Efficient Tensor Contraction Algorithms for Coupled Cluster

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Outline

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- scalability must be achieved both for intranode (shared memory) and internode (distributed memory) parallelism

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- optimized for distributed networks, shared memory, and accelerators
- open source, BSD license, `https://github.com/solomonik/ctf`

Distributed-memory tensor objects

CTF is orchestrated by bulk synchronous operations on a set of processors

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CTF::World dw(MPI_COMM_WORLD);
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- tensors are templated by the element type (double by default)
- custom algebraic structures (set, group, monoid, semiring, ring) may be defined by the user

Tensor algebra interface (credit: Devin Matthews)

CTF can express a tensor contraction like

$$Z_{ij}^{ab} = \frac{1}{2} \cdot W_{ij}^{ab} + 2 \cdot P(a,b) \sum_k F_k^a \cdot T_{ij}^{kb}$$

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

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- $P(a,b)$ is applied implicitly if **Z** is antisymmetric in ab
- **Z**, **F**, **T**, **W** should all be defined on the same world and all processes in the world must call the contraction bulk synchronously
- user-defined (mixed-type) scalar tensor functions can be applied instead of $+$ and $*$

Quantum chemistry codes using CTF

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- **Libtensor** has been integrated with CTF by Evgeny Epifanovsky
- **Q-Chem** can leverage Libtensor and integration with CTF is almost complete

