Fast tensor contractions for Coupled Cluster

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Motivation and goals

Cyclops (cyclic-operations) Tensor Framework

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- allow for efficient tensor redistribution and slicing
- exploit permutational tensor symmetry efficiently
- uses only MPI, BLAS, and OpenMP and is a library

Define a parallel world

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

- a set of processors in MPI corresponds to a communicator (MPI_Comm)
- MPI_COMM_WORLD is the default communicators containing all processes
- CTF_World dw(comm) defines an instance of CTF on any MPI communicator

Define a tensor

A tensor is a multidimensional array, e.g.

$$T^{ab}_{ij}$$

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

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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,

- Z["abij"] += 2.0*F["ak"]*T["kbij"]

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  - 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

Write a Coupled Cluster code

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"];
```

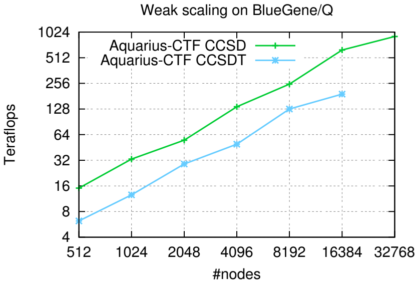
Write more Coupled Cluster code

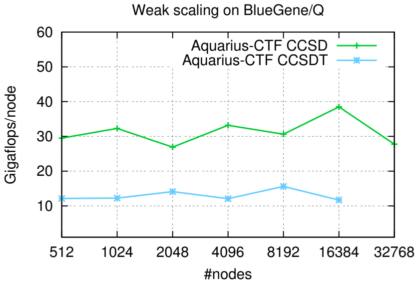
Extracted from Aquarius (Devin Matthews' code)

