Cyclops Tensor Framework

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Definition of a tensor

A rank r tensor is r-dimensional representation of a dataset, for example,

- a rank one tensor is a vector (e.g. a set of nodes V)
- a rank two tensor is a matrix (e.g. a set of edges E in a graph $E \subset V \times V$)

Graphically, a rank r tensor is a set of all possible paths P of length r through vertices V

$$P \subset \underbrace{V \times \ldots \times V}_{r\text{-times}}$$

Alternatively, P may be thought of as a set of hypergraph edges with cardinality r

Programmatically, a rank r tensor is an r-dimensional array

Tensor contractions

Given rank 4 tensors **T**, **V**, and **W** we may write perform tensor contraction as

$$W_{abij} = \sum_k \sum_l T_{abkl} \cdot V_{klij}$$

It is common to use raised and lowered index notation, which is sometimes related to the physical meaning of the indices,

$$W^{ab}_{ij} = \sum_{kl} T^{ab}_{kl} \cdot V^{kl}_{ij}$$

raised-indices are usually meant to be contracted with lowered indices.

Tensor folding

Since a tensor is a representation of any data set, we may always switch representations

- define transformation δ^{p}_{ab} to transform a and b into compound index p ($\delta^{p}_{ab} = 1$ when $p = a + b \cdot n$ and 0 otherwise)
- graphically, folding corresponds to replacing edges with vertices ($W = V \times V$)

The contraction

$$W^{ab}_{ij} = \sum_{kl} T^{ab}_{kl} \cdot V^{kl}_{ij}$$

may be folded into matrix multiplication as follows

$$\delta^{p}_{ab} \cdot W^{ab}_{ij} \cdot \delta^{ij}_{q} = \sum_{r} \delta^{p}_{ab} \cdot T^{ab}_{kl} \cdot \delta^{kl}_{r} \cdot \delta^{r}_{kl} \cdot V^{kl}_{ij} \cdot \delta^{ij}_{q}$$

$$W^{p}_{q} = \sum_{r} T^{p}_{r} \cdot V^{r}_{q}$$

Reasons to use tensor represenations

If all contractions can be folded into matrix multiplication, why use tensors of rank greater than two?

- permutational index symmetry: the tensors may express higher-dimensional structure
- expression of many different contractions with a single representation (each may require different folding)
- finding low-rank tensor decompositions, such as the CP (CANDECOMP/PARAFAC) decomposition

$$T_{ijk} \approx \sum_{r}^{R} v_{ir} \cdot w_{jr} \cdot z_{kr}$$

This talk will not address low-rank decompositions.

Application: Coupled Cluster

Coupled Cluster (CC) is a numerical approximation scheme to the time-independent many-body Schrödinger equation

$$|\Psi\rangle = e^{\mathbf{T_1}+\mathbf{T_2}+\mathbf{T_3}+\cdots}|\Phi_0\rangle$$

where $\mathbf{T_k}$ is a rank $2k$ 'ampltiude' tensor which correlates sets of k electrons over sets of k basis-functions (captures k-electron excitations)

- the CCSD method is a truncation at $\mathbf{T_1} + \mathbf{T_2}$
- the CCSDT method also includes $\mathbf{T_3}$

The CC methods produce a set of nonlinear equations for the amplitude tensors which are solved iteratively via tensor contractions

Given a system of n electrons, the methods require $O(n^{2k})$ memory and $O(n^{2k+2})$ operations

Motivation and goals

Cyclops (cyclic-operations) Tensor Framework (CTF)

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- exploits 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

Consider a rank four tensor **T** (in CC this is the 2-electron $\mathbf{T_2}$ amplitude)

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

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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  - 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

