Parallel Algorithms for CP and Tucker Decompositions

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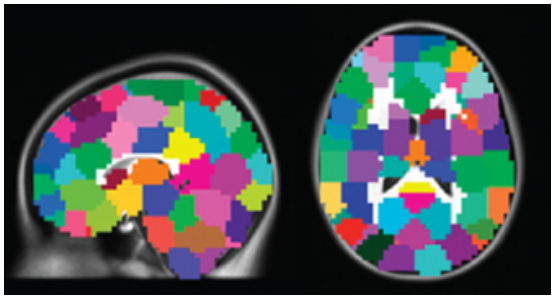
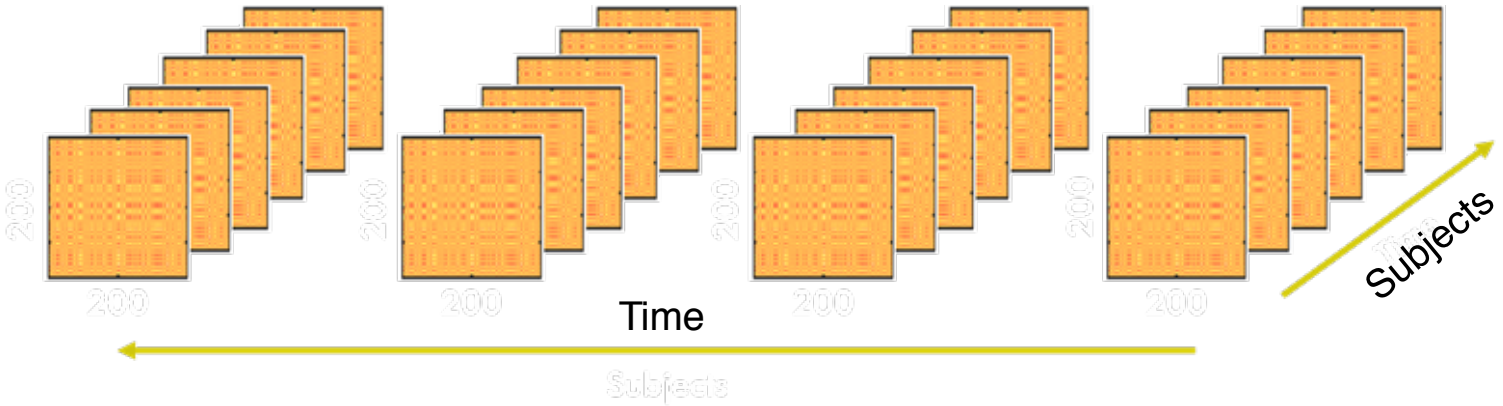
WAKE FOREST
UNIVERSITY

Motivation: multidimensional data analysis requires scalable algorithms



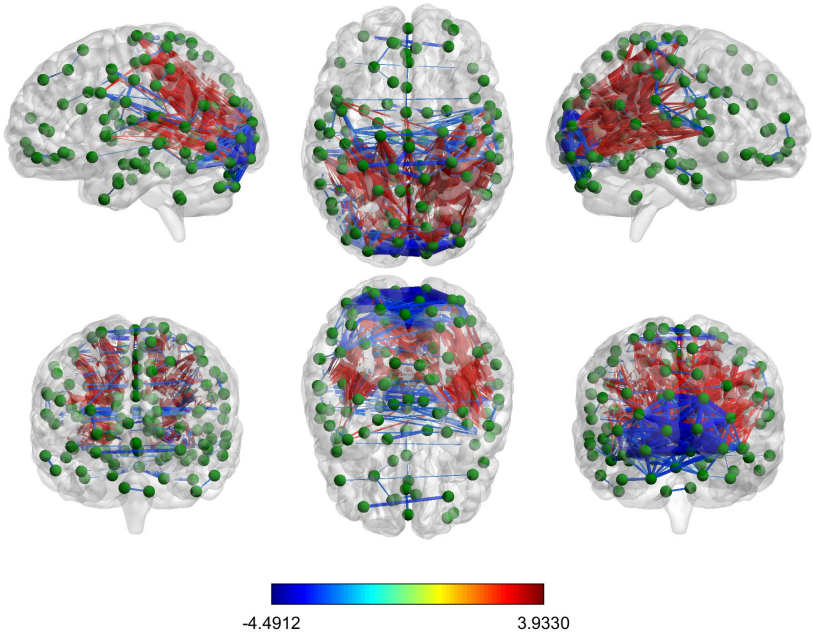
Dynamic functional connectivity fMRI data

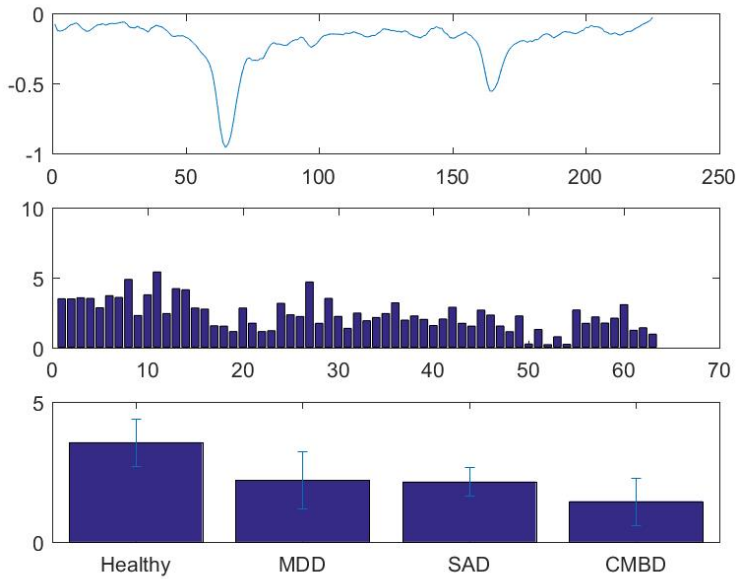
- measures correlation between regions of the brain over time
- experiments can include cognitive task
- study multiple subjects across groups



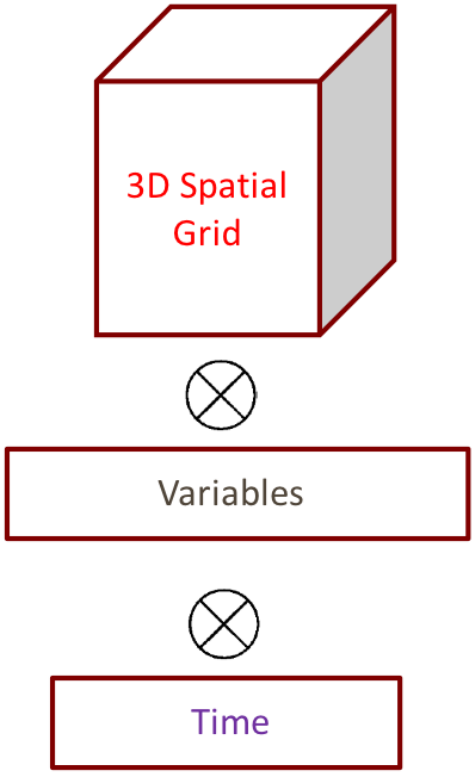
200 regions $\times$ 200 regions $\times$ 225 time steps $\times$ 59 subjects
4 GB of data

CP decomposition discovers patterns of synchronization across brain networks





Motivation: Numerical simulations producing more data than we can handle

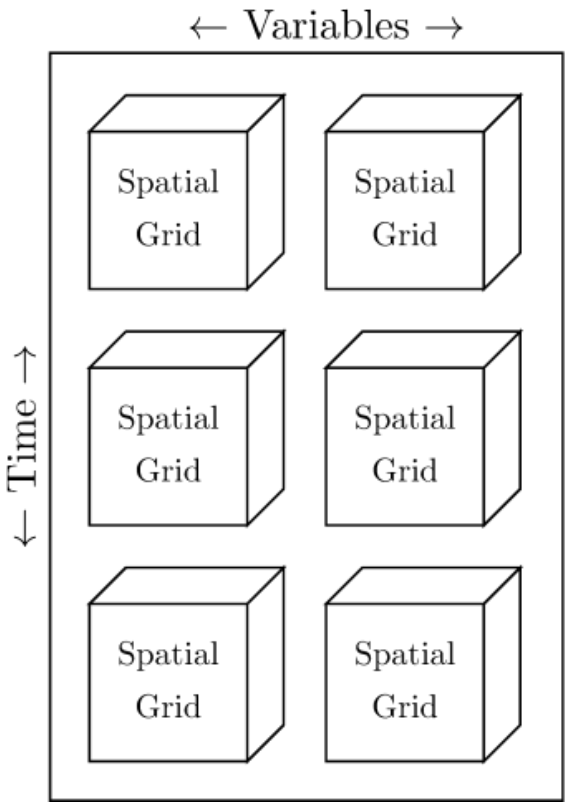


$512 \times 512 \times 512$ 3D grid,
128 time steps, 64 variables:
8 terabytes of data
(double precision)

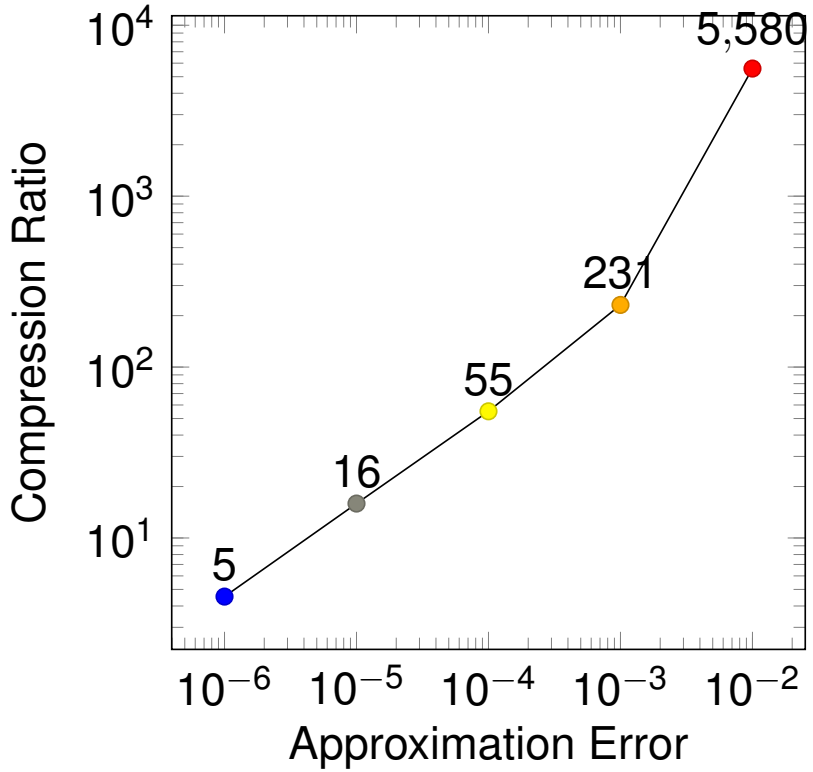
S3D MPI-based Combustion Code

- direct numerical simulation of engine combustion
- run on supercomputers
- single experiment produces terabytes of data
- storage resolution much less than computed resolution
- difficult to analyze or even transfer data