```
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"];
Z(3)["abcijk"] -= WAMEI["amei"]*T(3)["ebcmjk"];
```

Run your Coupled Cluster code on a IBM supercomputer

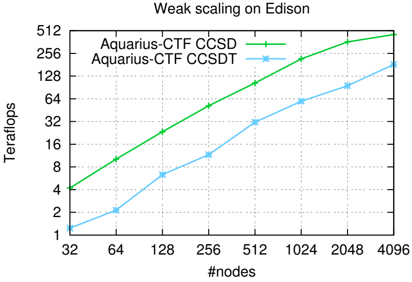
CCSD up to 55 water molecules with cc-pVDZ
CCSDT up to 10 water molecules with cc-pVDZ

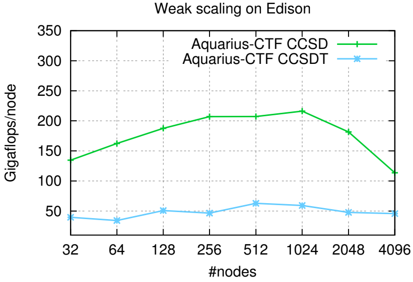




Run your Coupled Cluster code on the computer next door (Edison)

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





Run your Coupled Cluster code faster than NWChem

NWChem is a distributed-memory quantum chemistry method suite

- provides CCSD and CCSDT

CCSD performance on Edison (thanks to Jeff Hammond for building NWChem and collecting data)

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- NWChem 40 water molecules on 1024 nodes: 44 min
- CTF 40 water molecules on 1024 nodes: 9 min

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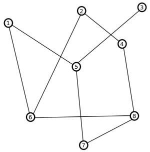
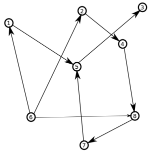
- Faster symmetric tensor contraction algorithms...

Graphs and hypergraphs

Examples of a undirected graph and directed graph





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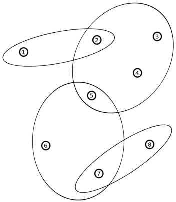

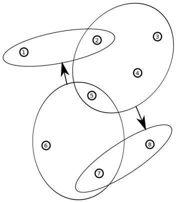

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- similarly we can represent any matrix as a graph with the connectivity of the graph corresponds to the sparsity of the matrix

Its useful to connect matrices with graphs

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- direct particle methods may be written in above form (for certain definition of $\cdot$), where $\mathbf{x}$ are particles and $\mathbf{A}$ corresponds to forces

Semirings

We typically work with the semiring $c + a \cdot b$, but we could employ the tropical semiring $\min(c, a + b)$

- let $\mathbf{y} = y \oplus \mathbf{A} \odot \mathbf{x}$ denote matrix vector multiplication on the tropical semiring, so

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- the closure of a matrix $\mathbf{B}$ corresponding to graph G on the tropical semiring $\mathbf{B}^* = \mathbf{I} \oplus \mathbf{B} \oplus \mathbf{B}^2 \ldots$ gives all shortest paths in G

Tensors are hypergraphs

Consider a $n \times n \times m \times m$ tensor

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

which is symmetric in *ab* and *ij*

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- We can represent any fully-symmetric tensor of dimension d as a hypergraph where all edges have cardinality d

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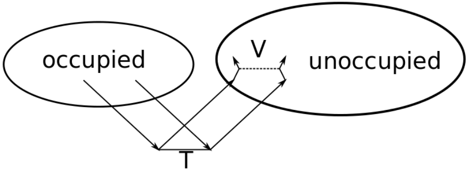
- for instance $Z^{ab}_{ij} = \sum_{cd} V^{ab}_{cd} T^{cd}_{ij}$ may be visualized as



Coupled Cluster as a hypergraph computation

Coupled Cluster iteratively refines the bipartite hypergraph H corresponding to **T**

- the integrals **V** may also be interpreted as hyperedges in H, but not bipartite
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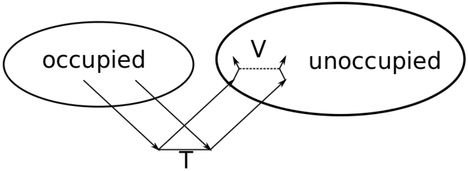

- Speculation: switch semirings and have CC compute shortest paths in a hypergraph

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Now lets consider a special case of semirings: commutative rings

- Let **b** be a vector of length n

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

Symmetrized product

We can apply a similar trick for the symmetrized outer product

- Let **a** and **b** be vectors of length n
- Compute symmetric matrix **A**

$$\mathbf{C} = \mathbf{a} \cdot \mathbf{b}^T + \mathbf{b} \cdot \mathbf{a}^T$$

$$C_{i \leq j} = a_i \cdot b_j + a_j \cdot b_i$$

- If $\cdot$ is an operator on a commutative ring, we can use half the multiplications,

$$C_{i \leq j} = (a_i + a_j) \cdot (b_i + b_j) - a_i \cdot b_i - a_j \cdot b_j.$$

A commutative ring of symmetric matrices

Given n-by-n symmetric matrices $\mathbf{A}, \mathbf{B}$ define commutative ring $\otimes$

$$\mathbf{A} \otimes \mathbf{B} = \mathbf{A} \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{A}$$

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- the operator $\otimes$ may be applied using $n^3/3! = n^3/6$ multiplications

$$w_i = \sum_{k=1}^{n} A_{ik} \quad x_i = \sum_{k=1}^{n} B_{ik} \quad y_i = \sum_{k=1}^{n} A_{ik} \cdot B_{ik}$$

$$Z_{i \le j \le k} = (A_{ij} + A_{ik} + A_{jk}) \cdot (B_{ij} + B_{ik} + B_{jk})$$