CCSD

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

```
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"];
Z(3)["abcijk"] += 0.5*WMNIJ["mnij"]*T(3)["abcmnk"];
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- extract permuted tensor slices (e.g. arbitrary subsets of rows and columns)

Tensor decomposition and mapping

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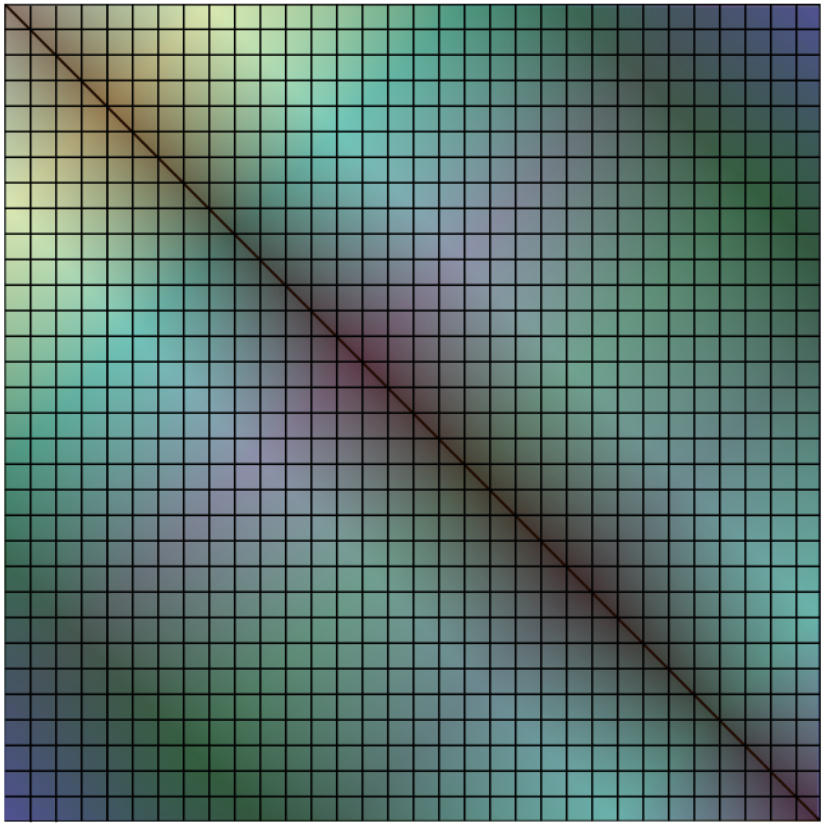
CTF mapping logic

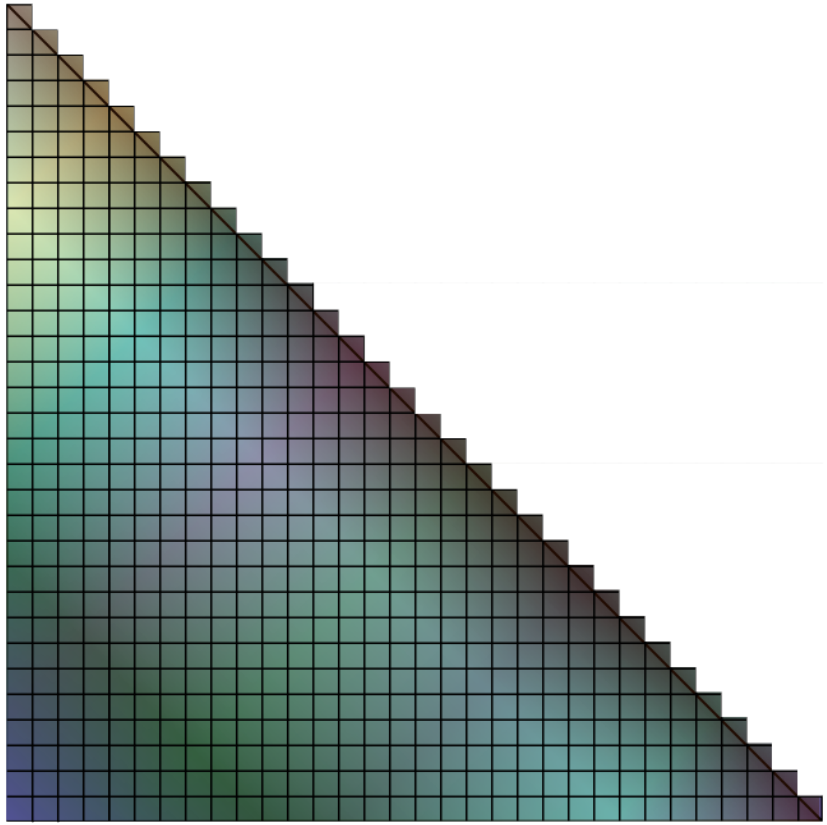
- arrange physical topology into all possible processor grids
