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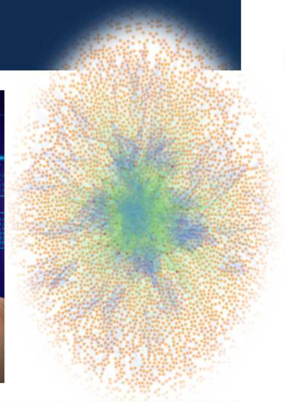

TuckerMPI: Optimised library for distributed data compression

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ECP Annual Meeting: Lossy Data Compression Breakout

Jan 16th, 2019, Houston

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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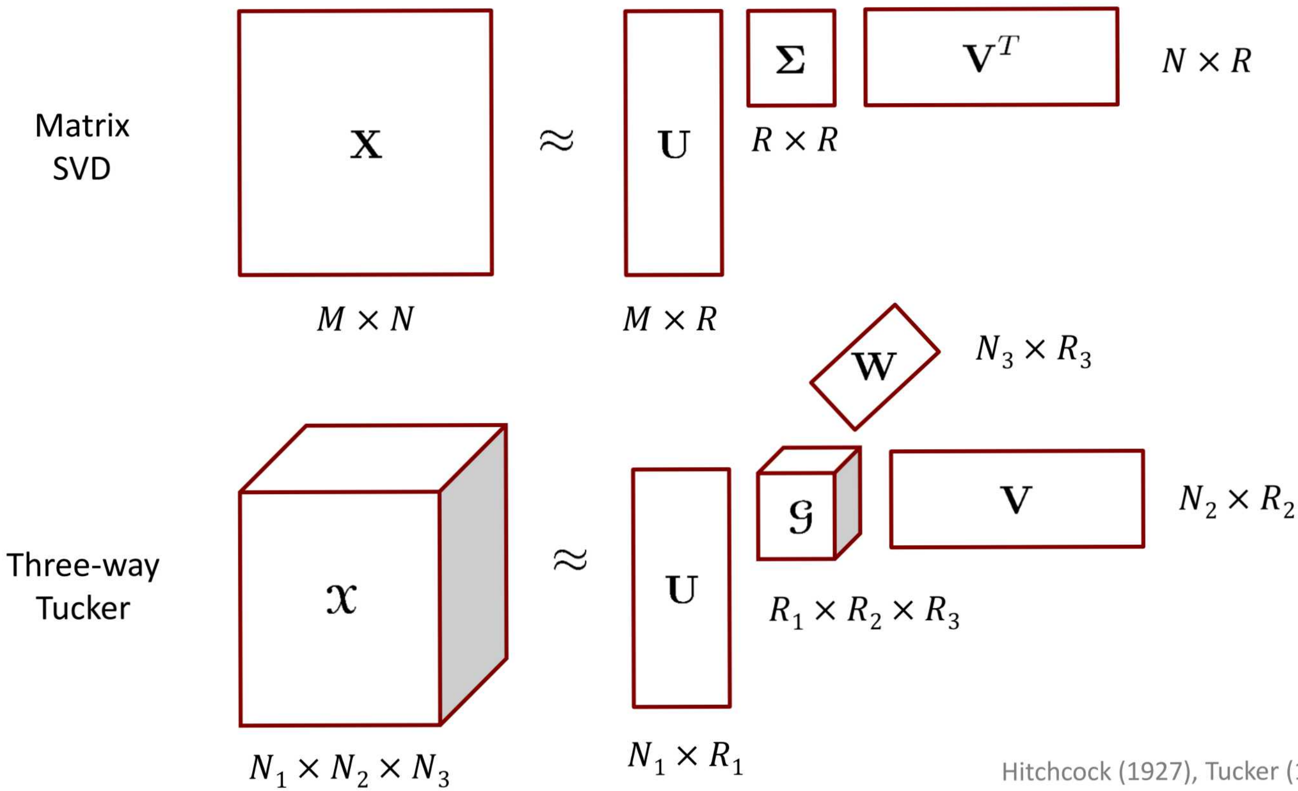
High level Objective

- Enable orders-of-magnitude (lossy) compression:
  - distributed data, *in-situ.*
  - scalable, efficient.
- Allow exploring the accuracy-compression-cost tradeoff.
- What are downstream implications (archival, analysis, sharing)?
- How do workflows change:
  - in-situ vs in-tandem vs offline.
  - Can we reconstruct partially?
  - Characterizing risks and mitigation factors.
- Augment the *in-situ* capability for SNL-ATDM apps.

