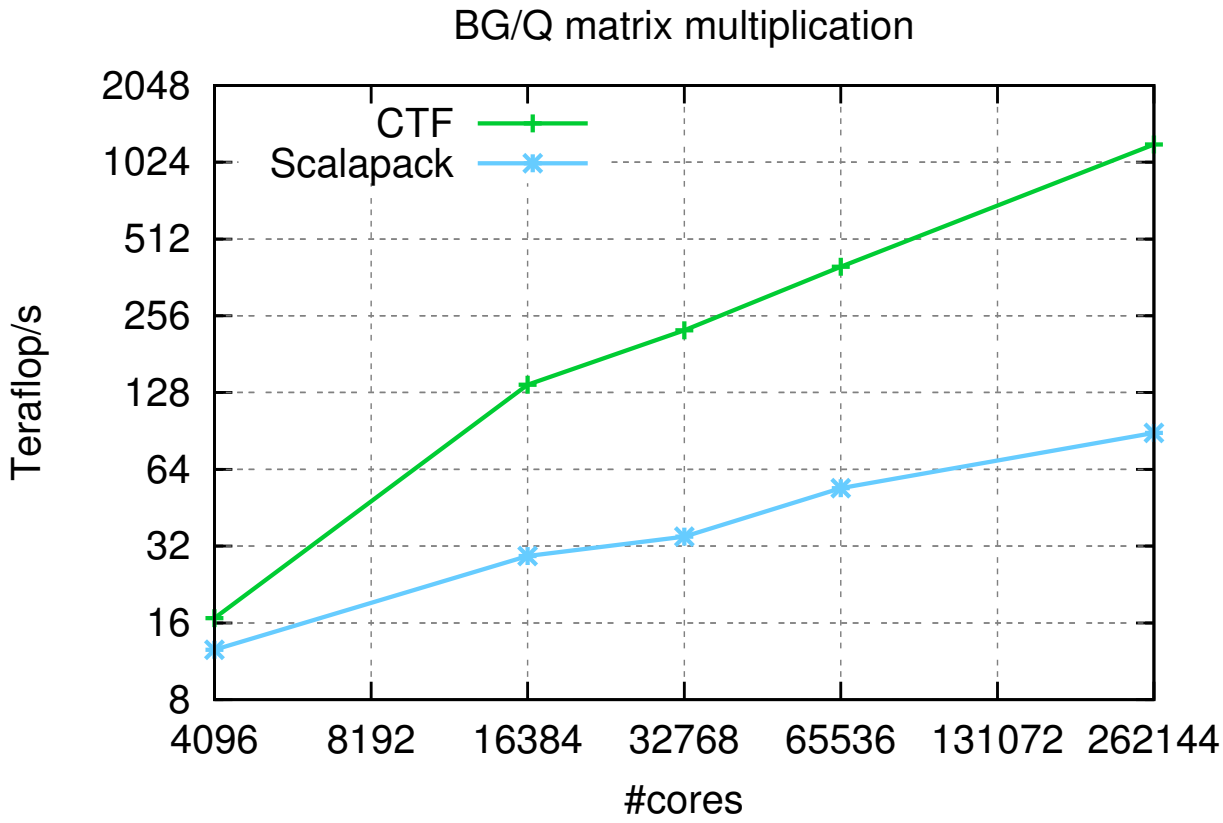
Algorithms for tensor redistribution

The following three redistribution kernels are provided by CTF

- Sparse (key-value) redistribution
  - requires all-to-all-v communication and local binning/sorting
  - well-fit for user-level data entry and sparse tensors
- Dense mapping-to-mapping (no-explicit-key) redistribution
  - send/recv counts precomputed analytically via (complicated) recurrence
  - subset of messages packed from data at a time
  - optimized via template-instantiated nested loops, threading
- Block-to-block redistribution
  - reassignment of block (virtual) decomposition to processors
  - processors send blocks via point-to-point messages

