Efficient Algorithms for Tensor Contractions in Coupled Cluster

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Outline

1. Cyclops Tensor Framework
   - Aim
   - Interface
   - Internal Mechanism
   - Performance
   - Ongoing and future work
2. Symmetry preserving algorithm
   - Instances in matrix computations
   - General symmetric contractions
   - Application to coupled-cluster
3. Conclusion

Motivation and goals

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- is packaged as a library and uses only MPI, BLAS, and OpenMP
- selects best mapping for tensors and contractions via performance models
- decomposes and redistributes tensor data dynamically

Distributed-memory context

CTF relies on MPI (Message Passing Interface) for bulk synchronous multiprocessor parallelism

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CTF_World dw(comm)
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- MPI_COMM_WORLD is the default communicator containing all processes
- data movement possible between a world and a ‘subworld’ (defined on a subcommunicator)

Tensor definition

A CTF tensor is a multidimensional distributed array, e.g.

$$T_{ij}^{ab}$$

where **T** is $m \times m \times n \times n$ antisymmetric in ab and in ij

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CTF_Tensor T(4,\{m,m,n,n\},\{AS,NS,AS,NS\},dw)
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- there are also obvious derived types for CTF_Tensor: CTF_Matrix, CTF_Vector, CTF_Scalar

Contract tensors

CTF can express a tensor contraction like

$$Z_{ij}^{ab} = Z_{ij}^{ab} + 2 \cdot P(a,b) \sum_k F_k^a \cdot T_{ij}^{kb}$$

where $P(a,b)$ implies antisymmetrization of index pair ab, as

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Z["abij"] += 2.0*F["ak"]*T["kbij"]
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- **for** loops and summations implicit in syntax
- $P(a,b)$ is applied implicitly if **Z** is antisymmetric in ab
- **Z**, **F**, **T** should all be defined on the same world and all processes in the world must call the contraction bulk synchronously

CCSD

Extracted from Aquarius (Devin Matthews' code)

