Parallel Tensor Computations in Python or C++ Using Cyclops

Edgar Solomonik

Department of Computer Science
University of Illinois at Urbana-Champaign

PASC 2018

July 3, 2018

L P N A @CS@Illinois

A library for parallel tensor computations

Cyclops Tensor Framework (`github.com/cyclops-community/ctf`)

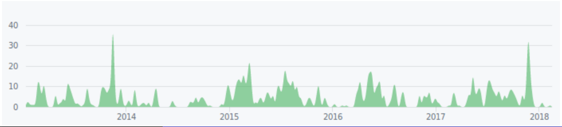
- distributed-memory symmetric/sparse/dense tensor objects

```
Matrix<int> A(n, n, AS|SP, World(MPI_COMM_WORLD));
Tensor<float> T(order, is_sparse, dims, syms, ring, world);
T.read(...); T.write(...); T.slice(...); T.permute(...);
```

- parallel contraction/summation of tensors

```
C["ij"]    = A["ik"]*B["kj"];      // matmul
C["ijl"]  += A["ikl"]*B["kjl"];    // batched matmul
Z["abij"] += V["ijab"];            // tensor transpose
T["wxyz"] += U["uw"]*T["uxyz"];    // TTM
T["abij"]  = T["abij"]*D["abij"]; // Hadamard product
S["ii"]    = v["i"]                // S = diag(v)
v["i"]    += S["ii"]               // v += diag(S)
M["ij"] += Function<>([](double x){ return 1/x; })(v["j"]);
```

- ∼2000 commits since 2011, open source since 2013



Electronic structure calculations with cyclops

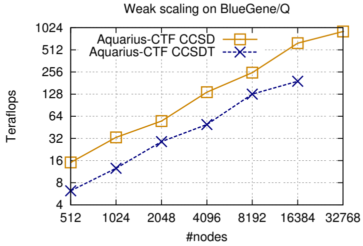
Extracted from Aquarius (lead by Devin Matthews)
https://github.com/devinamatthews/aquarius

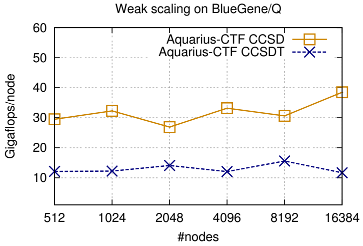
```
FMI["mi"]      += 0.5*WMNEF["mnef"]*T2["efin"];
WMNIJ["mnij"] += 0.5*WMNEF["mnef"]*T2["efij"];
FAE["ae"]      -= 0.5*WMNEF["mnef"]*T2["afmn"];
WAMEI["amei"] -= 0.5*WMNEF["mnef"]*T2["afin"];

Z2["abij"]  = WMNEF["ijab"];
Z2["abij"] += FAE["af"]*T2["fbij"];
Z2["abij"] -= FMI["ni"]*T2["abnj"];
Z2["abij"] += 0.5*WABEF["abef"]*T2["efij"];
Z2["abij"] += 0.5*WMNIJ["mnij"]*T2["abmn"];
Z2["abij"] -= WAMEI["amei"]*T2["ebmj"];
```

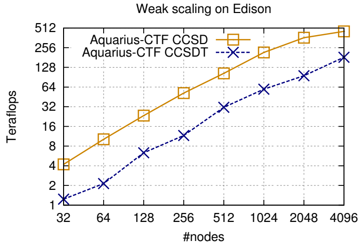
- CTF has been integrated with **QChem, VASP (CC4S), and PySCF**
- Is also being used for other applications, e.g. by IBM+LLNL collaboration to perform 49-qubit quantum circuit simulation

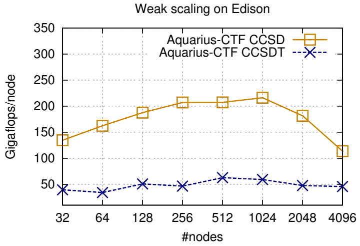
Electronic structure calculations with Cyclops

CCSD up to 55 (50) water molecules with cc-pVDZ
CCSDT up to 10 water molecules with cc-pVDZ