Benefit of topology aware mapping

CTF can leverage rectangular collectives on BG/Q

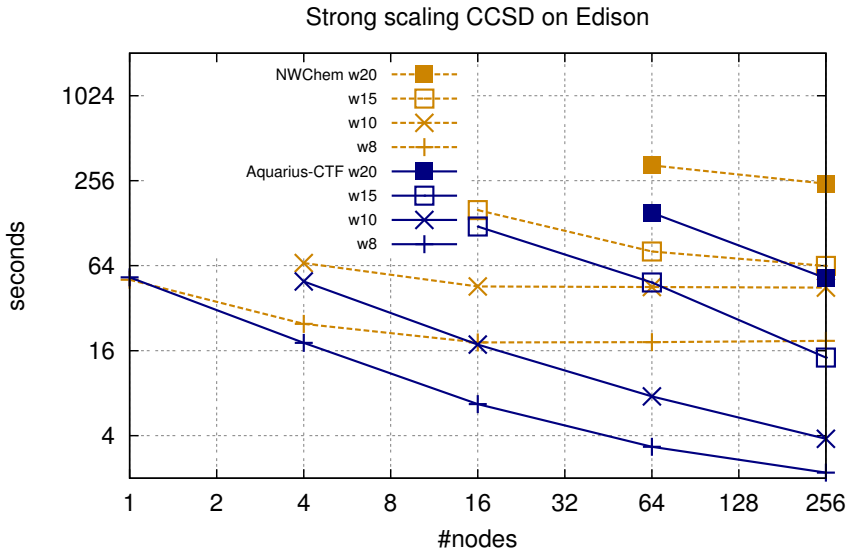


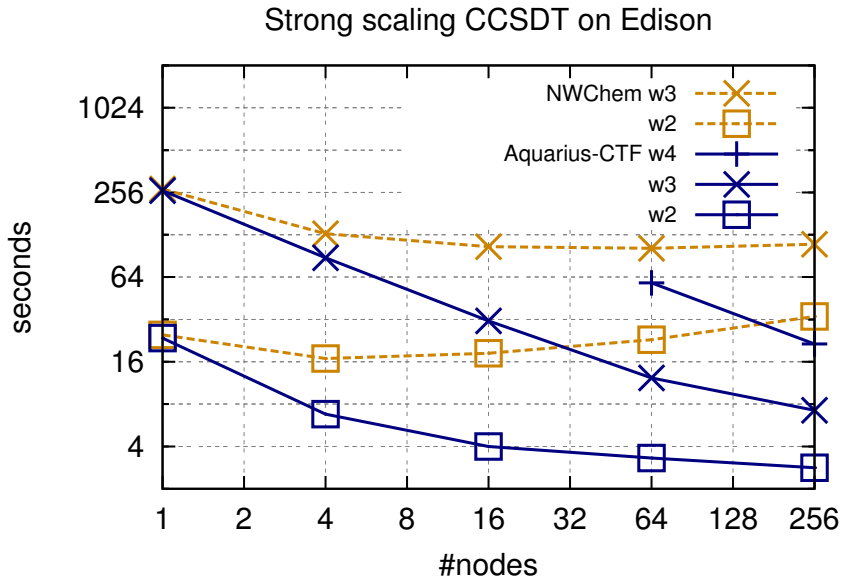
The QBall (QBox) density functionional theory (DFT) code has leveraged CTF just to accelerate matrix multiplication