Tucker decomposition yields huge compression for combustion simulation data



Natural five-way multiway structure of scientific data



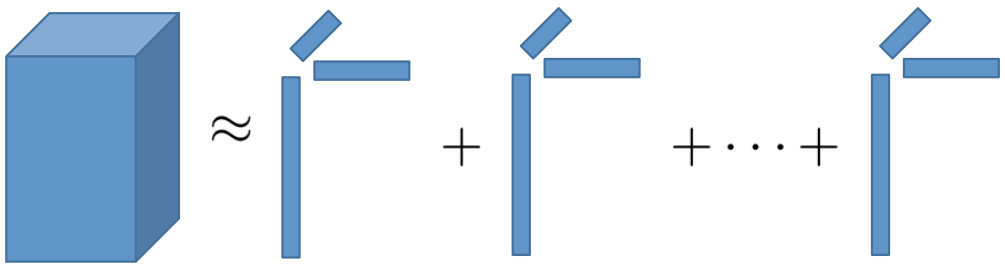
Compression rates as fidelity varies for 550GB simulation dataset

Parallel Computation of CP Decompositions with Nonnegativity Constraints

joint work with Srinivas Eswar[1], Koby Hayashi[1], Ramakrishnan Kannan[2], and Haesun Park[1]

[1] Georgia Tech
[2] Oak Ridge National Lab

CP Notation



$$\mathcal{X} \approx \mathbf{u}_1 \circ \mathbf{v}_1 \circ \mathbf{w}_1 + \cdots + \mathbf{u}_R \circ \mathbf{v}_R \circ \mathbf{w}_R, \qquad \mathcal{X} \in \mathbb{R}^{I \times J \times K}$$

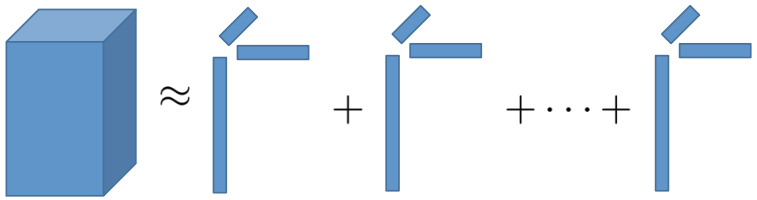
$$\mathcal{X} \approx [\![\mathbf{U}, \mathbf{V}, \mathbf{W}]\!], \qquad \mathbf{U} \in \mathbb{R}^{I \times R}, \mathbf{V} \in \mathbb{R}^{J \times R}, \mathbf{W} \in \mathbb{R}^{K \times R}$$

are *factor matrices*

$$x_{ijk} \approx \sum_{r=1}^{R} u_{ir} v_{jr} w_{kr}, \qquad 1 \leq i \leq I, 1 \leq j \leq J, 1 \leq k \leq K$$

Notation convention: scalar dimension N, index n with $1 \leq n \leq N$

NNCP Optimization Problem



For fixed rank R, we want to solve

$$\underset{\mathbf{U},\mathbf{V},\mathbf{W}\geq 0}{\arg\min} \left\| \mathcal{X} - \sum_{r=1}^{R} \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r \right\|$$

Alternating Optimization (AO)

Fixing all but one factor matrix, we have a linear nonnegative least squares (NNLS) problem:

$$\arg\min_{\mathbf{V}\geq 0} \left\| \mathcal{X} - \sum_{r=1}^{R} \hat{\mathbf{u}}_r \circ \mathbf{v}_r \circ \hat{\mathbf{w}}_r \right\|$$

or equivalently

$$\arg\min_{\mathbf{V}\geq 0} \left\| \mathbf{X}_{(2)} - \mathbf{V}(\hat{\mathbf{W}} \odot \hat{\mathbf{U}})^{\mathsf{T}} \right\|_F$$

$\odot$ is the *Khatri-Rao* product, a column-wise Kronecker product

AO works by alternating over factor matrices, updating one at a time by solving the corresponding linear NNLS problem

Nonnegative (Linear) Least Squares

Generic problem:

$$\arg\min_{\mathbf{Y} \geq 0} \|\mathbf{AY} - \mathbf{B}\|_F$$

Many possible algorithms:

- Multiplicative Updates [LS99]
- Hierarchical Alternating Least Squares [CZPA09]
- Block Principal Pivoting [KP11]
- Alternating Direction Method of Multipliers [LS15]
- Nesterov-type Algorithm [LKL+17]

Nonnegative (Linear) Least Squares

Generic problem:

$$\arg\min_{\mathbf{Y}\geq 0} \|\mathbf{AY} - \mathbf{B}\|_F$$

Our problem:

$$\arg\min_{\mathbf{V}\geq 0} \left\|\mathbf{X}_{(2)} - \mathbf{V}(\hat{\mathbf{W}} \odot \hat{\mathbf{U}})^{\mathsf{T}}\right\|_F$$

All algorithms compute $\mathbf{A}^T\mathbf{B}$ and $\mathbf{A}^T\mathbf{A}$, which for us are

$$\mathbf{A}^T\mathbf{B} \rightarrow \mathbf{X}_{(2)}(\hat{\mathbf{W}} \odot \hat{\mathbf{U}}) \quad \text{and} \quad \mathbf{A}^T\mathbf{A} \rightarrow (\hat{\mathbf{W}} \odot \hat{\mathbf{U}})^T(\hat{\mathbf{W}} \odot \hat{\mathbf{U}})$$

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- $\mathbf{X}_{(2)}(\hat{\mathbf{W}} \odot \hat{\mathbf{U}})$ is called Matricized-Tensor Times Khatri-Rao Product (MTTKRP) and is expensive to compute
- $(\hat{\mathbf{W}} \odot \hat{\mathbf{U}})^T(\hat{\mathbf{W}} \odot \hat{\mathbf{U}})$ can be computed relatively cheaply as $\hat{\mathbf{W}}^T\hat{\mathbf{W}} * \hat{\mathbf{U}}^T\hat{\mathbf{U}}$, where $*$ is elementwise product

Parallelizing MTTKRP

Our goal is to perform MTTKRP in parallel as fast as possible

- How do we distribute the tensor across processors?
- How do we distribute the matrices across processors?
- How do we divide up the computation?
- How much interprocessor communication will that require?

Parallel Communication Lower Bound

Theorem ([BKR18])

Any parallel MTTKRP algorithm involving a tensor with $I_k = I^{1/N}$ for all k and that evenly distributes one copy of the input and output performs at least

$$\Omega\left(\left(\frac{NIR}{P}\right)^{\frac{N}{2N-1}} + NR\left(\frac{I}{P}\right)^{1/N}\right)$$

sends and receives. (Second term will typically dominate.)

- N is the number of modes
- I is the number of tensor entries
- I_k is the dimension of the kth mode
- R is the rank of the CP model
- P is the number of processors

Parallelization Approach

1. Logically organize processors into N-D grid (match tensor)

$$P_1 \times P_2 \times \cdots \times P_N$$

2. Each processor is assigned a (cubical) subtensor of size

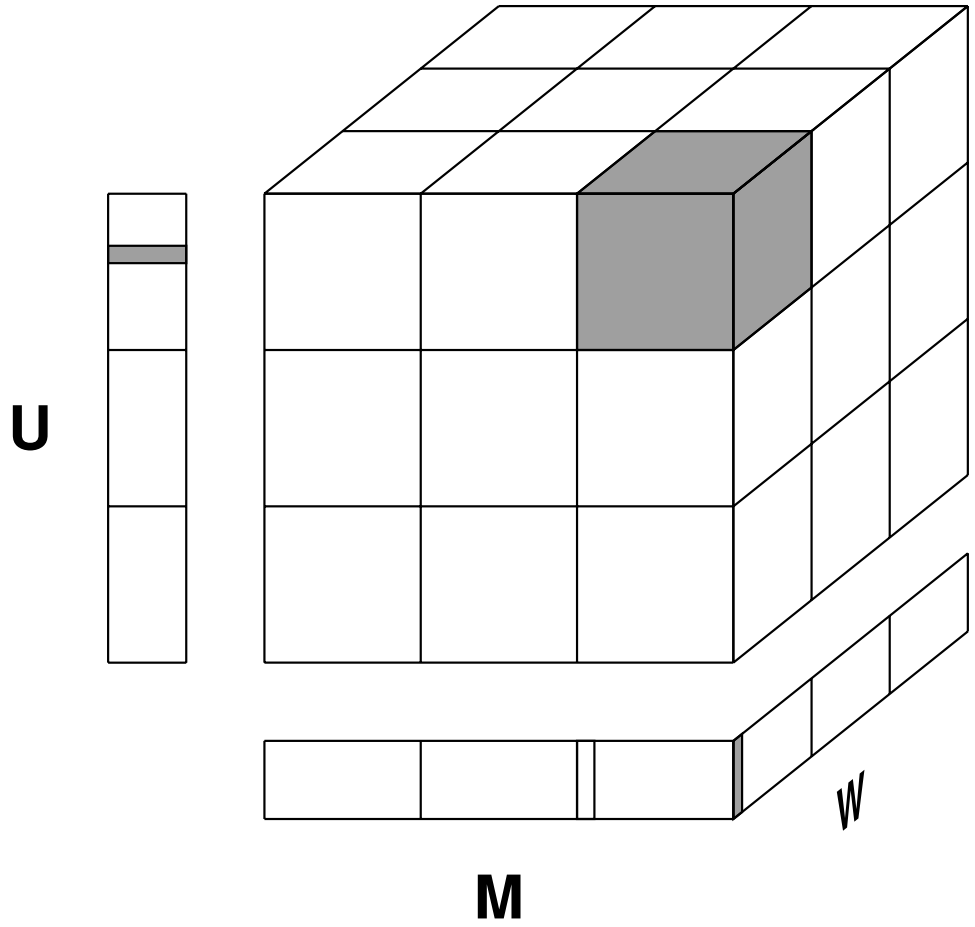
$$\frac{I_1}{P_1} \times \frac{I_2}{P_2} \times \cdots \times \frac{I_N}{P_N}$$