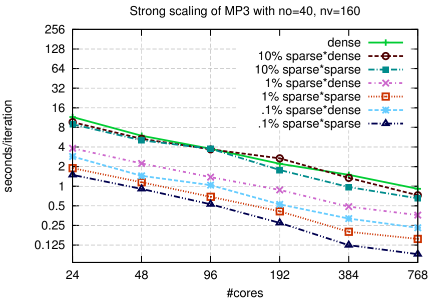
compares well to NWChem (up to 10x speed-ups for CCSDT)

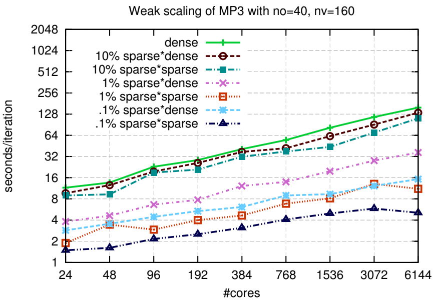
MP3 method

```
Tensor<> Ea, Ei, Fab, Fij, Vabij, Vijab, Vabcd, Vijkl, Vaibj;
... // compute above 1-e an 2-e integrals

Tensor<> T(4, Vabij.lens, *Vabij.wrld);
T["abij"] = Vabij["abij"];

divide_EaEi(Ea, Ei, T);

Tensor<> Z(4, Vabij.lens, *Vabij.wrld);
Z["abij"]  = Vijab["ijab"];
Z["abij"] += Fab["af"]*T["fbij"];
Z["abij"] -= Fij["ni"]*T["abnj"];
Z["abij"] += 0.5*Vabcd["abef"]*T["efij"];
Z["abij"] += 0.5*Vijkl["mnij"]*T["abmn"];
Z["abij"] += Vaibj["amei"]*T["ebmj"];

divide_EaEi(Ea, Ei, Z);

double MP3_energy = Z["abij"]*Vabij["abij"];
```

Sparse MP3 code

Strong and weak scaling of sparse MP3 code, with
(1) dense V and T (2) sparse V and dense T (3) sparse V and T





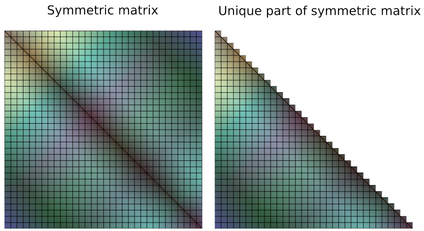
Custom tensor element types

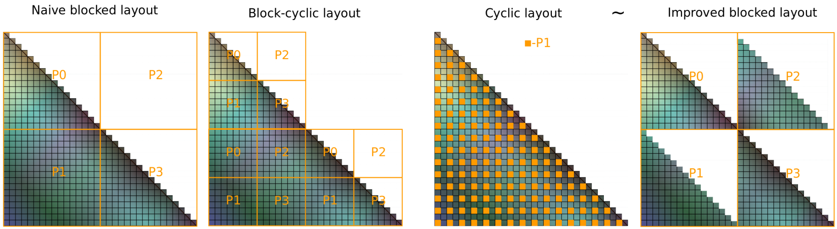
Cyclops permits arbitrary element types and custom functions

- CombBLAS/GraphBLAS-like functionality
- See examples for SSSP, APSP, betweenness centrality, MIS, MIS-2
- Functionality to handle serialization of pointers within user-defined types is under development
- Block-sparsity via sparse tensor (local) of dense tensors (parallel)

```
// Define Monoid tmon to perform matrix summation as addition
...

Matrix< Matrix<> > C(nblk, nblk, SP, self_world, tmon);

C["ij"] = Function< Matrix<> >(
            [](Matrix<> mA, Matrix<> mB){
              Matrix<> mC(mA.nrow, mB.ncol);
              mC["ij"] += mA["ik"]*mB["kj"];
              return mC;
            }
          )(A["ik"],B["kj"]);
```