Comparison with NWChem

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

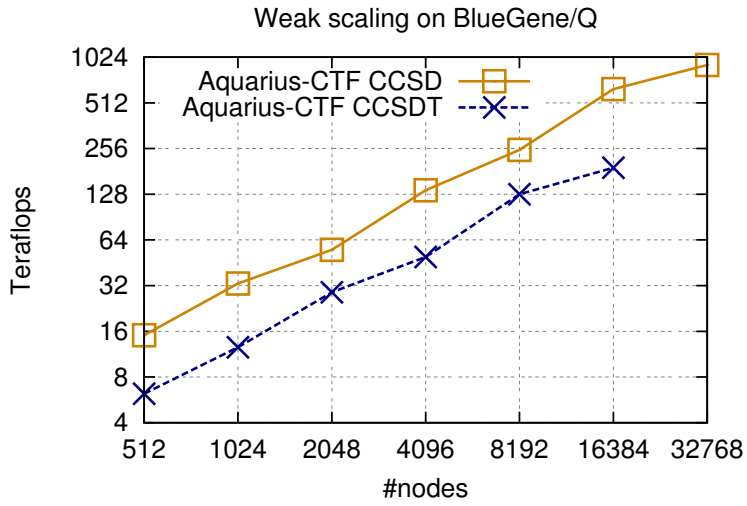
- provides Coupled Cluster methods: CCSD and CCSDT
- derives equations via Tensor Contraction Engine (TCE)
- generates contractions as blocked loops leveraging Global Arrays