3. Each processor is assigned a subset of rows of each factor matrix, with dimensions

$$\frac{I_1}{P} \times R, \quad \frac{I_2}{P} \times R, \quad \cdots, \quad \frac{I_N}{P} \times R$$

4. Distribute computation based on where tensor data lives, communicating only the factor matrices as needed

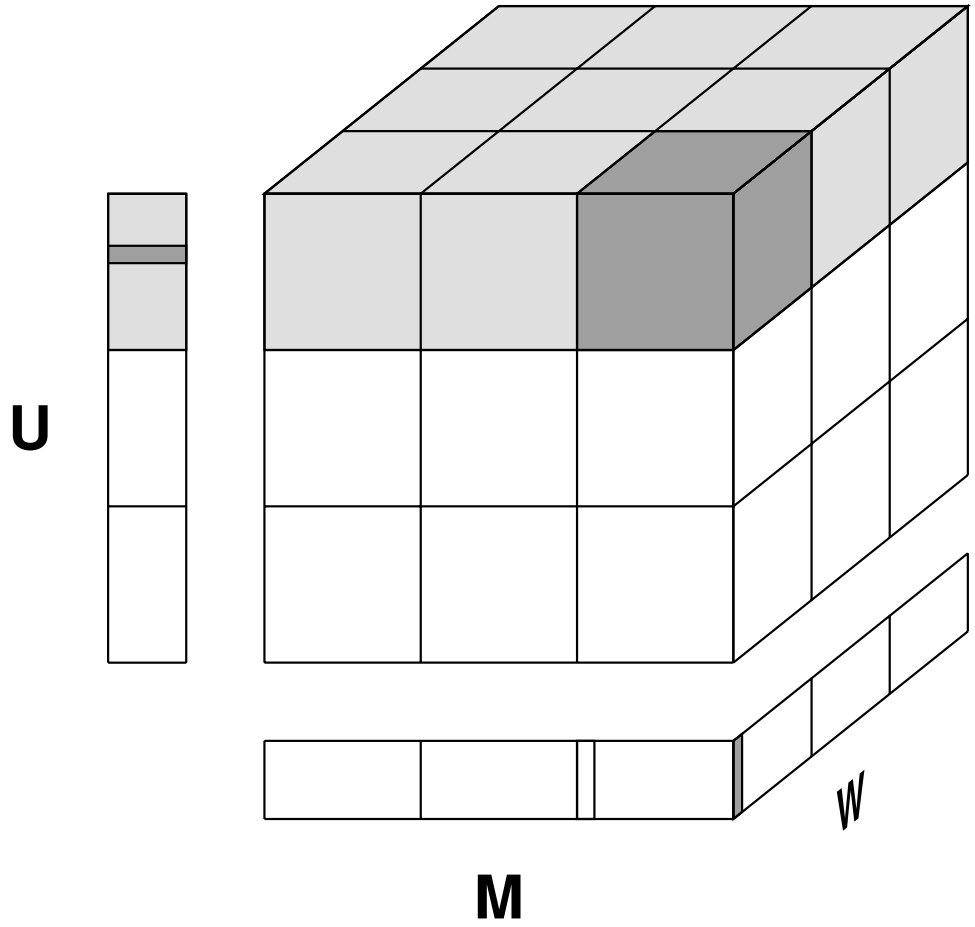
Communication-Optimal Parallel Algorithm (3D)



Each processor

1. Starts with one subtensor and subset of rows of each input factor matrix

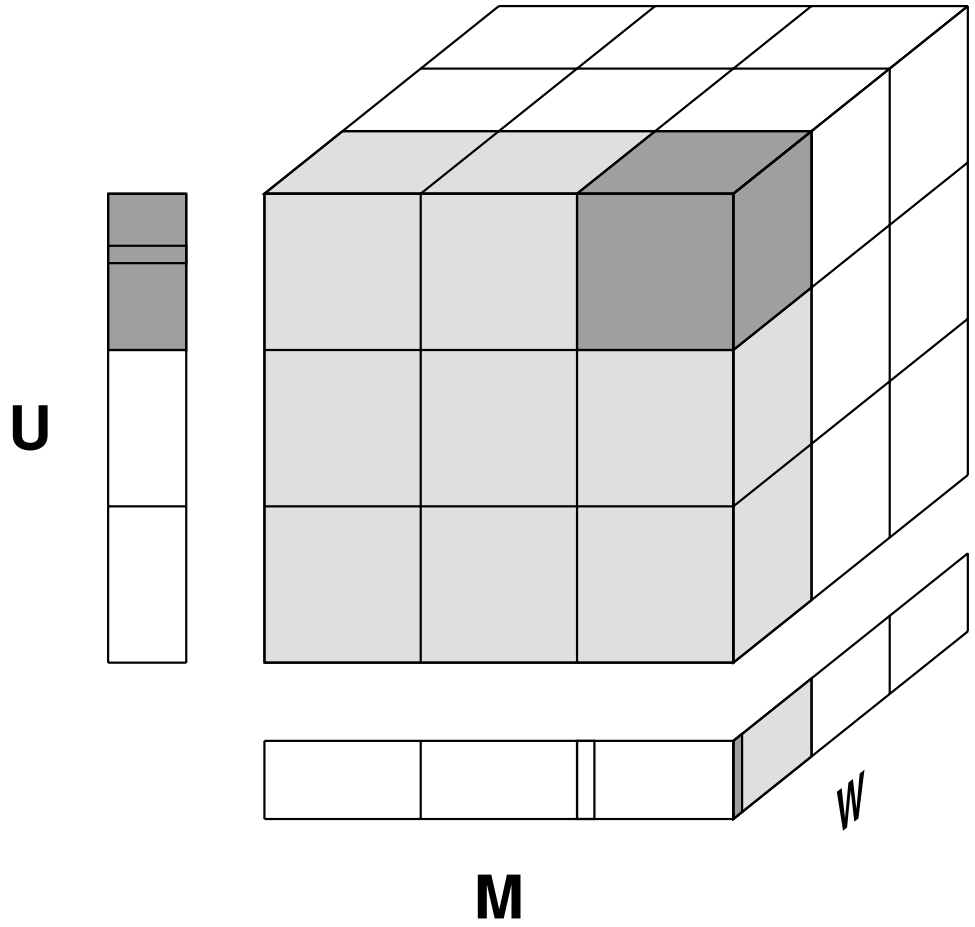
Communication-Optimal Parallel Algorithm (3D)



Each processor

1. Starts with one subtensor and subset of rows of each input factor matrix
2. All-Gathers all the rows needed from **U**

Communication-Optimal Parallel Algorithm (3D)



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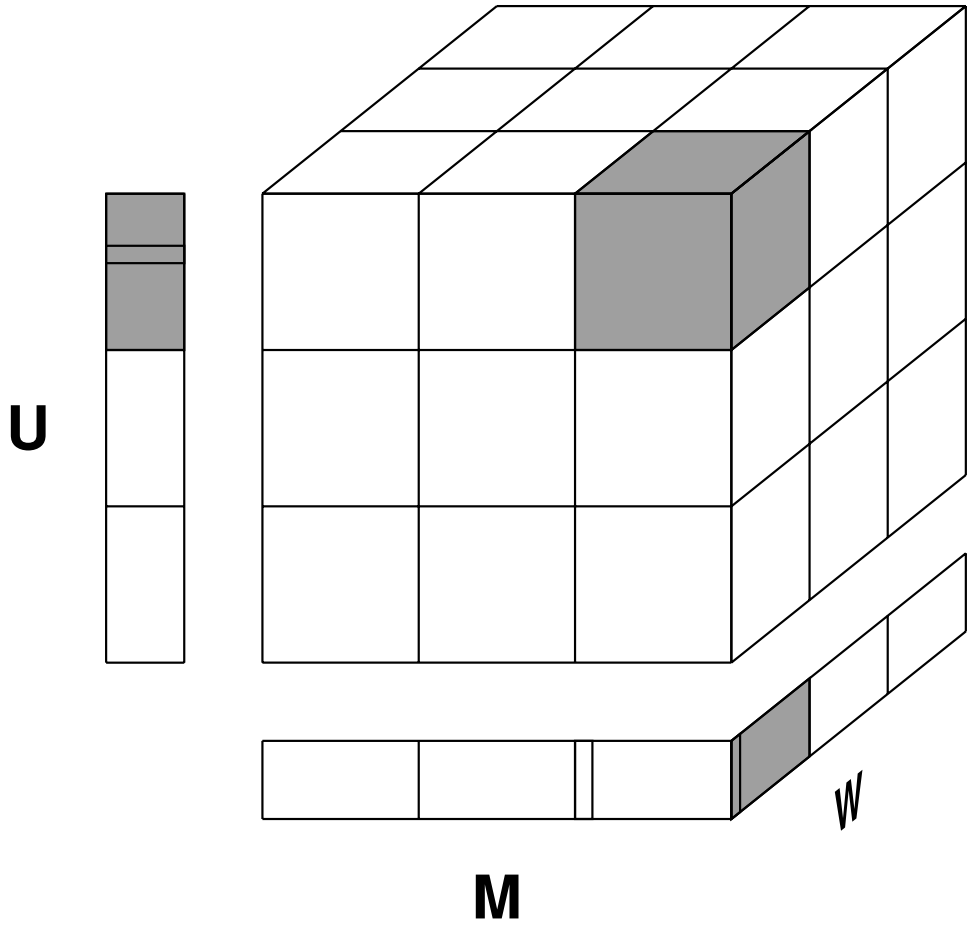

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1. Starts with one subtensor and subset of rows of each input factor matrix
2. All-Gathers all the rows needed from **U**
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4. Computes its contribution to rows of **M** (local MTTKRP)