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

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

CCSDT

Extracted from Aquarius (Devin Matthews' code)

```
Z(1)["ai"] += 0.25*WMNEF["mnef"]*T(3)["aefimn"];

Z(2)["abij"] += 0.5*WAMEF["bmef"]*T(3)["aefijm"];
Z(2)["abij"] -= 0.5*WMNEJ["mnej"]*T(3)["abeinm"];
Z(2)["abij"] += FME["me"]*T(3)["abeijm"];

Z(3)["abcijk"]  = WABEJ["bcek"]*T(2)["aeij"];
Z(3)["abcijk"] -= WAMIJ["bmjk"]*T(2)["acim"];
Z(3)["abcijk"] += FAE["ce"]*T(3)["abeijk"];
Z(3)["abcijk"] -= FMI["mk"]*T(3)["abcijm"];
Z(3)["abcijk"] += 0.5*WABEF["abef"]*T(3)["efcijk"];
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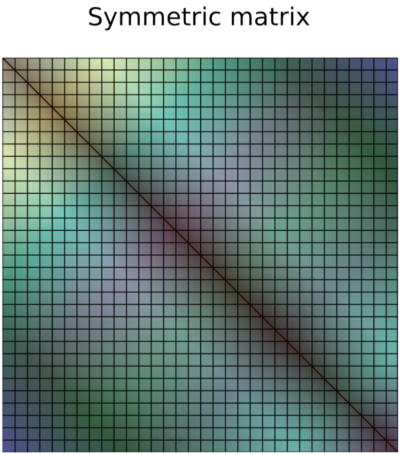
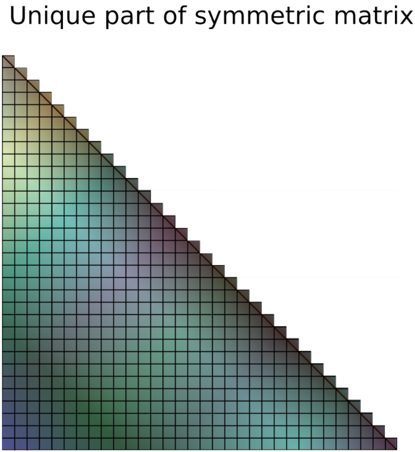
  - **B** may be defined on subworlds on the world on which **A** is defined and each subworld may specify different P and Q

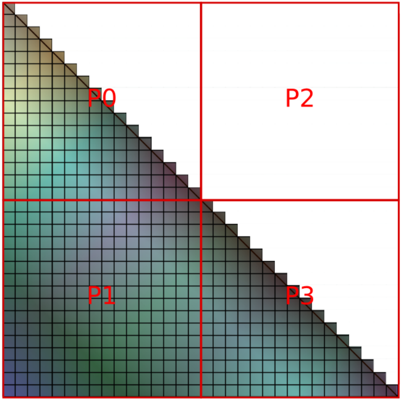
Symmetric matrix representation



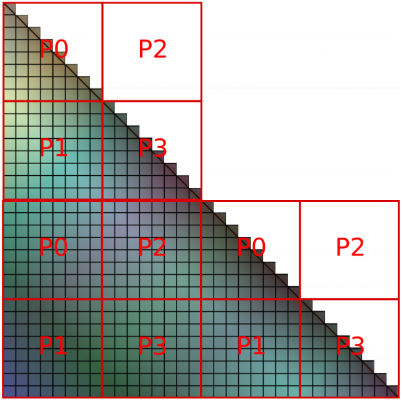


Blocked distributions of a symmetric matrix

Naive blocked layout

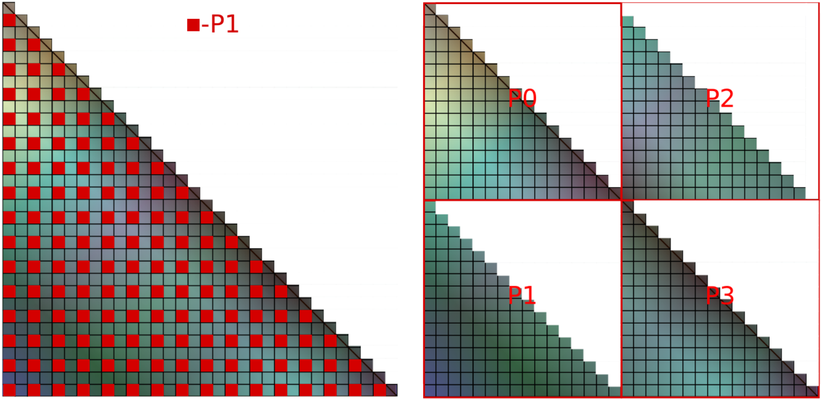


Block-cyclic layout



Cyclic distribution of a symmetric matrix

Cyclic layout ∼ Improved blocked layout



Tensor decomposition and mapping

CTF tensor decomposition

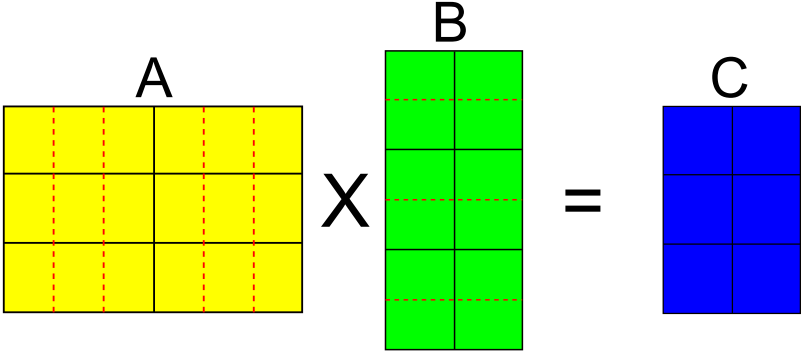
- cyclic layout used to preserve packed symmetric structure (hence Cyclops – cyclic ops)
- overdecomposition (virtualization) employed to decouple the decomposition from the physical processor grid

CTF mapping logic

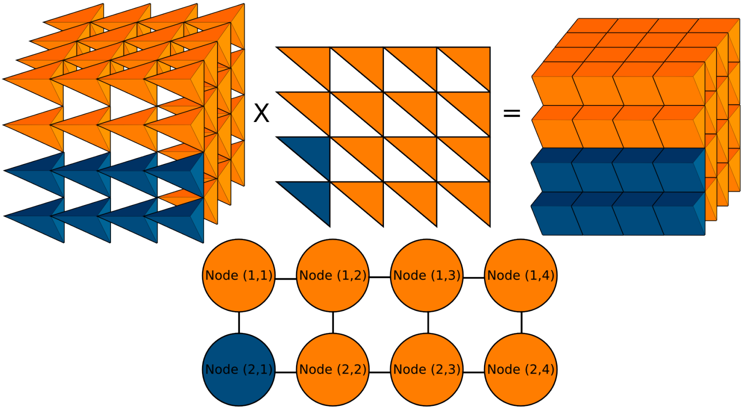
- arrange physical topology into all possible processor grids
- dynamically (in parallel) autotune over all topologies and over mapping strategies
- select best mapping based on model-based performance prediction

Virtualization (local blocking)

Matrix multiply on 2x3 processor grid. Red lines represent virtualized part of processor grid. Elements assigned to blocks by cyclic phase.



3D tensor mapping