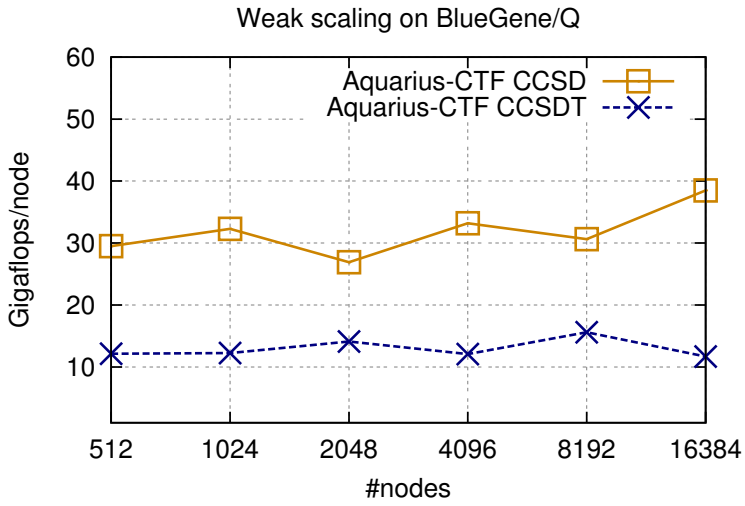


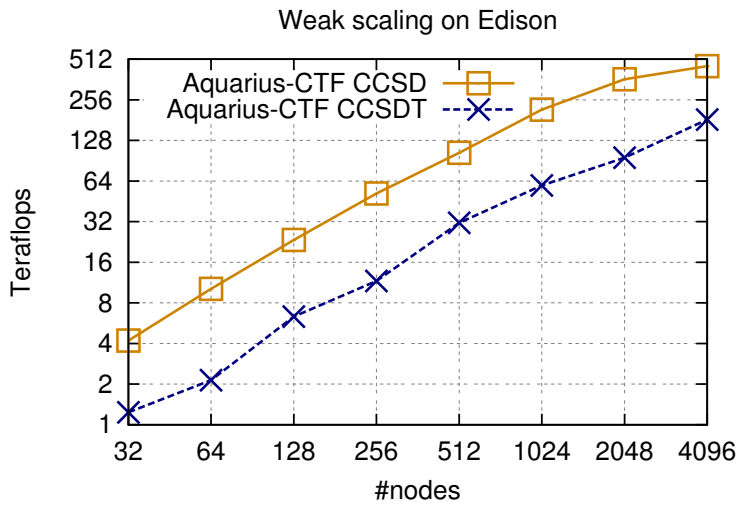


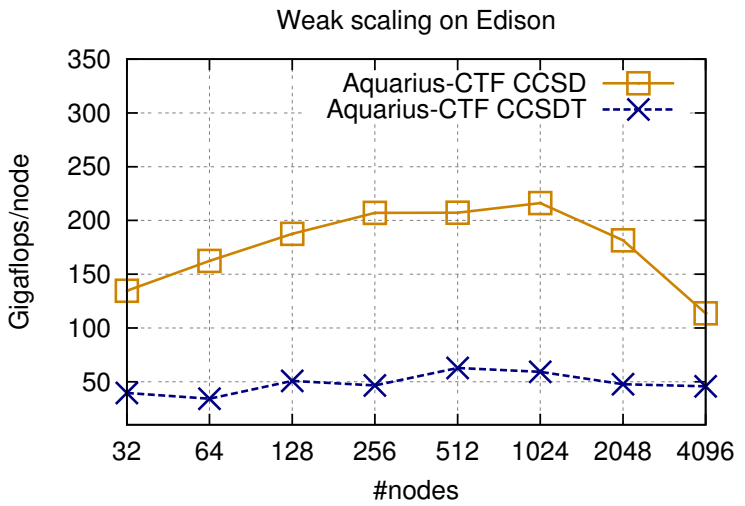
Coupled cluster on IBM BlueGene/Q and Cray XC30

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









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
n_v-orbitals, n_o-electrons, p-processors, M-local memory size

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

Algebraic Structures

CTF allows a tensor elements to have a user-defined algebraic structure:

algebraic str.	add.	add. id.	add. inv.	mul.	mul. id.
set					
monoid	✓	✓			
group	✓	✓	✓		
semiring	✓	✓		✓	✓
ring	✓	✓	✓	✓	✓

For each summation or contraction, the user may define custom functions, so we also have

semigroup = set + function
rng = group + function

user-defined types must be static-sized (migratable)

Algebraic Structure Interface

Tropical algebraic semiring

$$c \oplus a \odot b := \min(c, a + b)$$

Interface via C++11 Lambdas:

```
Semiring<int> ts(INT_MAX/2, //additive identity
                 [](int a, int b){ return min(a,b); }, //add
                 MPI_MIN, //add MPI op
                 0, //multiplicative identity
                 [](int a, int b){ return a+b; }); //mul
```

Adjacency matrix for n-node undirected graph with integer weights:

```
Matrix<int> A(n,n,SP|SH,ts);
```

SP – sparse, **SH** – symmetric-hollow (zero diagonal)