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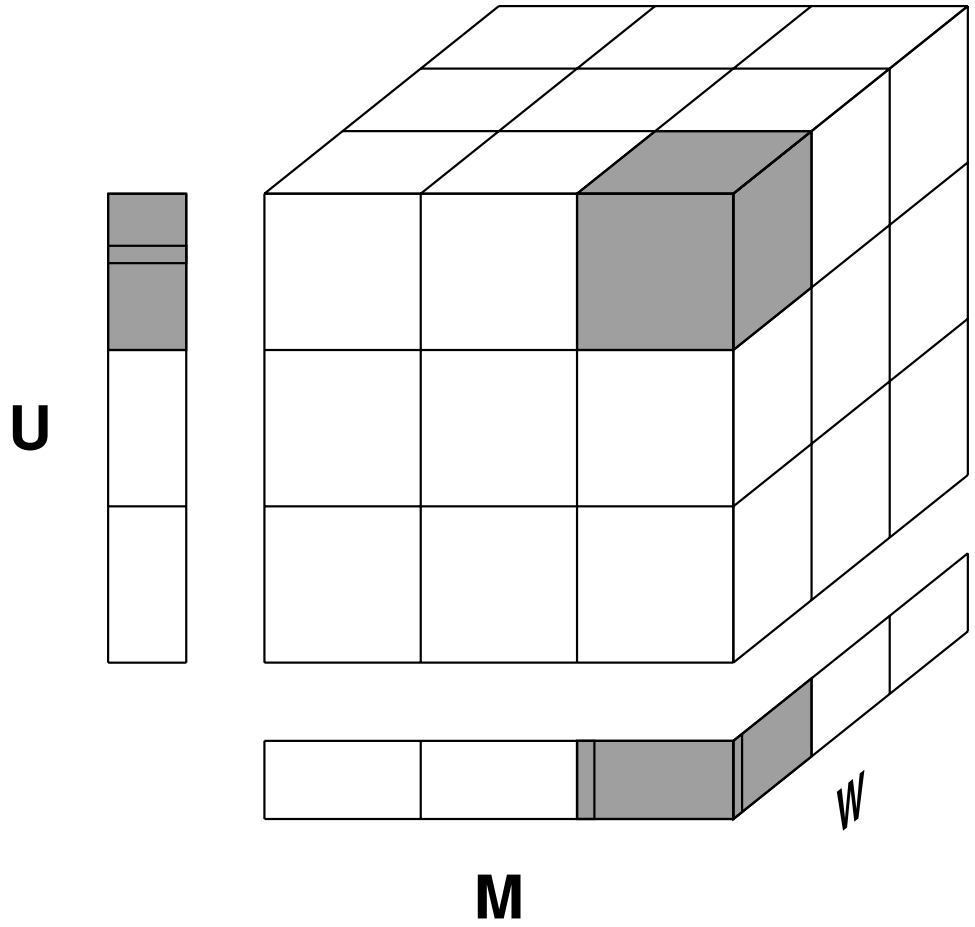

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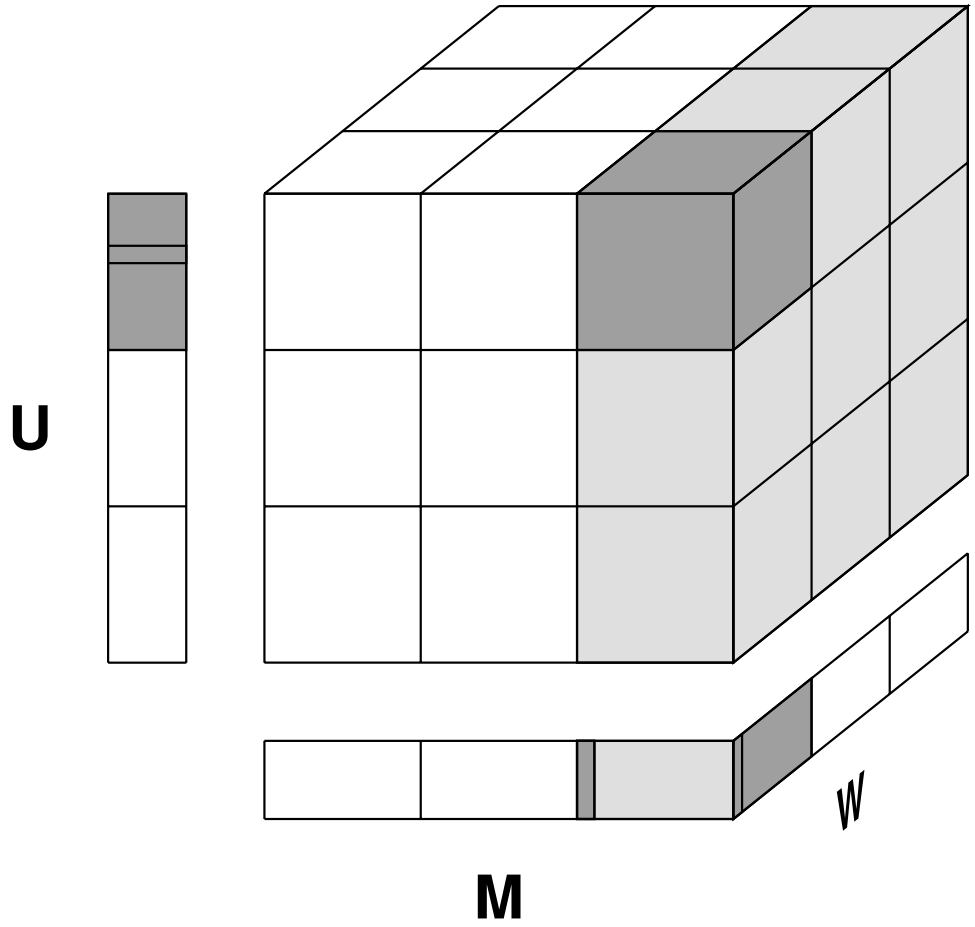

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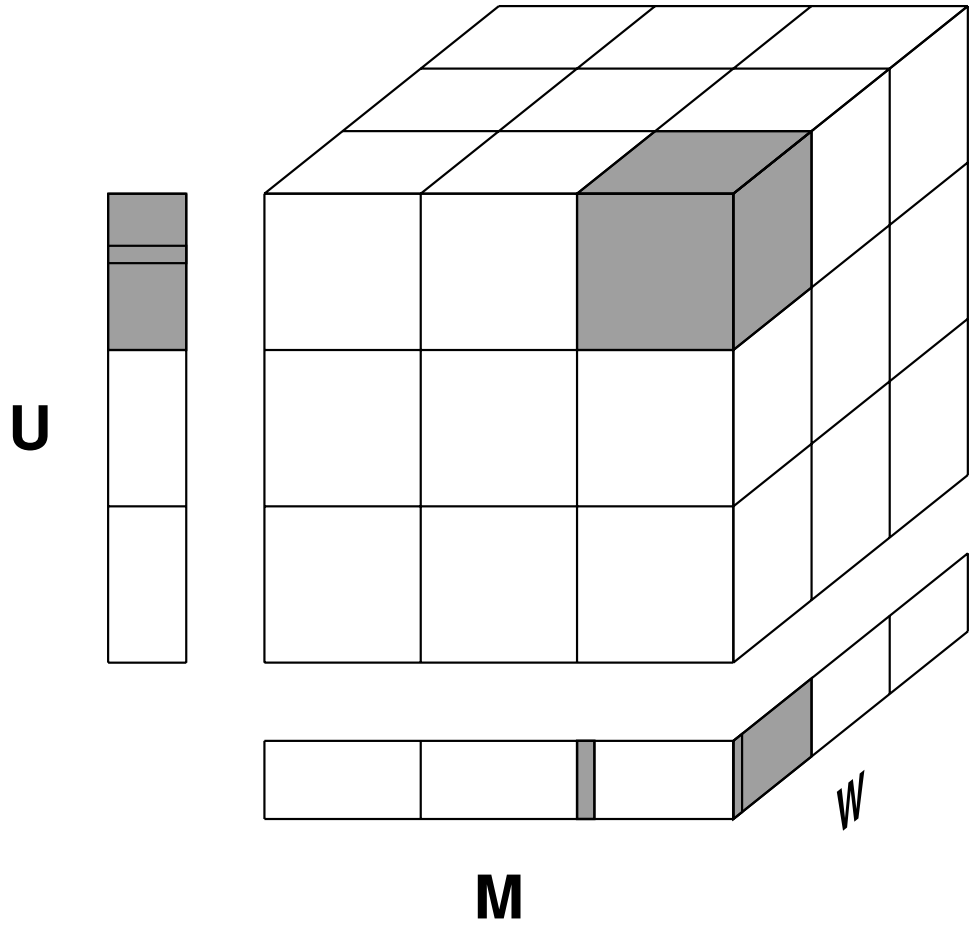
5. Reduce-Scatters to compute and distribute **M** evenly

Communication-Optimal Parallel Algorithm (3D)



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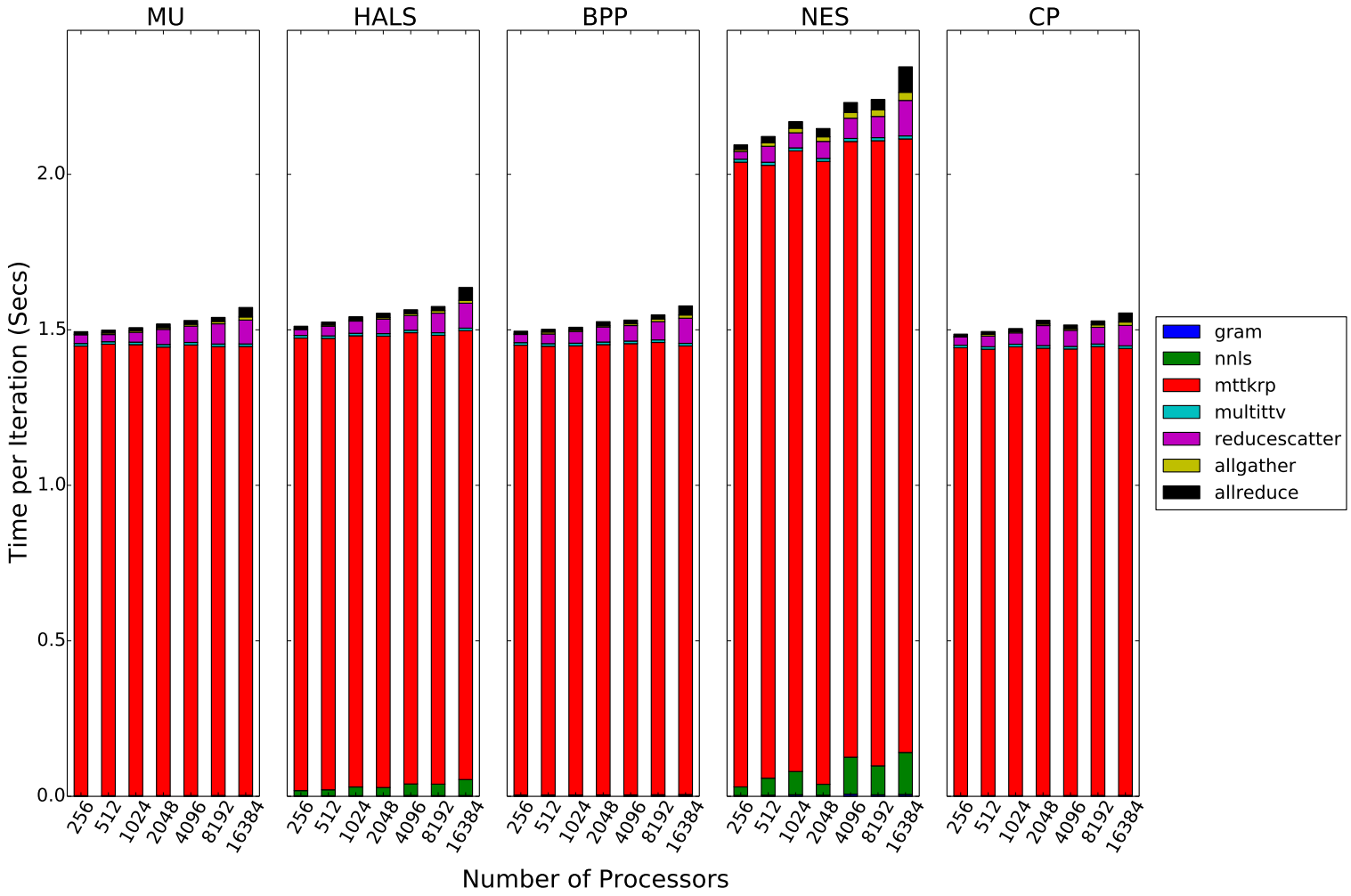
4. Computes its contribution to rows of **M** (local MTTKRP)
5. Reduce-Scatters to compute and distribute **M** evenly
6. Use **M** to solve NNLS problem for **V**