- for each contraction autotune over all topologies and mappings
- select best mapping based on performance models (communication cost, memory requirements, etc.)

Symmetric matrix representation

Symmetric matrix

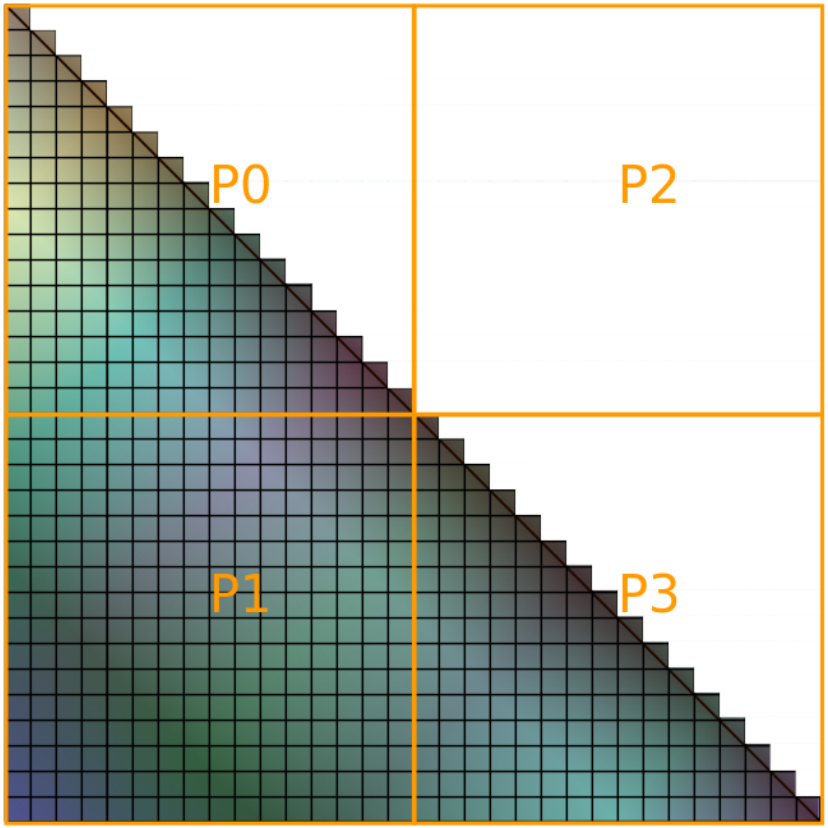


Unique part of symmetric matrix

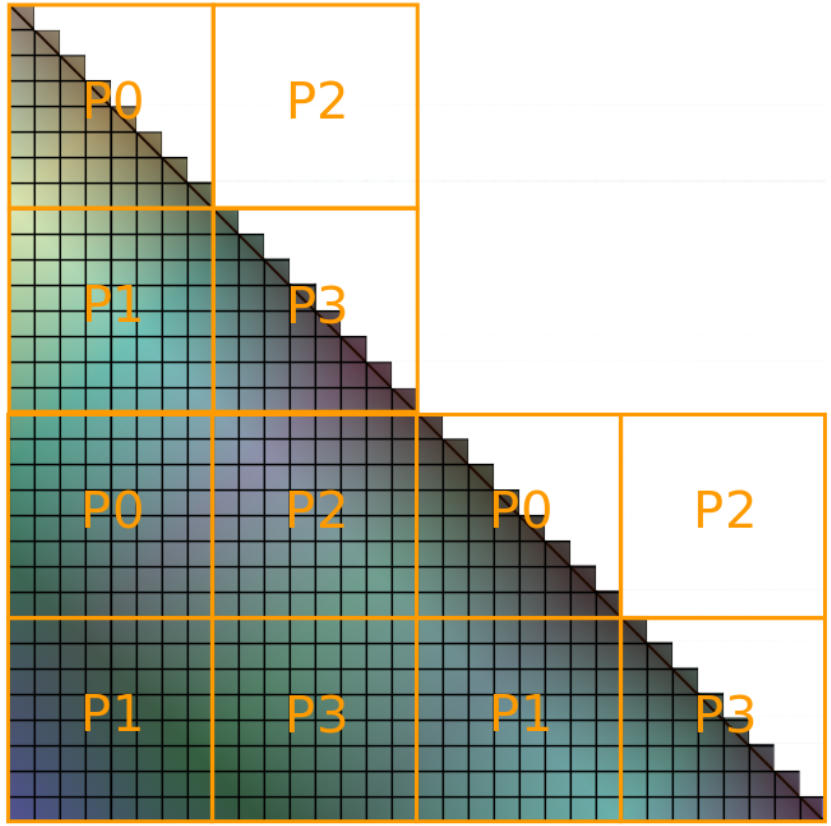


Blocked distributions of a symmetric matrix

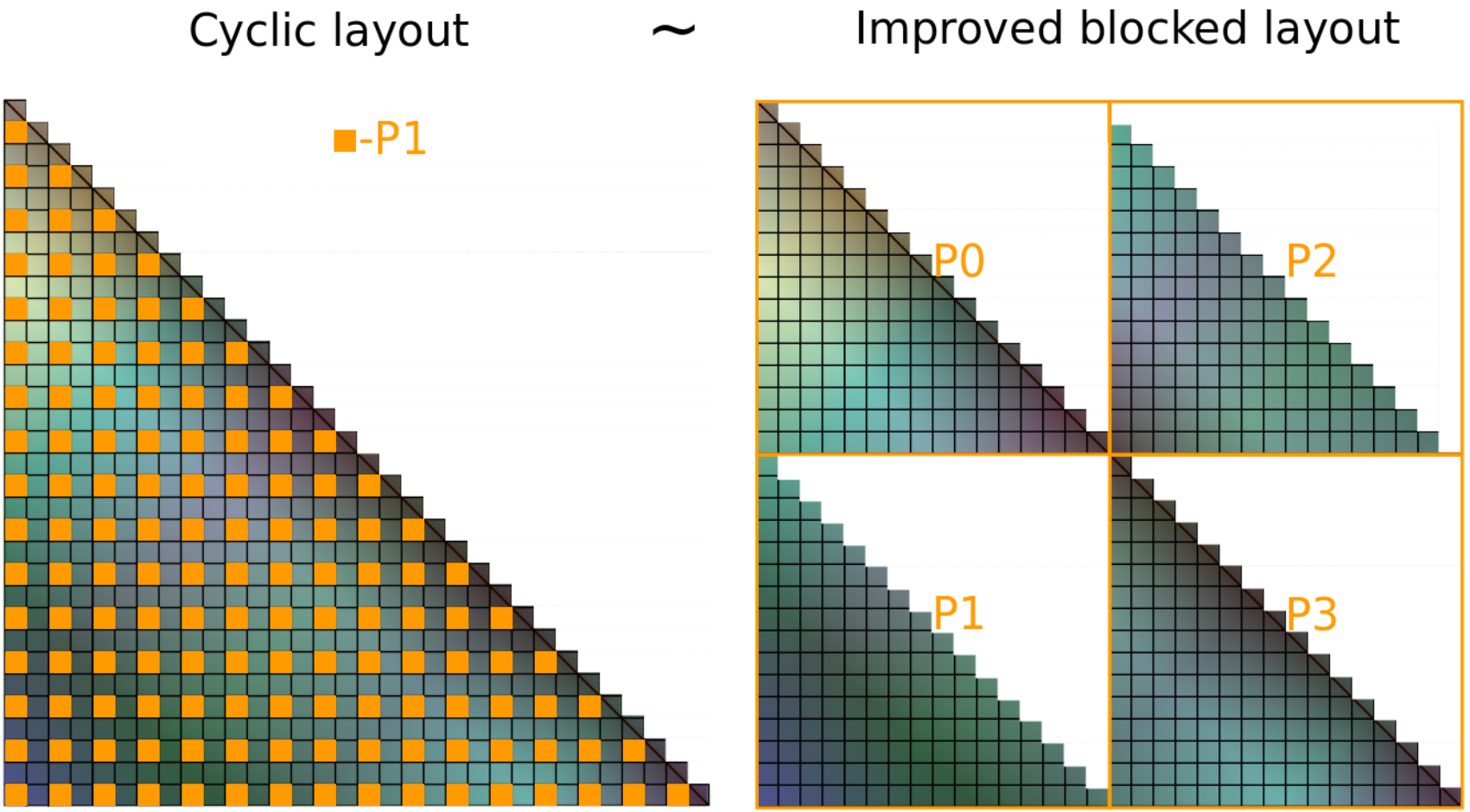
Naive blocked layout



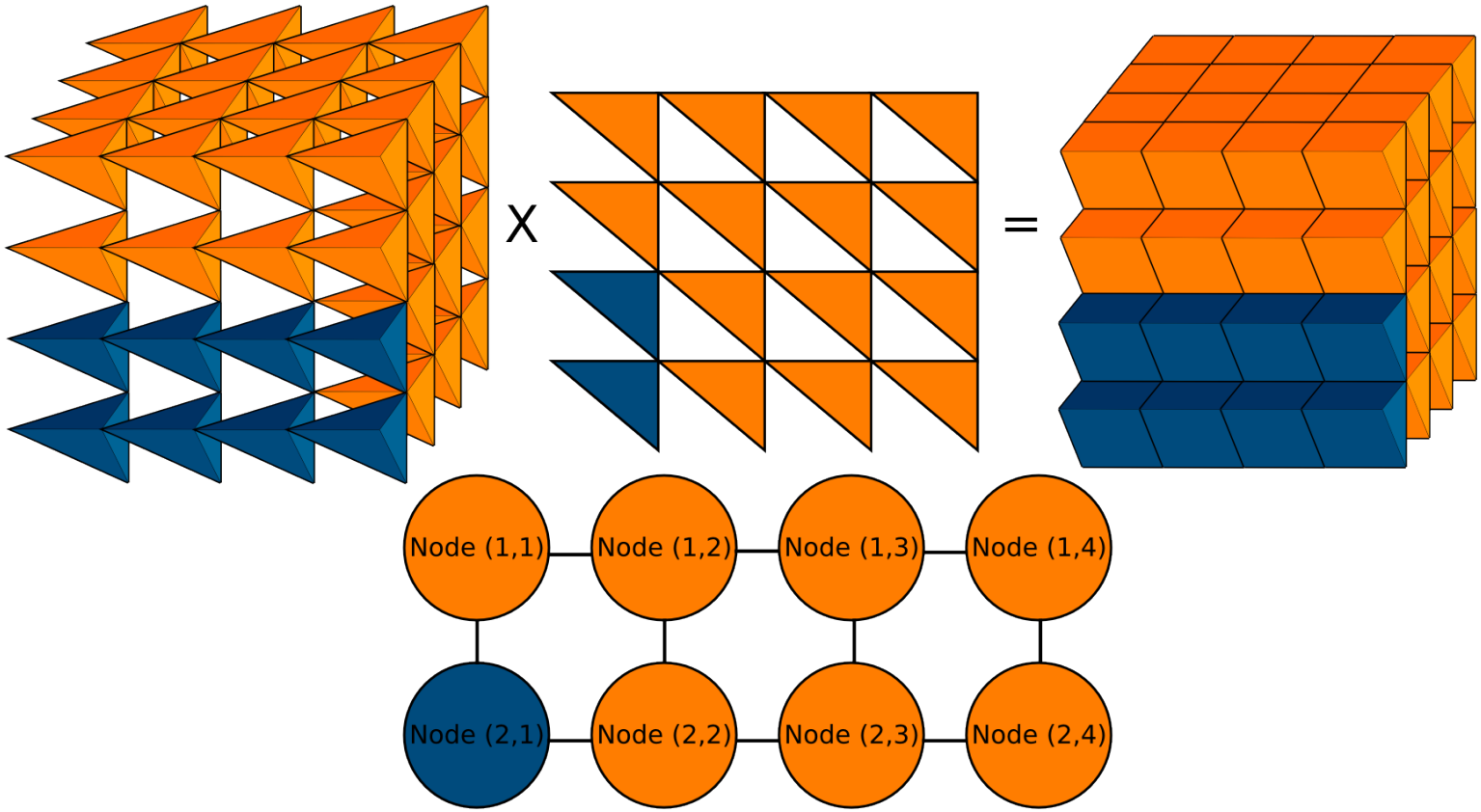
Block-cyclic layout