Extract from CCSD implementation

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"];
```

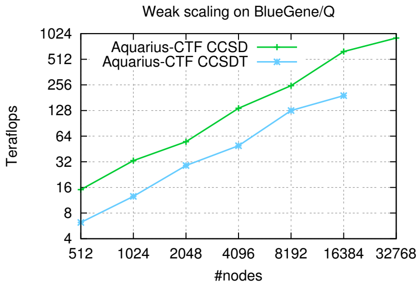
Extract from CCSDT implemetnation

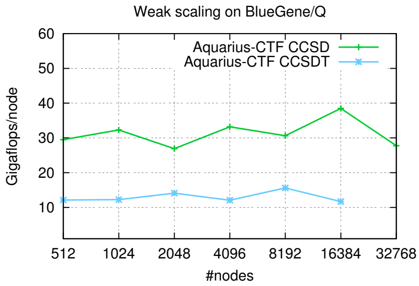
Extracted from Aquarius (Devin Matthews' code)

```
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"];
```

Coupled Cluster on IBM BlueGene/Q

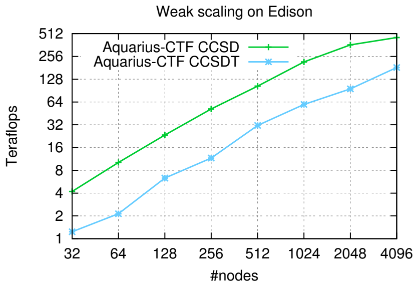
CCSD up to 55 water molecules with cc-pVDZ
CCSDT up to 10 water molecules with cc-pVDZ

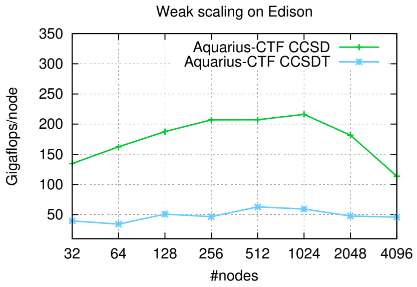




Coupled Cluster on Cray XC30 Edison

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





Comparison with NWChem

NWChem is a distributed-memory quantum chemistry method suite

- provides CCSD and CCSDT
- uses Global Arrays a Partitioned Global Address Space (PGAS) backend for tensor contractions
- derivation automatically done by Tensor Contraction Engine (TCE)

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

NWChem approach to contractions

A high-level description of NWChem's algorithm for tensor contractions:

- data layout is abstracted away by the Global Arrays framework
- Global Arrays uses one-sided communication for data movement
- packed tensors are stored in blocks
- for each contraction, each process does a subset of the block contractions
- each block is transposed and unpacked prior to contraction
- dynamic load balancing is employed among processors

CTF approach to contractions

A high-level description of CTF's algorithm for tensor contractions:

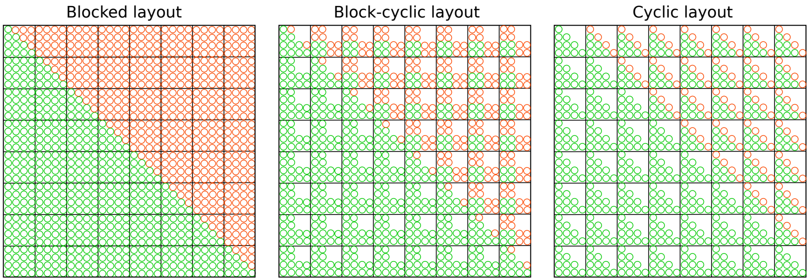
- packed tensors are decomposed cyclically among toroidal processor grids
- MPI collectives are used for all communication
- for each contraction, a distributed layout is selected based on internal performance models
- performance model considers all possible execution paths
- before contraction, tensors are redistributed to a new layout
- if there is enough memory, the tensors are (partially) unpacked
- all preserved symmetries and non-symmetric indices are folded in preparation for matrix multiplication
- nested distributed matrix multiply algorithms are used to perform the contraction in a load-balanced manner

Input via sparse tensor reads and writes

In CTF, tensors are defined on a communicator (subset or full set of processors)

- the data pointer is hidden from the user
- the user can perform block-synchronous bulk writes and reads of index-value pairs
- to avoid communication, the user may read the current local pairs
- it is possible to perform overlapped writes (accumulate)