Rest of the Algorithm

- With correct processor grid, MTTKRP algorithm achieves communication lower bound
- Also need to compute $\mathbf{G} = \mathbf{U}^T\mathbf{U} * \mathbf{W}^T\mathbf{W}$
  - involves communication
  - generally lower order cost
- Lots of overlap across MTTKRP computations
  - save communication: keep temporary copies around
  - save computation: use dimension tree optimization
  - $O(N)$ savings, where N is the number of modes
- Can choose algorithm to compute $\mathbf{V}$ from $\mathbf{M}$ and $\mathbf{G}$
  - for some algorithms, this is all local computation
  - some algorithms require extra computation of global information, can add significant cost

Weak Scaling Results for 4D Synthetic Data



- local tensor is fixed at $128 \times 128 \times 128 \times 128$

Mouse Brain Data

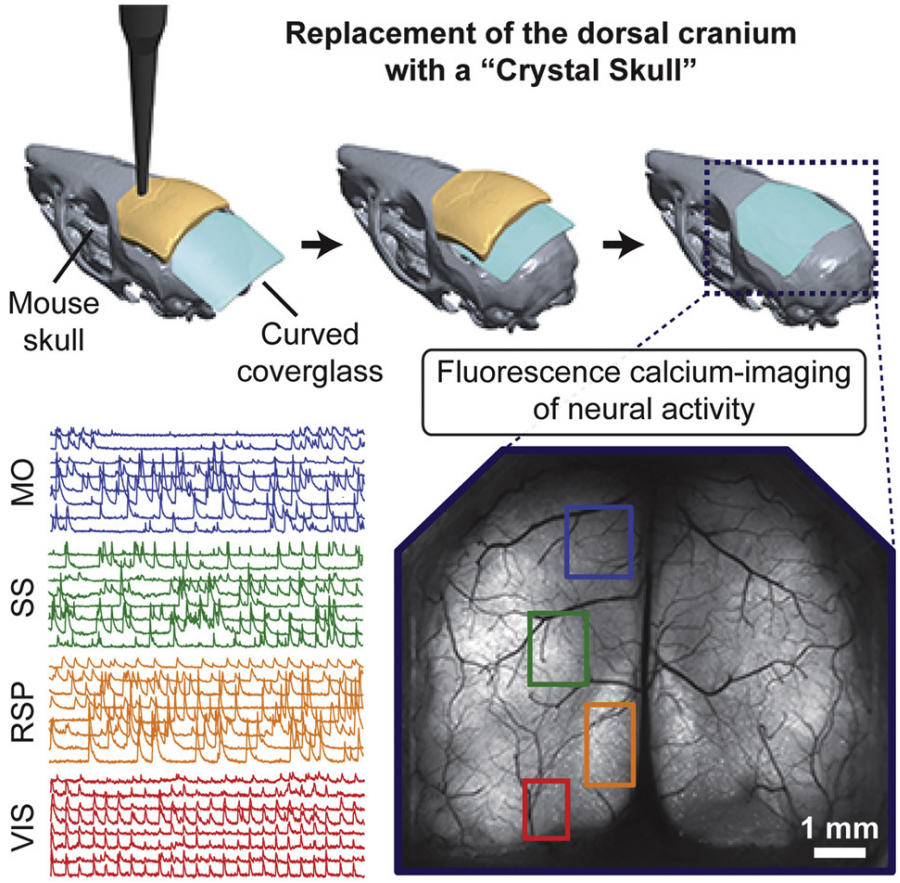
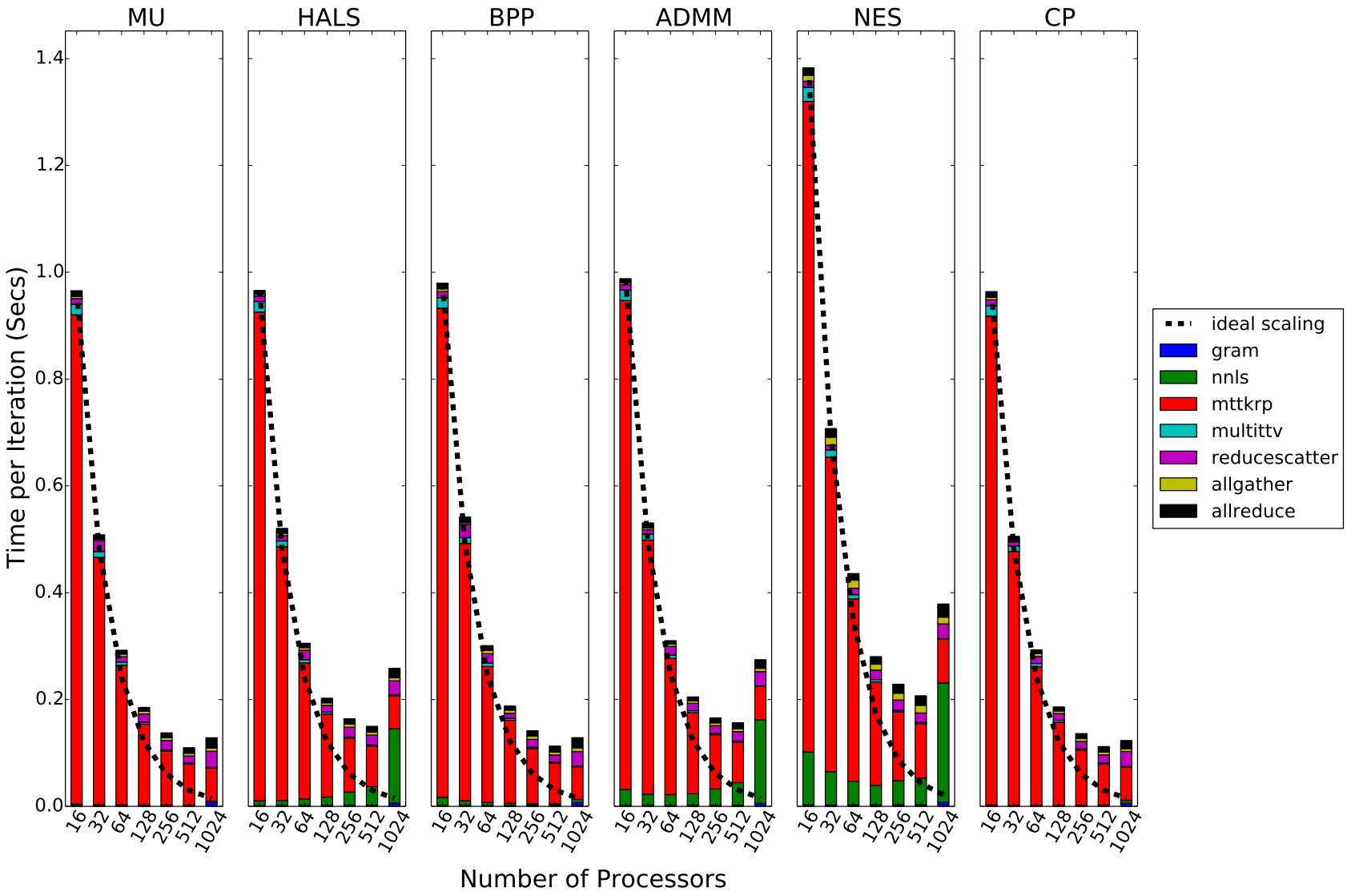