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- Block-to-block redistribution
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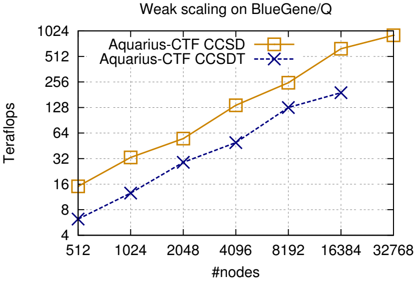
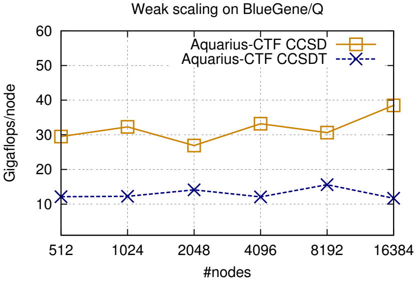
  - processors send blocks via point-to-point messages

Coupled-cluster code on BlueGene/Q (Mira)

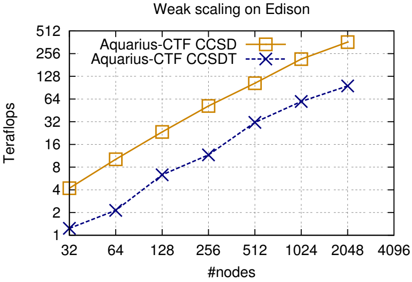
CCSD up to 55 water molecules with cc-pVDZ
CCSDT up to 10 water molecules with cc-pVDZ

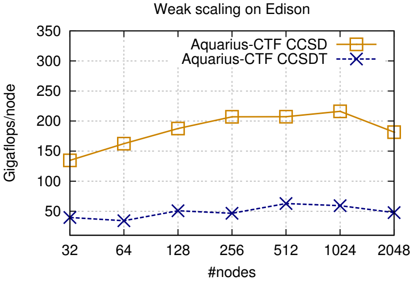




Coupled-cluster code on Cray XC30 (Edison)

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

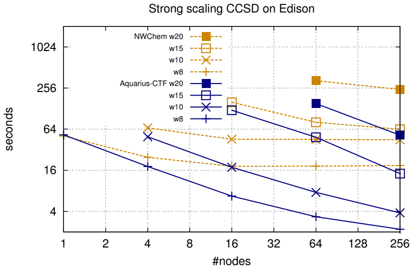


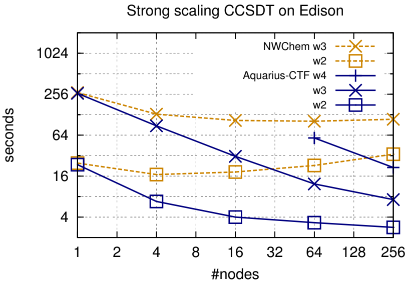


Comparison with NWChem

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)





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    - enables graph algorithms on the (min,+) semiring
    - more exotic use-cases possible such as tensors of particles

Future work for CTF

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Future work for CTF

- (Aquarius) CCSD(T), CCSDT(Q), CCSDTQ
- time-accurate performance models
- simultaneous multi-contraction scheduling
- sparse tensors and contractions
- faster algorithms for symmetric contractions (theory in next part of this talk)

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$$Z_{ij} = A_{ij} \cdot (b_i + b_j) \qquad\qquad c_i = \sum_{j=1}^{n} Z_{ij} - \left(\sum_{j=1}^{n} A_{ij}\right) \cdot b_i$$

which requires $\frac{n^2}{2}$ multiplications and $\frac{5n^2}{2}$ additions

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- The *symmetry preserving algorithm* employs a *symmetric* intermediate tensor $\mathbf{Z}$ using $n^3/6$ multiplications and $7n^3/6$ additions,

$$Z_{ijk} = (A_{ij} + A_{ik} + A_{jk}) \cdot (B_{ij} + B_{ik} + B_{jk}) \qquad v_i = \sum_{k=1}^{n} A_{ik} \cdot B_{ik}$$

$$C_{ij} = \sum_{k=1}^{n} Z_{ijk} - n \cdot A_{ij} \cdot B_{ij} - v_i - v_j - \left(\sum_{k=1}^{n} A_{ik}\right) \cdot B_{ij} - A_{ij} \cdot \left(\sum_{k=1}^{n} B_{ik}\right)$$