Tucker Compression: Overview

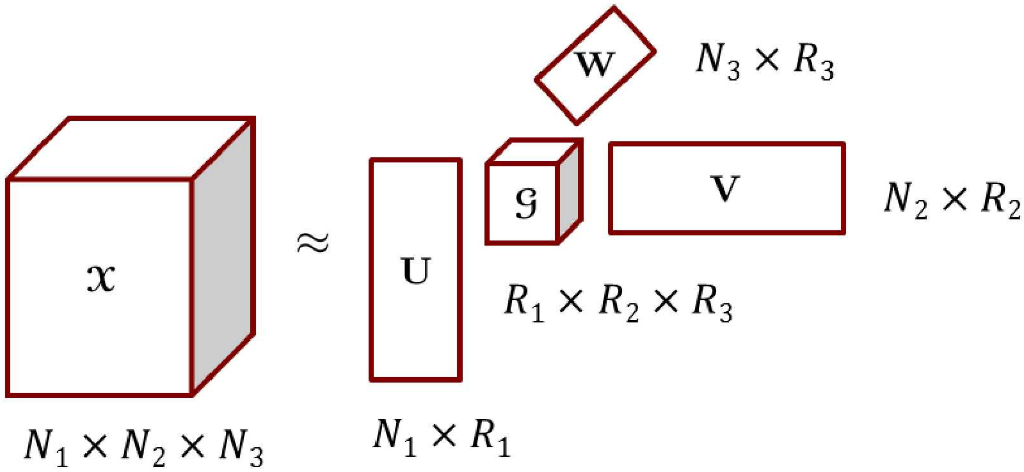
Extend Matrix SVD to multi-way arrays (tensors)



$$\text{CR} \approx \frac{N_1 \times N_2 \times N_3}{R_1 \times R_2 \times R_3}$$

Hitchcock (1927), Tucker (1966)

Tucker Compression - Overview



- For specified relative error, choose projection ranks R_1, R_2, R_3 such that:

$$\|\mathcal{X} - (\mathcal{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{W})\| \leq \epsilon \|\mathcal{X}\|$$

- Find orthogonal matrices **U**, **V**, **W** that reduce the tensor size but retain its "mass".

$$\mathcal{G} = \mathcal{X} \times_1 \mathbf{U}' \times_2 \mathbf{V}' \times_3 \mathbf{W}' \quad \Longrightarrow \quad \|\mathcal{X}\|^2 - \|\mathcal{G}\|^2 \leq \epsilon^2 \|\mathcal{X}\|^2$$

- User can specify either ϵ or $R_1/R_2/R_3$.