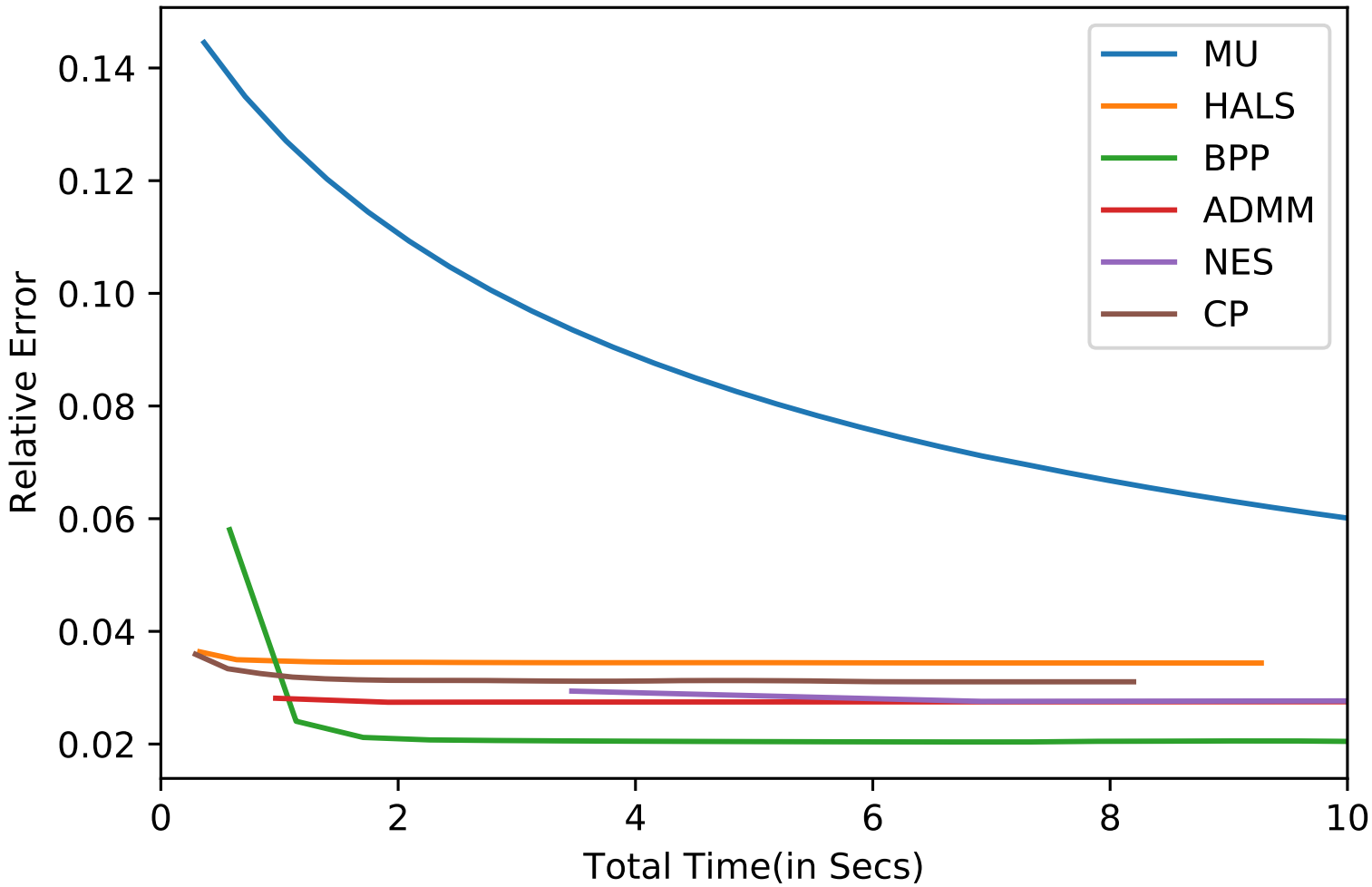
Image from [KZL+16]

- tensor is pixels $\times$ time $\times$ trial: $1.4M \times 69 \times 25$
- about 20 GB when stored in double precision

Strong Scaling Results for Mouse Brain Data

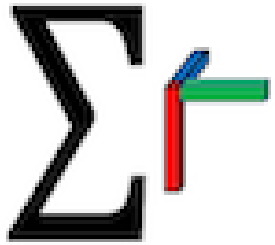


Convergence Results for Mouse Brain Data



Software: PLANC

Parallel Low-rank Approximations with Non-negativity Constraints



`https://github.com/ramkikannan/planc`

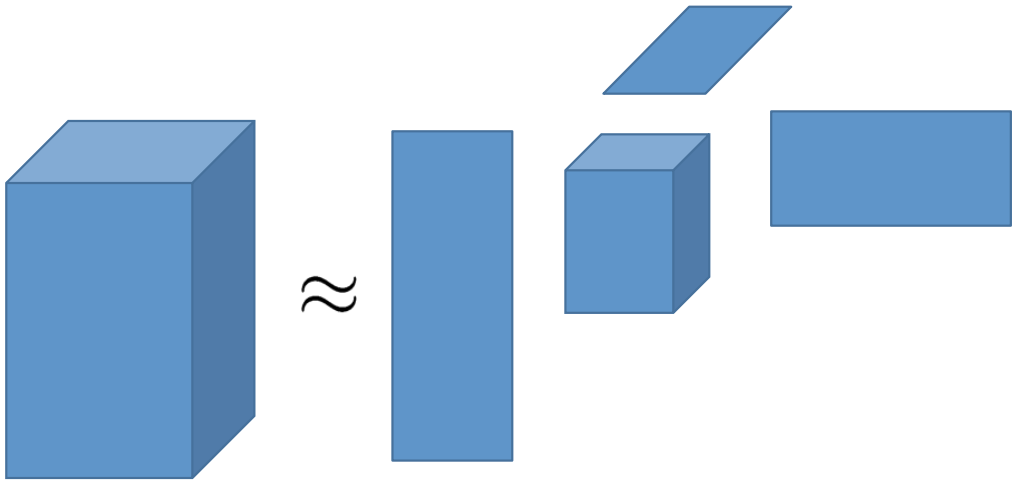
- Open source code for computing NMF and NNCP
- MPI/BLAS/LAPACK/C++11
- Designed for dense tensors and dense/sparse matrices
- Can offload computation to GPUs if available

Efficient Parallel Algorithm for Tucker Decompositions of Dense Tensors

joint work with Woody Austin[4], Alicia Klinvex[5], Tammy Kolda[6], and Hemanth Kolla[6]

[4] UT Austin
[5] Bettis Atomic Power Laboratory
[6] Sandia National Labs

Tucker Notation



$$\mathcal{X} \approx \mathcal{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{W}$$

$$\mathcal{X} \in \mathbb{R}^{I \times J \times K}, \mathcal{G} \in \mathbb{R}^{P \times Q \times R}$$
is *core tensor*

$$\mathcal{X} \approx [\![\mathcal{G}; \mathbf{U}, \mathbf{V}, \mathbf{W}]\!],$$

$$\mathbf{U} \in \mathbb{R}^{I \times P}, \mathbf{V} \in \mathbb{R}^{J \times Q}, \mathbf{W} \in \mathbb{R}^{K \times R}$$
are *factor matrices*

$$x_{ijk} \approx \sum_{p=1}^{P} \sum_{q=1}^{Q} \sum_{r=1}^{R} g_{pqr} u_{ip} v_{jq} w_{kr}, \quad 1 \leq i \leq I, 1 \leq j \leq J, 1 \leq k \leq K$$

Algorithm: ST-HOSVD [VVM12]

ST-HOSVD($\mathcal{X}, \varepsilon$)

1. Compute $\mathbf{U}$ with dimension $I \times P$
   (a) Compute Gram matrix $\mathbf{X}_{(1)}\mathbf{X}_{(1)}^T$
   (b) Use eigendecomposition to determine P and $\mathbf{U}$
   (c) TTM to shrink to size $P \times J \times K$: $\mathcal{Y} = \mathcal{X} \times_1 \mathbf{U}^T$
2. Compute $\mathbf{V}$ with dimension $J \times Q$
   (a) Compute Gram matrix $\mathbf{Y}_{(2)}\mathbf{Y}_{(2)}^T$
   (b) Use eigendecomposition to determine Q and $\mathbf{V}$
   (c) TTM to shrink to size $P \times Q \times K$: $\mathcal{Z} = \mathcal{Y} \times_2 \mathbf{V}^T$
3. Compute $\mathbf{W}$ with dimension $K \times R$
   (a) Compute Gram matrix $\mathbf{Z}_{(3)}\mathbf{Z}_{(3)}^T$
   (b) Use eigendecomposition to determine R and $\mathbf{W}$
   (c) TTM to shrink to size $P \times Q \times R$: $\mathcal{G} = \mathcal{Z} \times_3 \mathbf{W}^T$

Key kernels

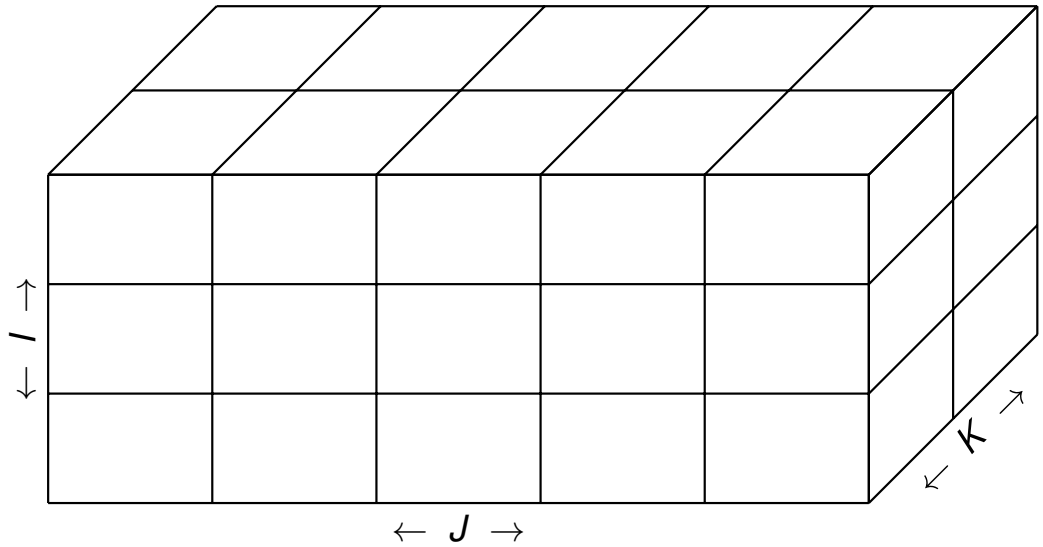
Key kernels of ST-HOSVD are

- Gram: short, fat matrix times its transpose ($\mathbf{X}_{(1)}\mathbf{X}_{(1)}^T$)
- Evecs: eigendecomposition of small symmetric matrix
- TTM: tensor times matrix to shrink problem ($\mathbf{U}^T\mathbf{X}_{(1)}$)

Our goal is to parallelize Gram and TTM efficiently

Tensor data distribution across processors

For N-way tensor, we use N-way processor grid with Cartesian block distribution (same as for CP)