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- Numerical stability confirmed via proof and experiments

Application to CCSD

The CCSD contraction

$$Z^{a\bar{k}}_{i\bar{c}} = \sum_{b}\sum_{j} T^{ab}_{ij} \cdot V^{j\bar{k}}_{b\bar{c}}$$

usually requires $2n^6$ total operations.
The symmetry-preserving algorithm can be applied over the indices

$$\mathbf{Z^a} = \sum_{b} \mathbf{T^{ab}} \cdot \mathbf{V_b}$$

with each multiplication being a contraction over the other four indices $i,j,\bar{c},\bar{k}$, which is more expensive than the addition operations, yielding n^6 operations to leading order.

Application to CCSD(T) and CCSDT(Q)

The CCSD(T) contraction

$$T^{ab\bar{c}}_{ij\bar{k}} = P(a,b)P(i,j)\sum_{\bar{l}=1}^{n} T^{a\bar{c}}_{i\bar{l}} \cdot W^{\bar{l}b}_{j\bar{k}}$$

usually requires $2n^7$ total operations.
The symmetry-preserving algorithm can be applied over the indices

$$\mathbf{T^{ab}} = P(a,b)\mathbf{T^{a}} \cdot \mathbf{W^{b}} \qquad \text{and} \qquad \mathbf{T_{ij}} = P(i,j)\mathbf{T_{i}} \cdot \mathbf{T_{j}}$$

with each multiplication in the latter being a contraction over the remaining three indices $\bar{c}$,$\bar{k}$, and $\bar{l}$, for a total of $n^7/2$ leading order operations.
For a similar CCSDT(Q) contraction, which usually requires $n^9/2$ operations, the symmetry preserving algorithm achieves $n^9/36$.

Conclusion

Future work on symmetry-preserving algorithms

- Full cost derivations for CC methods
- High performance implementation and integration into CTF

References

- CTF (latest): E.S., D. Matthews, J.R. Hammond, J.F. Stanton, J. Demmel, "A massively parallel tensor contraction framework for coupled-cluster", JPDC, 2015. computations
- symmetry preserving algorithms: E.S., J. Demmel, "Contracting symmetric tensors using fewer multiplications", ETH Report, 2015.
- communication cost of symmetry preserving algorithms: E.S., J. Demmel, T. Hoefler, "Communication lower bounds for tensor contraction algorithms", ETH Report, 2015.

Backup slides