Algorithm: ST-HOSVD

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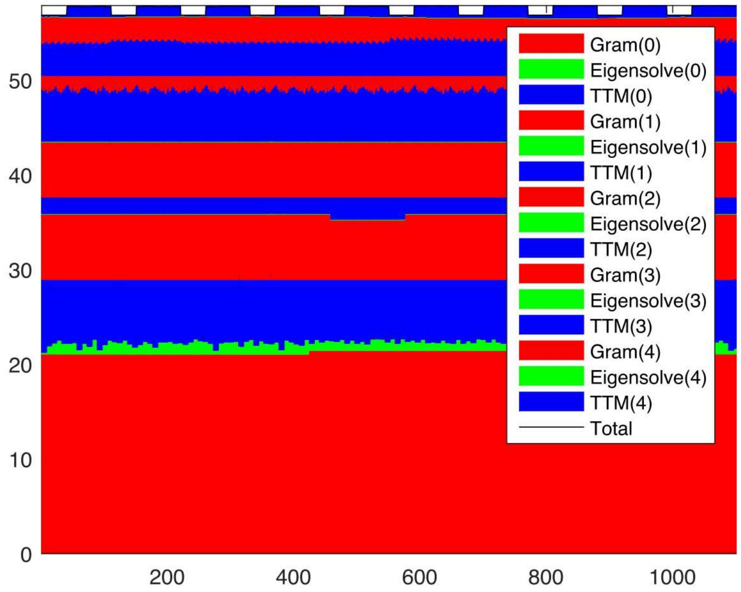
1. Choose $\mathbf{U}$ with projection rank R_1 such that: $\|\mathbf{X}_{(1)}\|^2 - \|\mathbf{U}'\mathbf{X}_{(1)}\|^2 \leq \epsilon^2\|\mathcal{X}\|^2/3$
    a) Compute gram matrix: $\mathbf{X}_{(1)}\mathbf{X}_{(1)}'$
    b) Use eigendecomposition of N_1 x N_1 matrix to choose R_1
    c) Set $\mathbf{U}$ = R_1 leading eigenvectors of gram matrix
2. Shrink to size R_1 x N_2 x N_3: $\mathcal{Y} = \mathcal{X} \times_1 \mathbf{U}'$
3. Choose $\mathbf{V}$ with projection rank R_2 such that: $\|\mathbf{Y}_{(2)}\|^2 - \|\mathbf{V}'\mathbf{Y}_{(2)}\|^2 \leq \epsilon^2\|\mathcal{X}\|^2/3$
    a) Compute gram matrix: $\mathbf{Y}_{(2)}\mathbf{Y}_{(2)}'$
    b) Use eigendecomposition of N_2 x N_2 matrix to choose R_2
    c) Set $\mathbf{V}$ = R_2 leading eigenvectors of gram matrix
4. Shrink to size R_1 x R_2 x N_3: $\mathcal{Z} = \mathcal{Y} \times_2 \mathbf{V}'$
5. Choose $\mathbf{W}$ with projection rank R_3 such that: $\|\mathbf{Z}_{(3)}\|^2 - \|\mathbf{W}'\mathbf{Z}_{(3)}\|^2 \leq \epsilon^2\|\mathcal{X}\|^2/3$
    a) Compute gram matrix: $\mathbf{Z}_{(3)}\mathbf{Z}_{(3)}'$
    b) Use eigendecomposition of N_3 x N_3 matrix to choose R_3
    c) Set $\mathbf{W}$ = R_3 leading eigenvectors of gram matrix
6. Shrink to size R_1 x R_2 x R_3: $\mathcal{G} = \mathcal{Z} \times_3 \mathbf{W}'$

Vannieuwenhoven, Vandebril, Meerbergen (SISC 2012)

Scalable Parallel implementation

- Three main kernels (Gram, Evecs, TTM) have been parallelized.
- MPI implementation of Tucker available (open):
  - `git@gitlab.com:tensors/TuckerMPI.git`



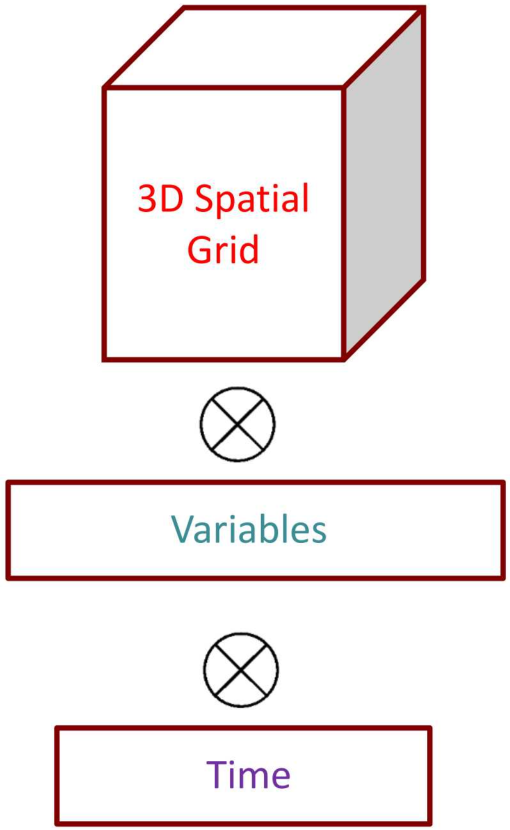
- 4.4TB -> 10GB (410X).
- Total of 55s; 1100 cores.
- Bulk of time is in first mode (GRAM computation).
- Fast BLAS for Eigensolve.
- Time for I/O is order of magnitude greater (~450s)