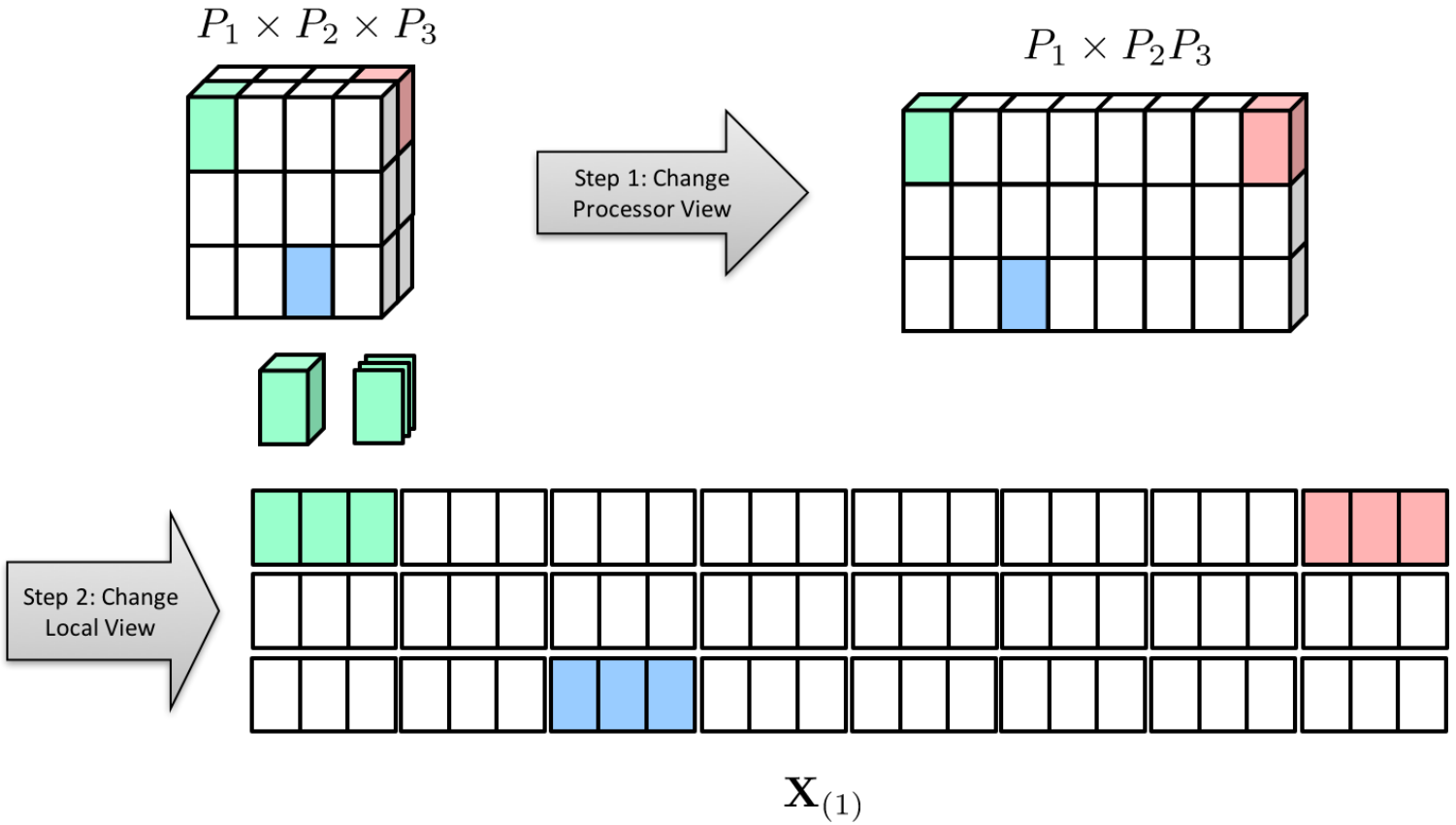


Example: $P_1 \times P_2 \times P_3 = 3 \times 5 \times 2$

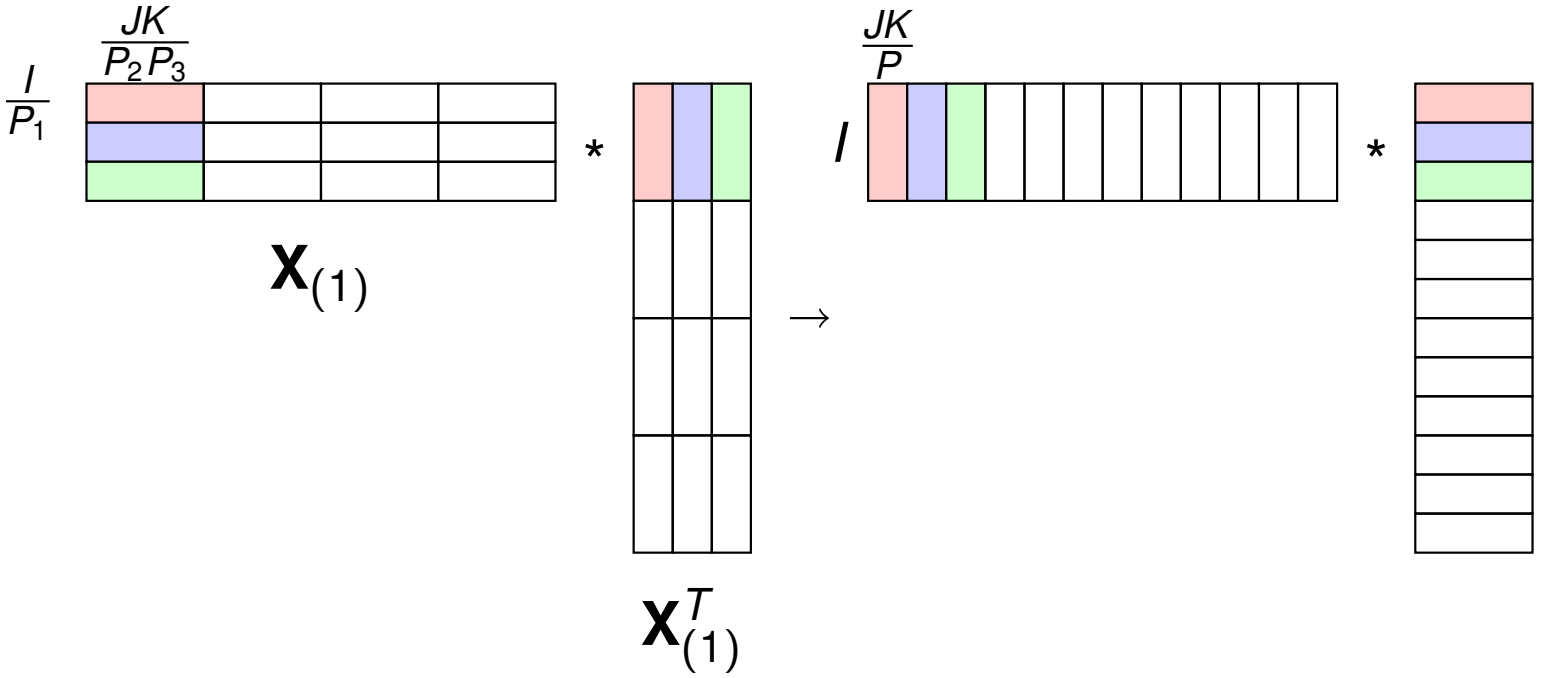
Local tensor size: $\frac{I}{P_1} \times \frac{J}{P_2} \times \frac{K}{P_3}$

Parallel matricization

Matricizing distributed tensor requires no data movement: matricized tensor already in standard matrix distribution

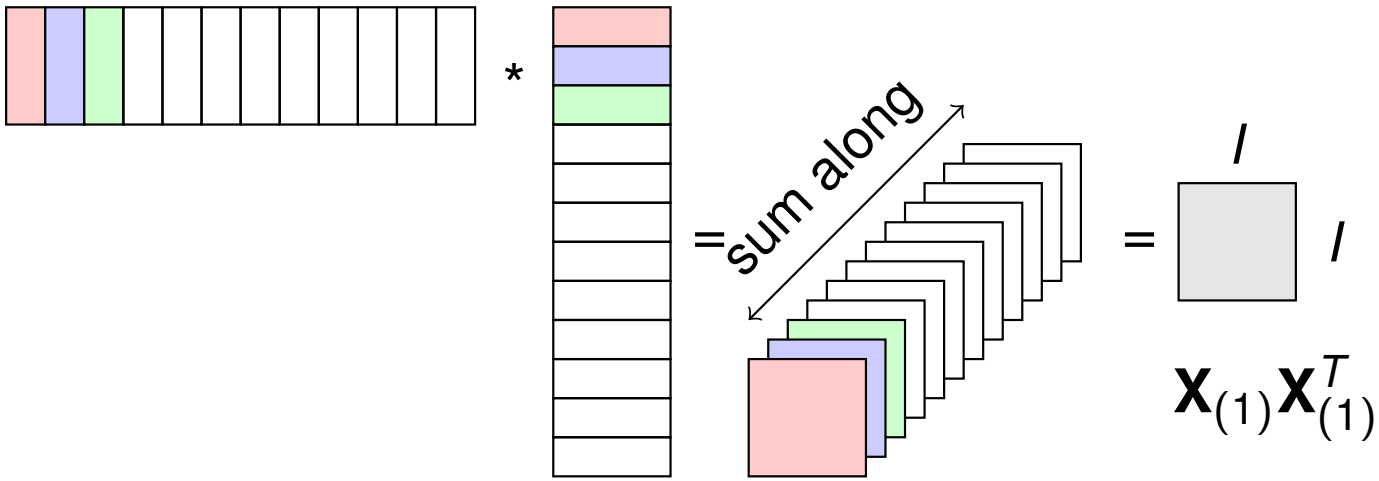


Parallel Gram Computation



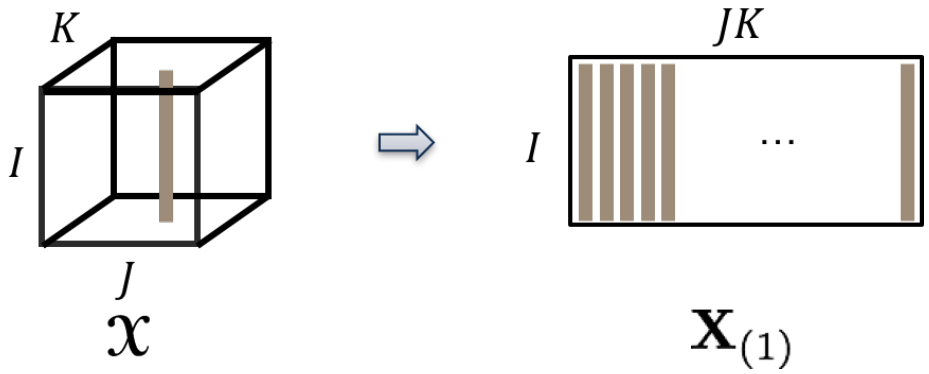
- each processor column redistributes its tensor data