$$C_{i \le j} = C_{i \le j} + \sum_{k=1}^{n} Z_{ijk} - n \cdot A_{ij} \cdot B_{ij} - y_i - y_j - w_i \cdot B_{ij} - A_{ij} \cdot x_j$$

General fast symmetric tensor contractions

Given *fully* symmetric **A**, **B**, and **C**, compute $\mathbf{C} = A \otimes B$

$$C_{i_1 \ldots i_{s+t}} = \sum_{((j_1 \ldots j_s),(l_1 \ldots l_t)) \in \chi_s(i_1 \ldots i_{s+t})} \left(\sum_{k_1 \ldots k_v} A^{k_1 \ldots k_v}_{j_1 \ldots j_s} \cdot B^{l_1 \ldots l_t}_{k_1 \ldots k_v} \right).$$

Typically computed by (implicitly) forming partially-symmetric $\bar{\mathbf{C}}$

$$\bar{C}^{l_1 \ldots l_t}_{j_1 \ldots j_s} = \sum_{k_1 \ldots k_v} A^{k_1 \ldots k_v}_{j_1 \ldots j_s} \cdot B^{l_1 \ldots l_t}_{k_1 \ldots k_v}.$$

This requires $\frac{n^{s+t+v}}{s!t!v!}$ multiplications, via fully symmetric intermediates it becomes,

$$\binom{n}{s+t+v} \approx \frac{n^{s+t+v}}{(s+t+v)!}$$

General symmetric contraction algorithm

Compute $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}$, using the notation $(j_1 \dots j_s, k_1 \dots k_t) \in \{i_1 \dots i_{s+t+v}\}$ to denote a partition into two disjoint sets:

$$Z_{i_1 \leq \dots i_{s+t+v}} = \sum_{(j_1 \dots j_s, k_1 \dots k_v) \in \{i_1 \dots i_{s+t+v}\}} A^{k_1 \dots k_v}_{j_1 \dots j_s} \cdot \sum_{(l_1 \dots l_t, k_1 \dots k_v) \in \{i_1 \dots i_{s+t+v}\}} B^{l_1 \dots l_t}_{k_1 \dots k_v}$$

$$W_{i_1 \leq \dots i_{s+t+v-1}} = \sum_{(j_1 \dots j_s, k_1 \dots k_v) \in \{i_1 \dots i_{s+t+v-1}\}} A^{k_1 \dots k_v}_{j_1 \dots j_s} \cdot \sum_{(l_1 \dots l_t, k_1 \dots k_v) \in \{i_1 \dots i_{s+t+v-1}\}} B^{l_1 \dots l_t}_{k_1 \dots k_v}$$

$$V_{i_1 \leq \dots i_{s+t+v-1}} = \sum_{(j_1 \dots j_s, k_1 \dots k_{v-1}) \in \{i_1 \dots i_{s+t+v-1}\}} \sum_{k_v} A^{k_1 \dots k_v}_{j_1 \dots j_s}$$
$$\cdot \sum_{(l_1 \dots l_t, k_1 \dots k_{v-1}) \in \{i_1 \dots i_{s+t+v-1}\}} \sum_{k_v} B^{l_1 \dots l_t}_{k_1 \dots k_v}$$

$$C_{i_1 \dots i_{s+t}} = \sum_{k_1 \dots k_v} Z_{i_1 \dots i_{s+t}, k_1, \dots k_v} - n \cdot \sum_{k_1 \dots k_{v-1}} W_{i_1 \dots i_{s+t}, k_1, \dots k_{v-1}}$$
$$- \sum_{k_1 \dots k_{v-1}} V_{i_1 \dots, i_{s+t}, k_1, \dots k_{v-1}}$$

Any tensor is a fully symmetric tensor

Realizing that a vector is a symmetric tensor, we may express any tensor as a nested symmetric tensor

- A nonsymmetric matrix A_{ij} is a vector of vectors $\bar{a}$ where each element $\bar{\bar{a}} = \bar{a}_i$ is a vector with $\bar{\bar{a}}_j = A_{ij}$

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- Therefore, we can compute a contraction like

$$C_{abij} = P(a, b) \sum_{ck} A_{acik} \cdot B_{cbkj}$$

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- Unfortunately contractions of the above form do not exist in Coupled Cluster theory and cannot be written using raised and lowered index notation

Limited application of fast symmetric contraction to Coupled Cluster

For some CC contractions, we can at least gain a factor of two

- Consider the contraction

$$Z_{ij}^{ab} = P(i,j)P(a,b)\sum_{klcd} T_{ik}^{ac} V_{cd}^{kl} T_{lj}^{db}$$

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- Defining vector $\bar{W}^a$ with elements $W_{il}^{ad} \in \bar{W}^a$ for all d, i, l, and similarly vector $\bar{V}_c$ and symmetric matrix $\bar{T}^{ac}$, we may compute $\bar{\mathbf{W}} = \bar{\mathbf{T}} \otimes \bar{\mathbf{V}}$,

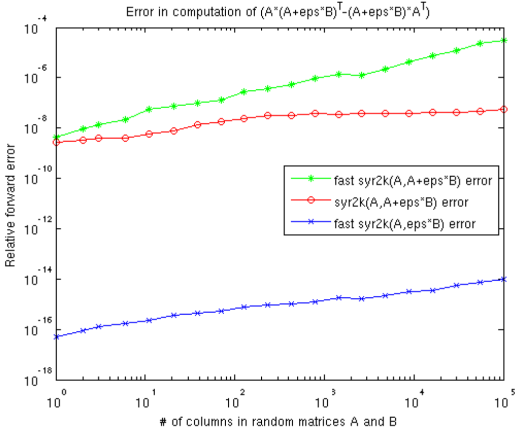
$$\bar{W}^a = \sum_c \bar{T}^{ac} \cdot \bar{V}_c$$

using half the multiplications, resulting in $n^2/2$ calls to subcontraction

$$\tilde{W}_{il}^{d} = \sum_k \tilde{T}_{ik} \cdot \tilde{V}_d^{kl}$$

Disclaimer: numerical characteristics

The fast contraction algorithms have different numerical characteristics in floating-point precision



Rewind

Stepping back from hypergraphs and rings...

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- Hopefully the hypergraph and fast contraction algorithms lead to some insight towards better understanding of CC

Collaborators and acknowledgements

Collaborators:

- Devin Matthews, UT Austin (contributions to CTF, teaching me CC, and development of Aquarius on top of CTF)
- Jeff Hammond, Argonne National Laboratory (initiated project, provides continuing advice, and runs NWChem for me when my patience runs out)
- James Demmel and Kathy Yelick, UC Berkeley (advising)

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Backup slides