[1] W. Austin, G. Ballard and T.G. Kolda, IPDPS'16 (arXiv:1510.06689).
[2] Tammy Kolda, SC16 talk.

TuckerMPI: Usage

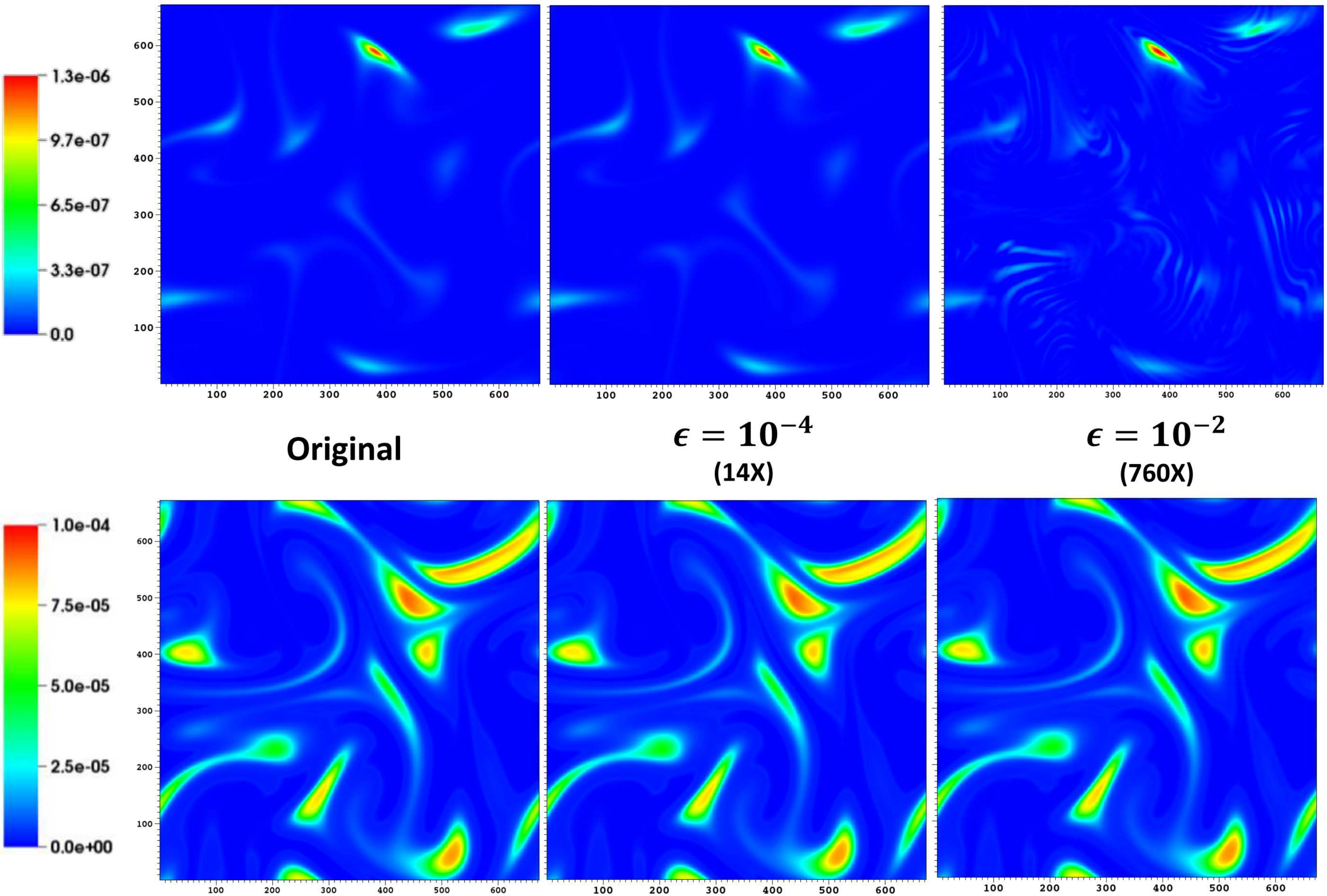
- Primary use case: structured mesh distributed data sets
  - Recently extended to handle multi-block capability.
  - Not currently usable for unstructured meshes, AMR meshes, particle data.
- Clean, portable C++ library with minimal dependencies (MPI, BLAS/LAPACK).
- Currently set up to work with parallel MPI-IO (read/write).
- Can be used offline, or *in-situ* (later slides).
- User need only specify:
  - Global dimensions of input data (tensor)
  - Desired global error threshold (ϵ), OR,
  - Desired ranks of truncation along each mode ($R_1/R_2/R_3$)