- CTF internal implementation (all parts threaded):
    1. bin keys by processor and redistribute
    2. bin key by virtual processor and then sort them
    3. iterate over the dense tensor, reading or writing keys along the way
    4. return keys to originating location if its a sparse read

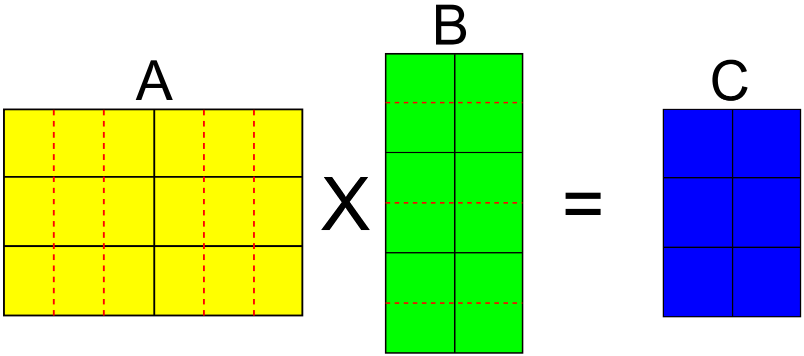
Blocked vs block-cyclic vs cyclic decompositions



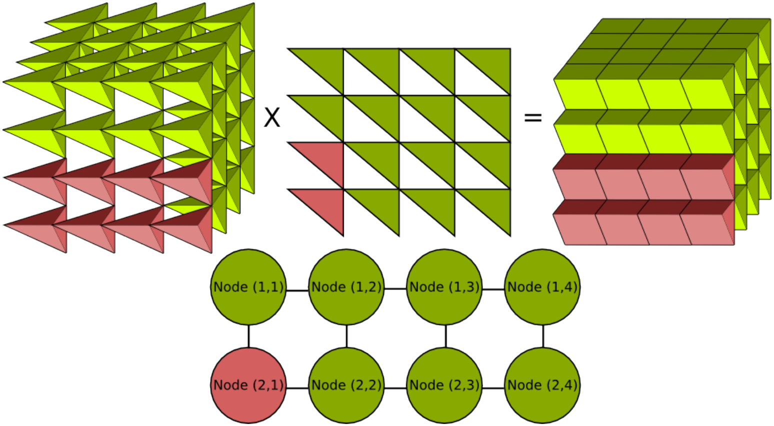
◯ Green denotes fill (unique values)   ◯ Red denotes padding / load imbalance

Virtualization

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



3D tensor mapping



The mapping process

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4. consider whether and what type of redistribution is necessary for the mapping
5. select the best mapping based on a performance model

Redistribution amongst different mappings

CTF must migrate tensors between different mappings between operations as well as for slice()

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- iterate over local piece of new tensor in global order and retrieve keys from bins
- kernel is threaded according to a global tensor partitioning

Transposition of a tensor on a virtual processor grid

In some cases, it is necessary to change the assignment of the tensor dimensions to virtual grid dimensions without changing the virtual processor grid itself

- in this case, CTF does not touch data within each block
- redistributed by block instead
- use MPI Isend and MPI Irecv for each sent and received block

Local transposition

Once the data is redistributed into the new mapping, we fold the tensors locally within blocks

- turns all non-symmetric block contractions into matrix multiplication
- 'preserved' symmetries may be folded into one dimension, but broken ones cannot
- maps dimensions which have symmetry that cannot be folded into matrix multiplication to have the longest stride

Distributed contraction

Once the tensors are distributed accordingly, the contraction algorithm begins

1. replicate small tensors over some processor grid dimensions (2.5D/3D matrix multiplication algorithms)
2. nested distributed SUMMA (2D matrix multiplication algorithm)
3. call to iterate over virtual blocks
4. call to iterate over broken symmetric dimensions
5. call to DGEMM

Rewind

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- CCSD(T) and CCSDT(Q) methods in development

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)

Grants:

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