Cyclic distribution of a symmetric matrix



Tensor contraction mapping visualization



Algorithms and optimization for tensor redistribution

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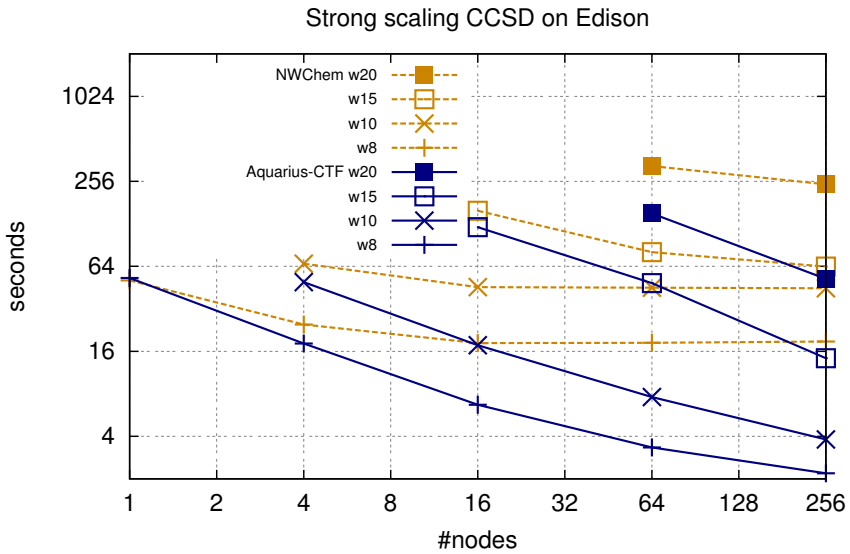
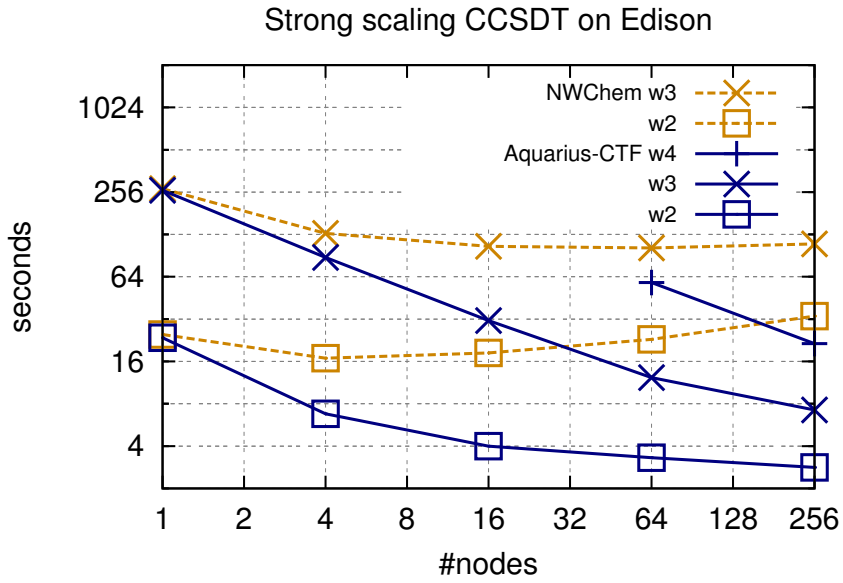
- Block-to-block redistribution between similar distributions on different processor grids
  - processors exchange blocks via point-to-point messages

Comparison with NWChem

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

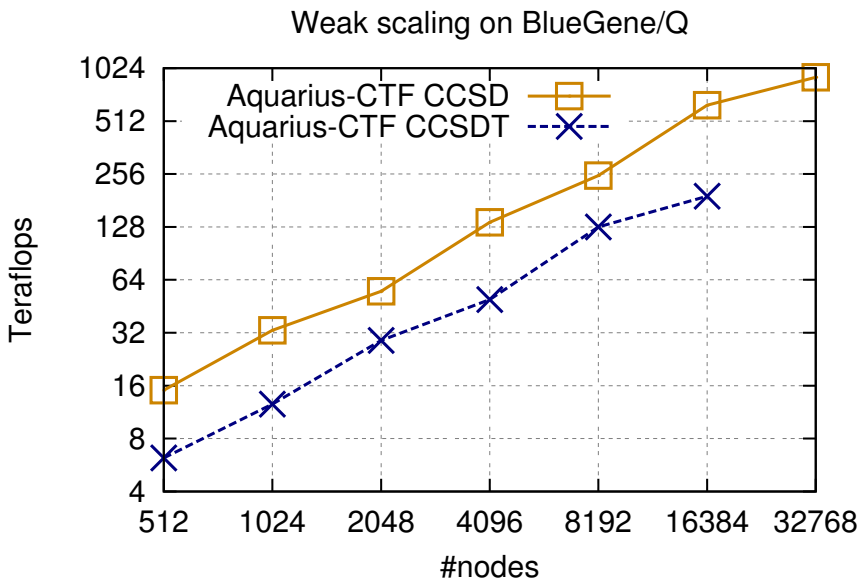