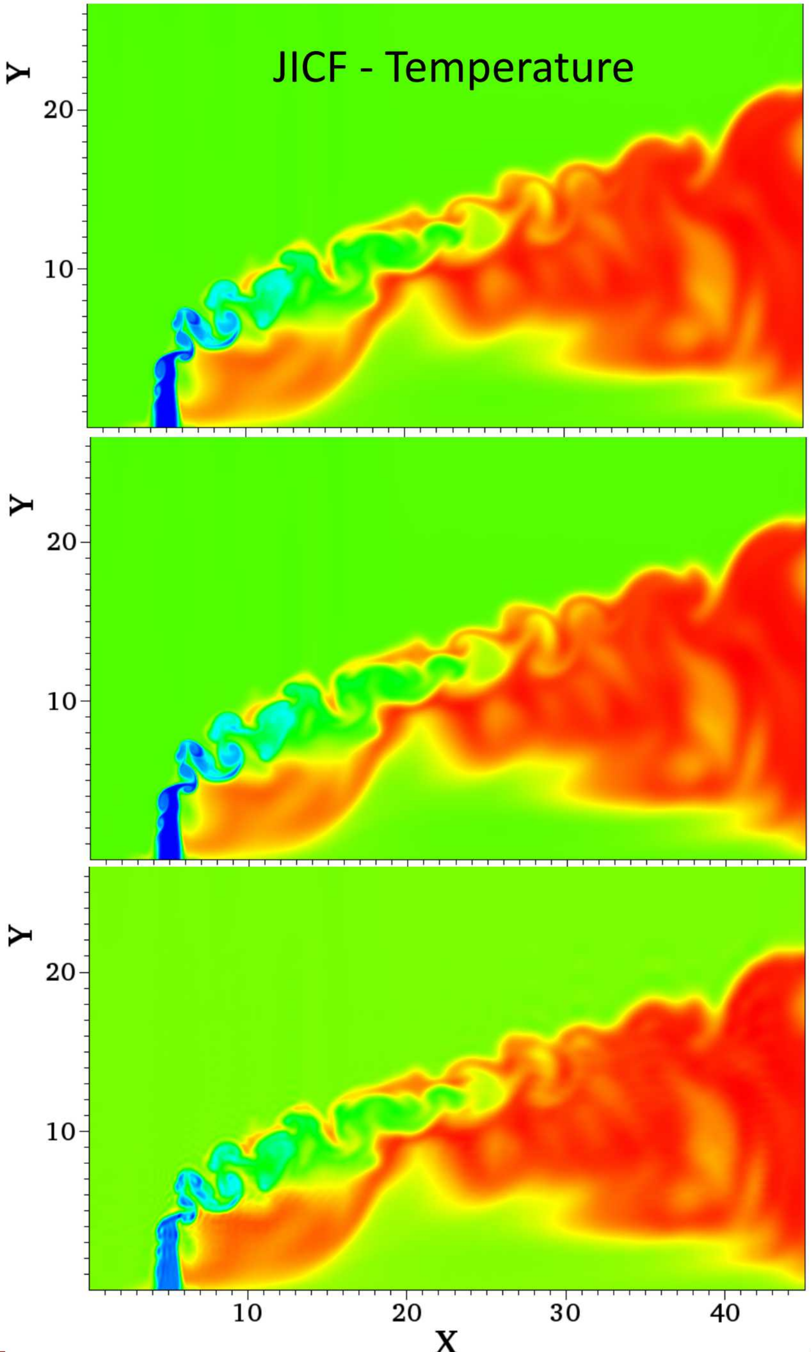
Sample Results: S3D datasets



	Original	$\epsilon = 10^{-4}$	$\epsilon = 10^{-2}$
HCCI	672 x 672 x 32 x 626	330 x 310 x 31 x 199 **(14 X)**	111 x 105 x 22 x 46 **(760 X)**
SP	500 x 500 x 500 x 11 x 400	95 x 129 x 125 x 7 x 125 **(410 X)**	30 x 38 x 35 x 6 x 11 **(20000 X)**
JICF	1500 x 2080 x 1500 x 18 x 10	424 x 387 x 261 x 18 x 10 **(110 X)**	90 x 61 x 48 x 13 x 6 **(40000 X)**

