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 \( ij \)

- `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 \( ab \),

- \( Z[" abij "] += 2.0*F[" ak"]*T[" kbij"] \)
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- $Z$, $F$, $T$ should all be defined on the same world and all processes in the world must call the contraction bulk synchronously
- the beginning of the end of all for loops...
Access and write tensor data

CTF takes away your data pointer
- Access arbitrary sparse subsets of the tensor by global index (coordinate format)
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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 \( Q \)
Write a Coupled Cluster code

Extracted from Aquarius (Devin Matthews’ code)

\[
\begin{align*}
\text{FMI["mi"]} & \text{ += 0.5*WMNEF["mnef"]*T(2)["efin"];} \\
\text{WMNIJ["mnij"]} & \text{ += 0.5*WMNEF["mnef"]*T(2)["efij"];} \\
\text{FAE["ae"]} & \text{ -= 0.5*WMNEF["mnef"]*T(2)["afmn"];} \\
\text{WAMEI["amei"]} & \text{ -= 0.5*WMNEF["mnef"]*T(2)["afin"];} \\
\text{Z(2)["abij"]} & \text{ = WMNEF["ijab"];} \\
\text{Z(2)["abij"]} & \text{ += FAE["af"]*T(2)["fbij"];} \\
\text{Z(2)["abij"]} & \text{ -= FMI["ni"]*T(2)["abnj"];} \\
\text{Z(2)["abij"]} & \text{ += 0.5*WABEF["abef"]*T(2)["efij"];} \\
\text{Z(2)["abij"]} & \text{ += 0.5*WMNIJ["mnij"]*T(2)["abmn"];} \\
\text{Z(2)["abij"]} & \text{ -= WAMEI["amei"]*T(2)["ebmj"];} \\
\end{align*}
\]
Write more Coupled Cluster code

Extracted from Aquarius (Devin Matthews’ code)

\[
\begin{align*}
Z(1)["ai"] & += 0.25*WMNEF["mnef"]*T(3)["aefimn"];
Z(2)["abij"] & += 0.5*WAMEF["bmef"]*T(3)["aefijm"];
Z(2)["abij"] & -= 0.5*WMNEJ["mnej"]*T(3)["abeinm"];
Z(2)["abij"] & += FME["me"]*T(3)["abeijm"];
Z(3)["abcijk"] & = WABEJ["bcek"]*T(2)["aeij"];
Z(3)["abcijk"] & -= WAMIJ["bmjk"]*T(2)["acim"];
Z(3)["abcijk"] & += FAE["ce"]*T(3)["abeijk"];
Z(3)["abcijk"] & -= FMI["mk"]*T(3)["abcijm"];
Z(3)["abcijk"] & += 0.5*WABEF["abef"]*T(3)["efcijk"];
Z(3)["abcijk"] & += 0.5*WMNIJ["mnij"]*T(3)["abcmnk"];
Z(3)["abcijk"] & -= WMAM["amei"]*T(3)["ebcmjk"];
\end{align*}
\]
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
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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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CCSD performance on Edison (thanks to Jeff Hammond for building NWChem and collecting data)

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

Lots of room for improvement, ongoing effort

- Multi-contraction scheduler being developed by Richard Lin (UCB)
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- Faster symmetric tensor contraction algorithms...
Graphs and hypergraphs

Examples of a undirected graph and directed graph

Examples of a undirected hypergraph and directed hypergraph
Matrices are graphs

A graph $G = (V, E)$ is a set of vertices $V$ and a set of edges $E$.

- we can associate a weight $w_{ij}$ for each edge $(i, j) \in E$. 

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- $W$ is symmetric if $G$ is undirected.
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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
It's useful to connect matrices with graphs.

Graphs give a natural visualization for
- any mesh

Matrices allow for numerical computation on graphs.
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\[ x^k = A \cdot x^{k-1} \]
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\[ x^k = A \cdot x^{k-1} \]

- direct particle methods may be written in above form (for certain definition of \( \cdot \)), where \( x \) are particles and \( A \) corresponds to forces
We typically work with the semiring $c + a \cdot b$, but we could employ the tropical semiring $\min(c, a + b)$

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

$$y_i = \min(y_i, \min_k (A_{ik} + x_k))$$
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- the closure of a matrix $B$ corresponding to graph $G$ on the tropical semiring $B^* = I \oplus B \oplus B^2 \ldots$ gives all shortest paths in $G$
Tensors are hypergraphs