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"];
}
```

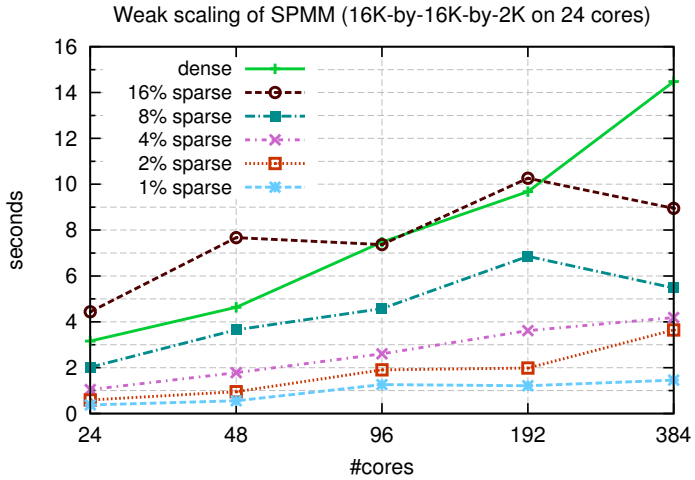
Betweenness centrality

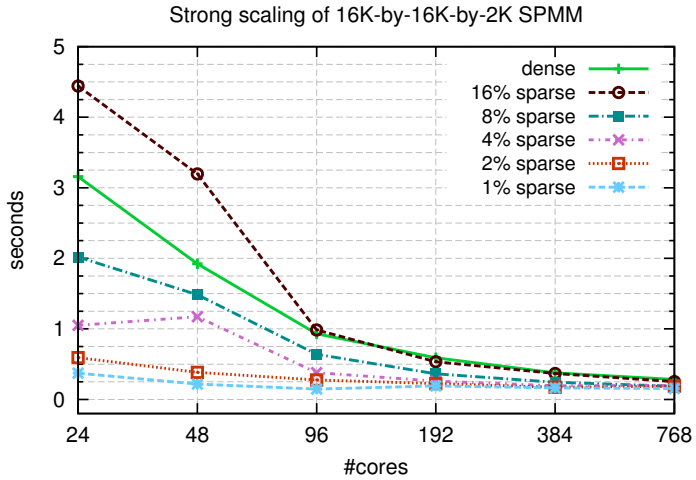
Betweenness centrality code snippet, for k of n nodes

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

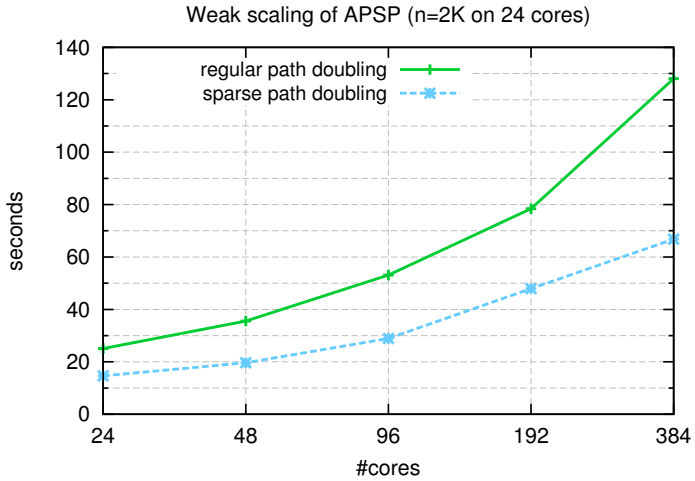
Performance of CTF for sparse computations

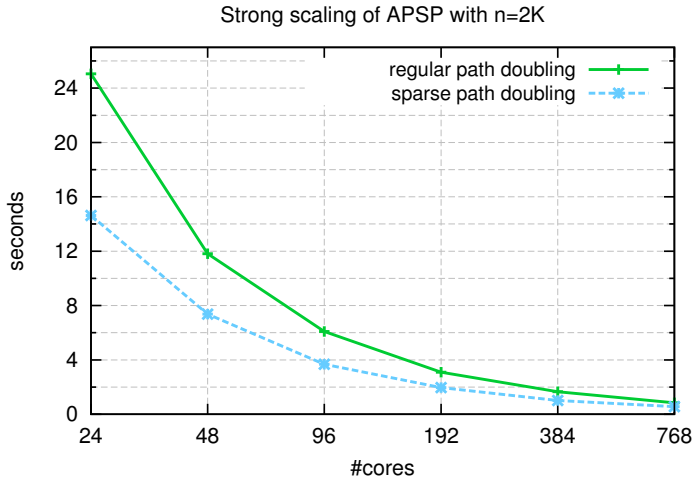
multiplication of a sparse matrix and a dense matrix





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





Conclusion

Summary of CTF:

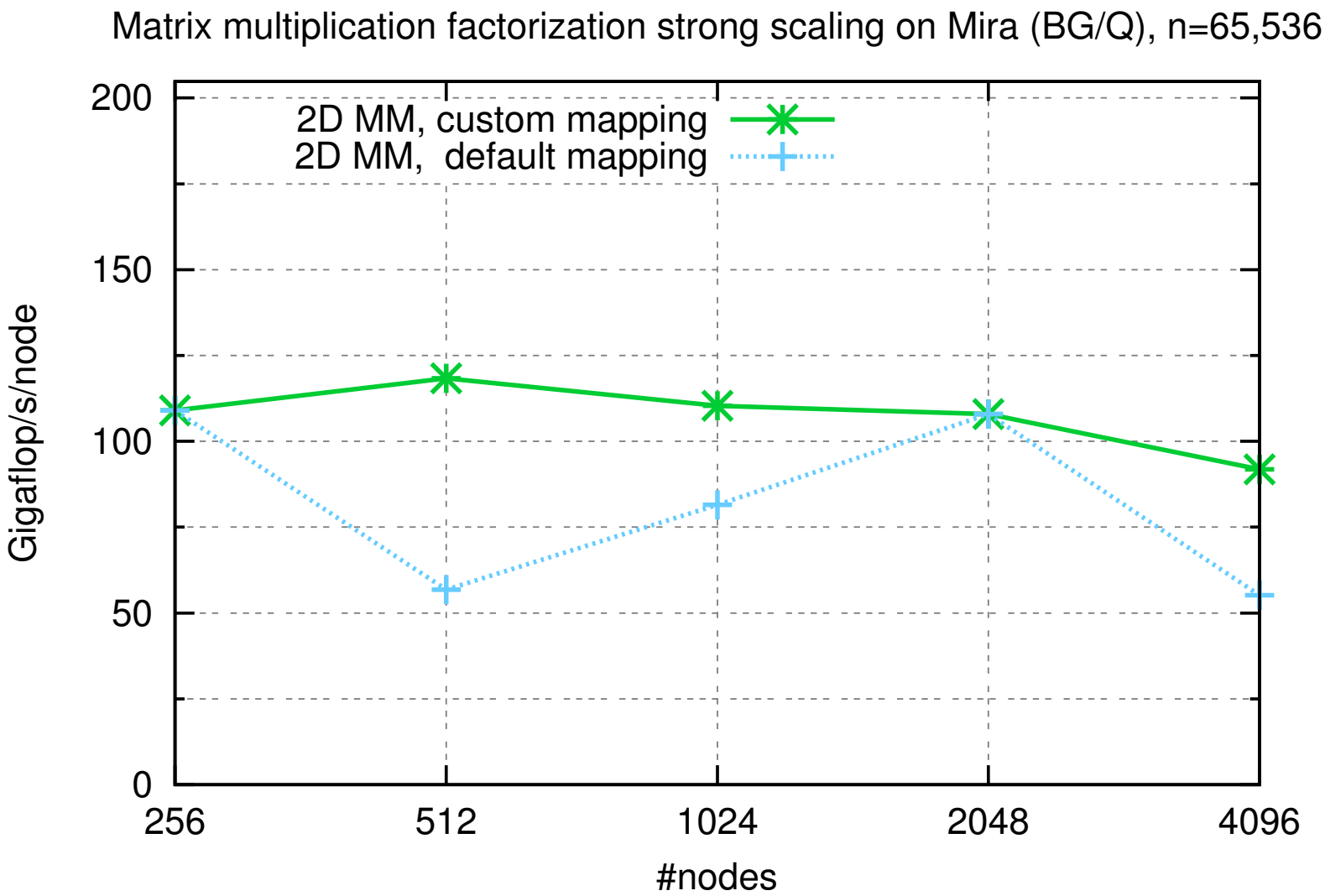
- distributed-memory tensor library leveraging MPI, OpenMP, and CUDA
- support for symmetric and sparse tensors
- similarities to Charm++ multidimensional chare arrays
  - overdecomposition (virtualization)
  - topology-aware mapping of tasks/blocks
  - application-driven development
- differences from Charm++
  - 'static' schedule selected at runtime vs dynamic load balancing
  - migration between regular distributions rather than greedy/refined
  - redistributions done processor-to-processor

Future work:

- generation of fast local 'dgemm' kernels for user-defined functions
- handling of contractions of two sparse tensors and sparse output
- multi-contraction scheduling, convolutions, tensor factorizations, ...

Backup slides

Topology-aware mapping on BG/Q



Algebraic shortest path computations

All-pairs shortest-paths (APSP):

- distance matrix is the closure of A,

$$A^* = I \oplus A \oplus A^2 \oplus \ldots A^n$$

- 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[1]:
  - let C be subset of B^k corresponding to paths containing *exactly* k edges,

$$B^{2k} = B^k \oplus (C \otimes B^k)$$

  - $O(n^3)$ cost, dependency paths length $O(\log^2 n)$

[1] Tiskin, Springer LNCS, 2001

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

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

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