HCCI – OH concentration

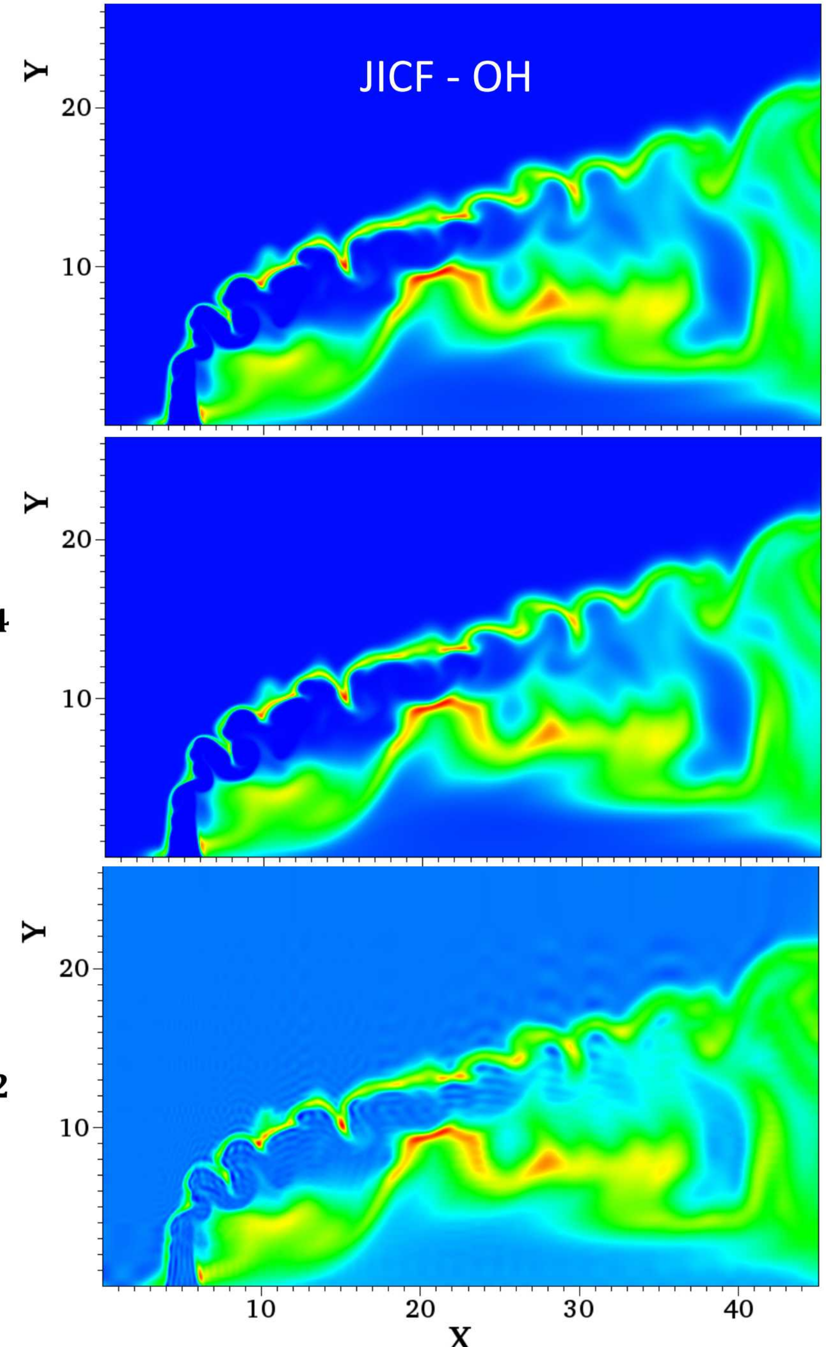




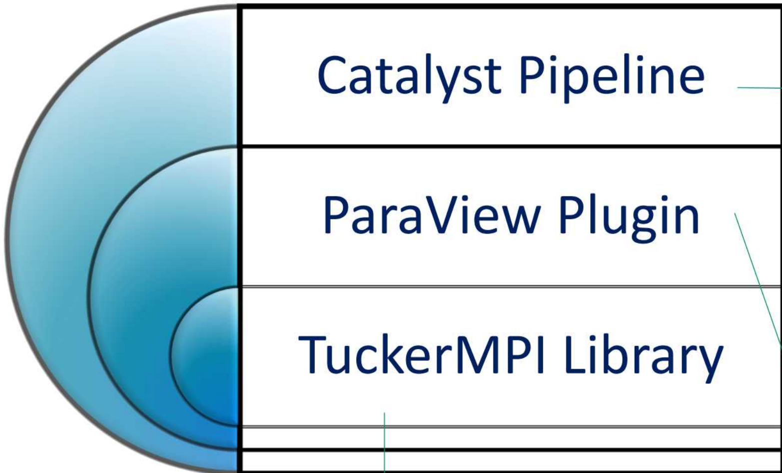
Original

$\epsilon = 10^{-4}$
(110X)

$\epsilon = 10^{-2}$
(40000X)



In-Situ capability with ParaView/Catalyst




```
def DoCoProcessing(datadescription):

    global coprocessor
    coprocessor.UpdateProducers(datadescription)

    LoadPlugin(‘/path/to/plugin/libSMTuckerMPICompression.so')

    vtk_test = coprocessor.CreateProducer(datadescription, 'input')

    ts = str(datadescription.GetTimeStep())
    SaveData('grid_compressed_' + ts + '.tucker', proxy=vtk_test)
```

- Dynamic library interface to TuckerMPI
- API for Tensor data structures, MPI domain decomposition maps/objects
- API for key kernels: tensor matricization, ST-HOSVD, Gram matrix computation.

- Plugin can be loaded into the ParaView GUI or Catalyst in-situ
- Plugin maps between ParaView and TuckerMPI data structures in parallel, MPI communicator re-mapping, and supports input types of vtkMultiBlockDataSet, vtkImageData, and vtkStructuredGrid
- Writer compresses vtkMultiBlockDataSet input by iterating over all blocks in parallel.

Ongoing Work

- In-situ reader (i.e. reconstruction) ParaView plugin.
- User-specified partial reconstruction.
- In-situ analysis on compressed data.
- Compress time snapshots in streaming manner.
- Compression of unstructured mesh data:
  - Key Idea: Unstructured mesh data are realizations of multi-D function
  - Compress by seeking low rank approximations of multi-D functions.

Thank you!