Symmetry and sparsity by cyclicity





for sparse tensors, a cyclic layout provides a load-balanced distribution

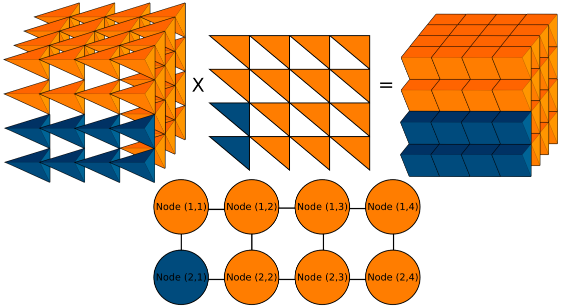
Parallel contraction in Cyclops

Cyclops uses nested parallel matrix multiplication variants

- 1D variants
  - perform a different *matrix-vector product* on each processor
  - perform a different *outer product* on each processor
- 2D variants
  - perform a different *inner product* on each processor
  - *scale a vector* on each processor then sum
- 3D variants
  - perform a different *scalar product* on each processor then sum
  - can be achieved by *nesting* 1D+1D+1D or 2D+1D or 1D+2D
- All variants are *blocked* in practice, naturally generalized to sparse matrix products

Tensor blocking/virtualization

Preserving symmetric-packed layout using cyclic distribution constrains possible tensor blockings



subdivision into more blocks than there are processors (virtualization)

Data mapping and redistribution

Transitions between contractions require redistribution and refolding

- 1D/2D/3D variants naturally map to 1D/2D/3D processor grids
- Initial tensor distribution is oblivious of contraction
  - by default each tensor distributed over all processors
  - user can specify any processor grid mapping
- Global redistribution done by one of three methods
  - reassign tensor blocks to processors (easy+fast)
  - reorder and reshuffle data to satisfy new blocking (fast)
  - treat tensors as sparse and sort globally by function of index
- Matricization/transposition is then done locally
  - dense tensor transpose done using HPTT (by Paul Springer)
  - sparse tensor converted to CSR sparse matrix format

Local summation and contraction

- For contractions, local summation and contraction is done via BLAS, including batched GEMM
- Threading is used via OpenMP and threaded BLAS
- GPU offloading is available but not yet fully robust
- For sparse matrices, *MKL provides fast sparse matrix routines*
- To support general (mixed-type, user-defined) elementwise functions, manual implementations are available
- User can specify blocked implementation of their function to improve performance

Performance modeling and intelligent mapping

- Performance models used to select best contraction algorithm
- Based on *linear cost model for each kernel*

$$T \approx \underbrace{\alpha S}_{\text{latency}} + \underbrace{\beta W}_{\text{comm. bandwidth}} + \underbrace{\nu Q}_{\text{mem. bandwidth}} + \underbrace{\gamma F}_{\text{flops}}$$

- Scaling of S, W, Q, F is a function of parameters of each kernel
- Coefficients for all kernels depend on compiler/architecture
- Linear regression with Tykhonov regularization used to select coefficients $\boldsymbol{x}^*$
- Model training done by benchmark suite that executes various end-functionality for growing problem sizes, collecting observations of parameters in rows of $\boldsymbol{A}$ and execution timing in $\boldsymbol{t}$

$$\boldsymbol{x}^* = \underset{\boldsymbol{x}}{\operatorname{argmin}}(||\boldsymbol{A}\boldsymbol{x} - \boldsymbol{t}||_2 + \lambda||\boldsymbol{x}||_2)$$

Cyclops with Python

- Using Cython, we have provided a Python interface for Cyclops
- Follows numpy.ndarray conventions, plus sparsity and MPI execution

```
Z["abij"]   += V["ijab"];                     // C++
Z.i("abij") << V.i("ijab")                    // Python
W["mnij"]   += 0.5*W["mnef"]*T["efij"];       // C++
W.i("mnij") << 0.5*W.i("mnef")*T.i("efij") // Python
einsum("mnef,efij->mnij",W,T)  // numpy-style Python
```

- Python interface is under active development, but is functional and available (DEMO)

Future directions and acknowledgements

Future/ongoing directions in Cyclops development

- General abstractions for tensor decompositions
- Concurrent scheduling of multiple contractions
- Fourier transforms along tensor modes
- Improvements to functionality and performance for linear algebra

Acknowledgements

- Devin Matthews (UT Austin), Jeff Hammond (Intel Corp.), James Demmel (UC Berkeley), Torsten Hoefler (ETH Zurich), Zecheng Zhang, Eric Song, Eduardo Yap, Linjian Ma (UIUC)
- Computational resources at NERSC, CSCS, ALCF, NCSA, TACC

Backup slides