- provides CCSD and CCSDT
- uses Global Arrays (GA) tensor partitioning and contraction
- Tensor Contraction Engine (TCE) factorizes CC equations and generated GA code

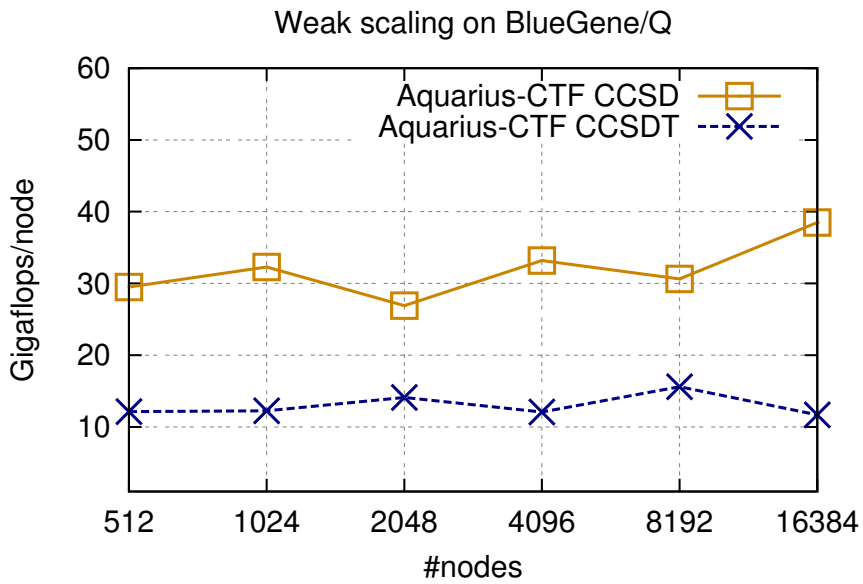




Coupled-cluster code on BlueGene/Q (Mira)

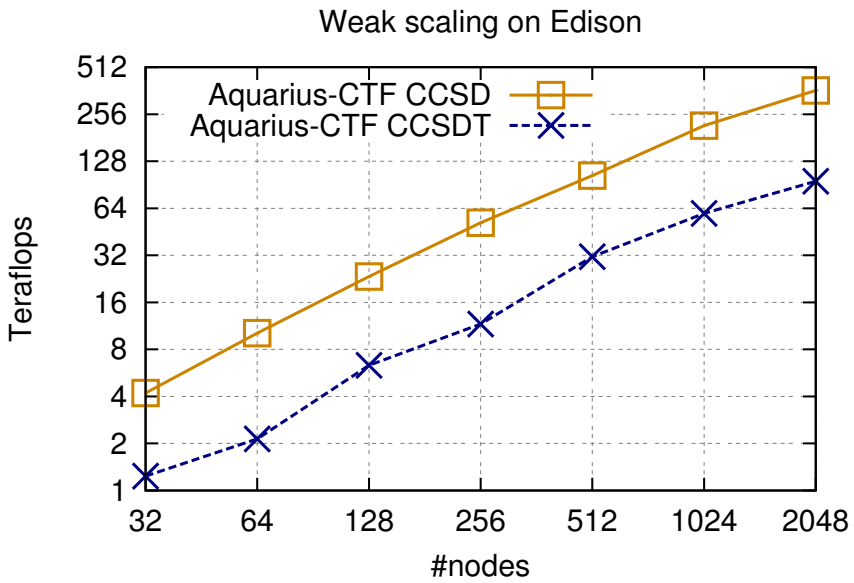
CCSD up to 55 water molecules with cc-pVDZ
CCSDT up to 10 water molecules with cc-pVDZ

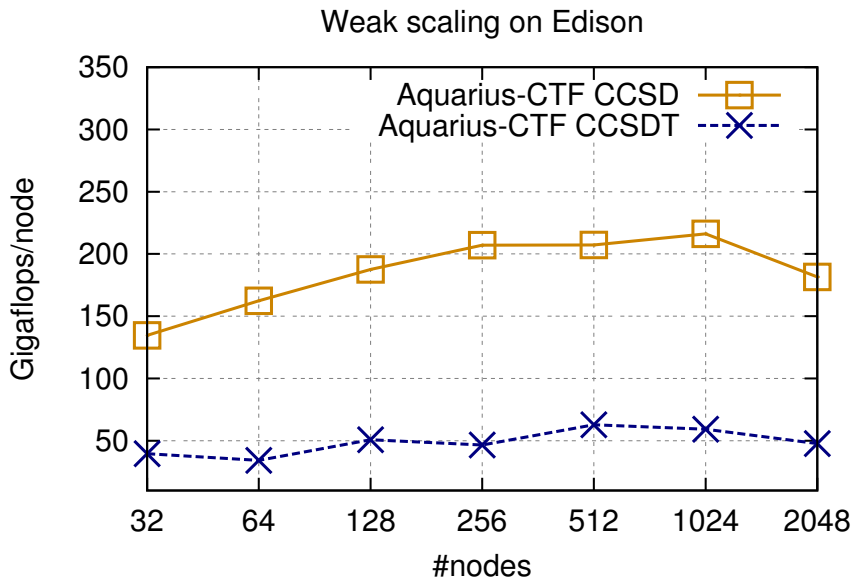




Coupled-cluster code on Cray XC30 (Edison)

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





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which requires n^2 multiplications and n^2 additions

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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
- Communication cost lower and upper bounds derived

Application to CCSD

The CCSD contraction

$$Z_{i\bar{c}}^{a\bar{k}} = \sum_{b} \sum_{j} T_{ij}^{ab} \cdot V_{b\bar{c}}^{j\bar{k}}$$

usually requires $2n^6$ total operations.

Application to CCSD

The CCSD contraction

$$Z_{i\bar{c}}^{a\bar{k}} = \sum_b \sum_j T_{ij}^{ab} \cdot V_{b\bar{c}}^{j\bar{k}}$$

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

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

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

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.

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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 $n^9/18$.

Conclusion

Future work on symmetry-preserving algorithms

- full cost derivations for CC methods

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