Consider a \( n \times n \times m \times m \) tensor

\[
T^{ab}_{ij}
\]

which is symmetric in \( ab \) and \( ij \)

- represent it as a directed hypergraph \( H = (V, E) \) with edges of the form \((\{a, b\}, \{i, j\}) \in E\)
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- If we can divide $V$ into two disjoint subsets $V_1 \cup V_2 = V$ (occupied and unoccupied orbitals), where all edges go from $V_1$ to $V_2$, $H$ is a bipartite hypergraph
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- We can represent any fully-symmetric tensor of dimension \( d \) as a hypergraph where all edges have cardinality \( d \)
Coupled Cluster as a hypergraph computation

Coupled Cluster iteratively refines the bipartite hypergraph $H$

- the integrals $V$ may also be interpreted as hyperedges in $H$, but not bipartite
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```
occupied  V  unoccupied
```

Speculation: switch semirings and have CC compute shortest paths in a hypergraph
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Symmetric matrix times vector

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- Typically, we say the symmetry of $\mathbf{A}$ is broken and compute

$$c_i = \sum_{j=1}^{n} A_{ij} \cdot b_j$$
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  \[
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  \]
- Typically, we say the symmetry of \( \mathbf{A} \) is broken and compute
  \[
  c_i = \sum_{j=1}^{n} A_{ij} \cdot b_j
  \]
- If \( \cdot \) is an operator on a ring, we can use half the number of multiplications
  \[
  c_i = \sum_{j=1}^{n} A_{ij} \cdot (b_i + b_j) - \left( \sum_{j=1}^{n} A_{ij} \right) b_i
  \]
Symmetrized product

We can apply a similar trick for the symmetrized outer product

- Let \( \mathbf{a} \) and \( \mathbf{b} \) be vectors of length \( n \)
- Compute symmetric matrix \( \mathbf{A} \)

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

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

- 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 $A, B$ define commutative ring $\otimes$

$$A \otimes B = A \cdot B + B \cdot A$$

- note that the product is still symmetric, unlike $A \cdot B$
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- note that the product is still symmetric, unlike \( A \cdot B \)
- the operator \( \otimes \) may be applied using \( n^3 / 3! = n^3 / 6 \) multiplications

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

\[
Z_{i \leq j \leq k} = (A_{ij} + A_{ik} + A_{jk}) \cdot (B_{ij} + B_{ik} + B_{jk})
\]

\[
C_{i \leq j} = C_{i \leq j} + \sum_{k=1}^{n} Z_{ijk} - n \cdot A_{ij} \cdot B_{ij} - y_i - y_j - w_i \cdot B_{ij} - A_{ij} \cdot x_j
\]
General fast symmetric tensor contractions

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

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

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

$$\tilde{C}_{j_1...j_s}^{l_1...l_t} = \sum_{k_1...k_v} A_{j_1...j_s}^{k_1...k_v} \cdot B_{l_1...l_t}^{k_1...k_v}.$$ 

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

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

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

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

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

$$- \sum_{k_1 \ldots k_v-1} V_{i_1 \ldots i_{s+t}, k_1 \ldots k_v-1}$$
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 $\bar{a} = \bar{a}_i$ is a vector with $\bar{a}_j = A_{ij}$
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- Therefore, we can compute a contraction like

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

where $A$ is symmetric in $ac$, $B$ is symmetric in $cb$ in $n^6 / 6$ operations
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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

$$Z_{ij}^{ab} = P(i, j)P(a, b) \sum_{klcd} T_{ik}^{ac} V_{kl}^c T_{lj}^{db}$$
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- Defining vector \( \tilde{W}^a \) with elements \( \tilde{W}_{il}^{ad} \in \tilde{W}^a \) for all \( d, i, l \), and similarly vector \( \tilde{V}_c \) and symmetric matrix \( \tilde{T}^{ac} \), we may compute \( \tilde{W} = \tilde{T} \otimes \tilde{V} \),

\[ \tilde{W}^a = \sum_c \tilde{T}^{ac} \cdot \tilde{V}_c \]

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.

![Graph showing error in computation of \((A^*(A + \text{eps}^*B)^T - (A + \text{eps}^*B)^*A^T)\)](image)
Rewind

Stepping back from hypergraphs and rings...

- Cyclops Tensor Framework is available at 
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- Hopefully the hypergraph and fast contraction algorithms lead to some insight towards better understanding of CC
Collaborators and acknowledgements

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- James Demmel and Kathy Yelick, UC Berkeley (advising)

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Backup slides