Parallel Gram Computation

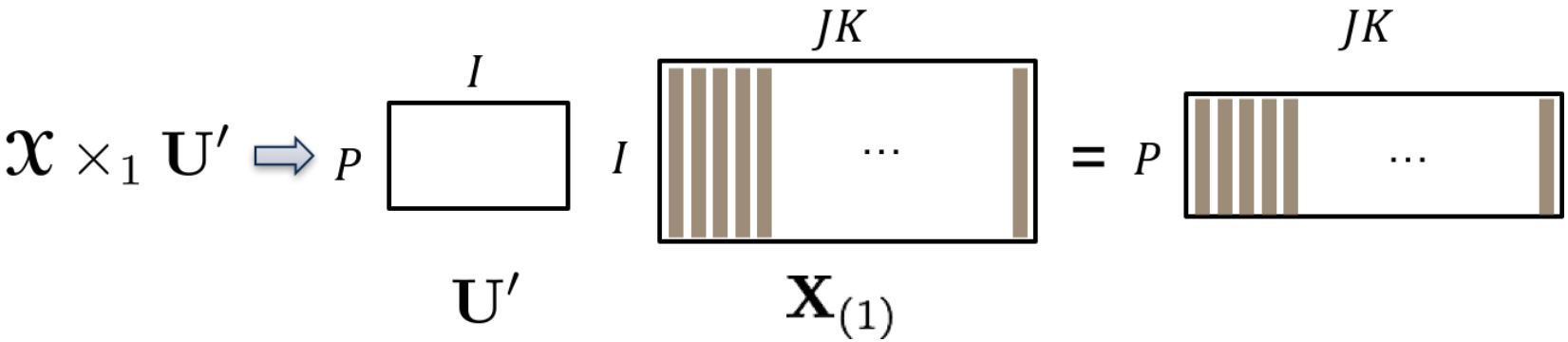


- each processor column redistributes its tensor data
- each processor computes local outer product
- sum across all processors via All-Reduce

Tensor Times Matrix

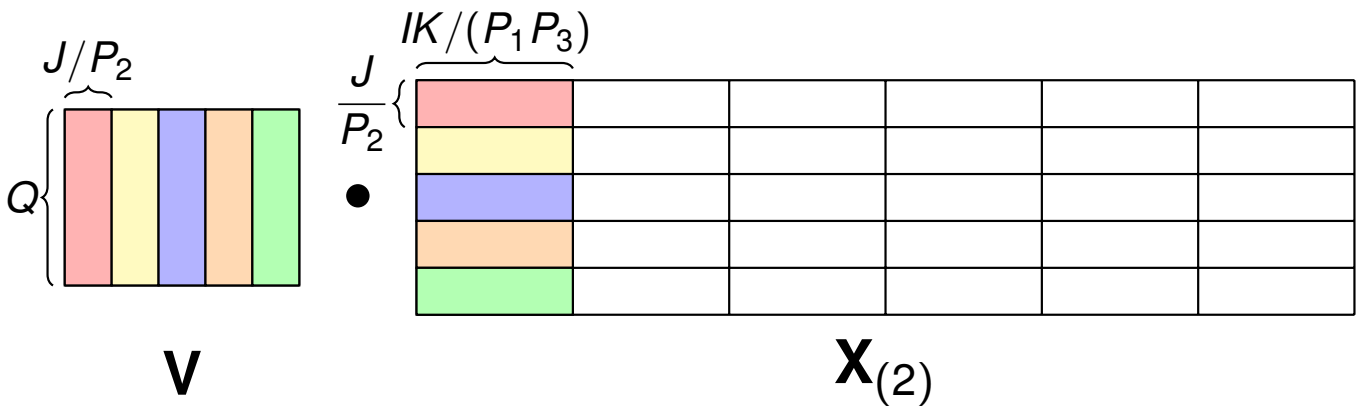


Tensor-times-matrix (TTM) is matrix multiplication with matricized tensor



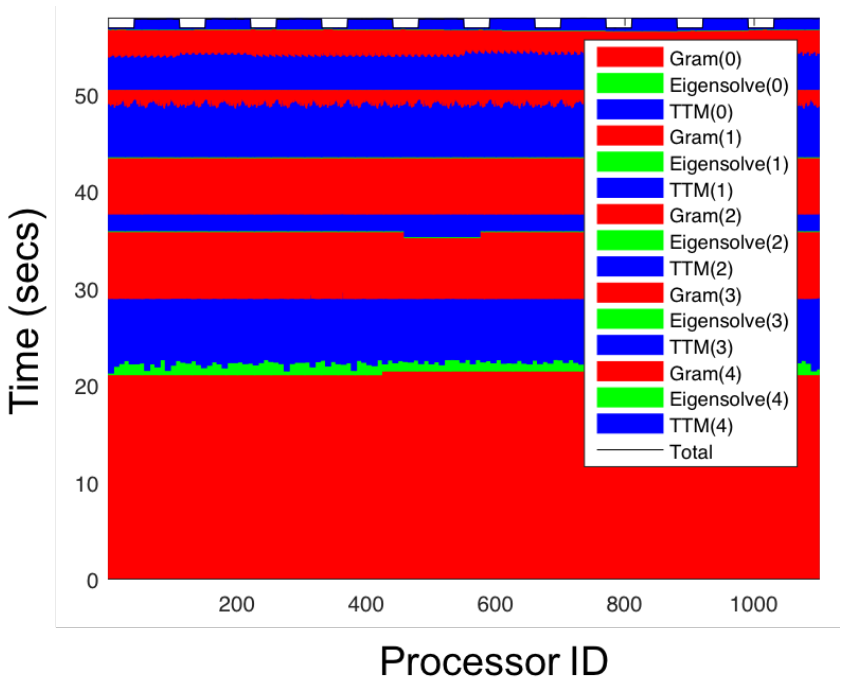
Parallel Tensor Times Matrix

Example: $P_1 \times P_2 \times P_3 = 3 \times 5 \times 2$



- Matrix $\mathbf{V}$ distributed conformally to 2nd mode of tensor $\mathcal{X}$
- Matrix $\mathbf{V}$ distributed redundantly on processor columns
- Local computation is matrix multiplication
- Communication pattern is reduce-scatter (MPI collective)

Time Breakdown of Parallel ST-HOSVD



Parallel running time example

- 5-way tensor of size 4.4 TB
- reduced to 10 GB (410X)
- 1100 processors (cores)
- 55 seconds total

Observations

- load-balanced execution
- cycle of Gram-Eig-TTM shrinks over time
- writing original tensor to disk is slower by 10X

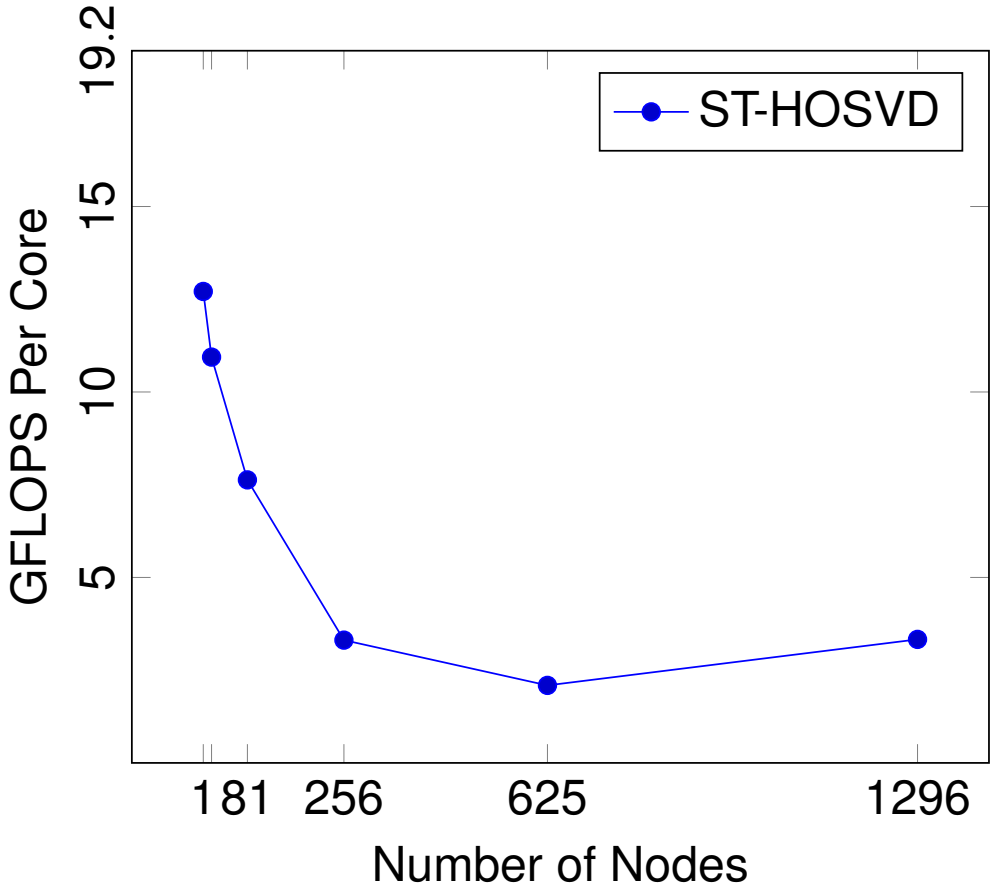
Weak Scaling on Synthetic Data

Problem Setup

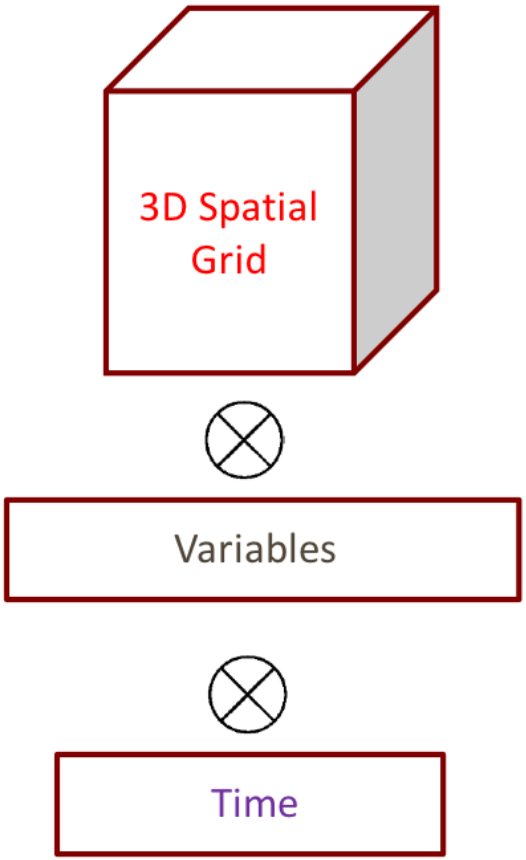
- local tensor fixed at $200 \times 200 \times 200 \times 200$
- local core fixed at $20 \times 20 \times 20 \times 20$

Result

- as problem size grows with number of processors, high efficiency maintained up to 31K cores



Combustion Simulation (S3D) Data



Stat-Planar dataset

- $500 \times 500 \times 500 \times 11 \times 400$
- 4.4 TB of total storage
- use 250 nodes to process

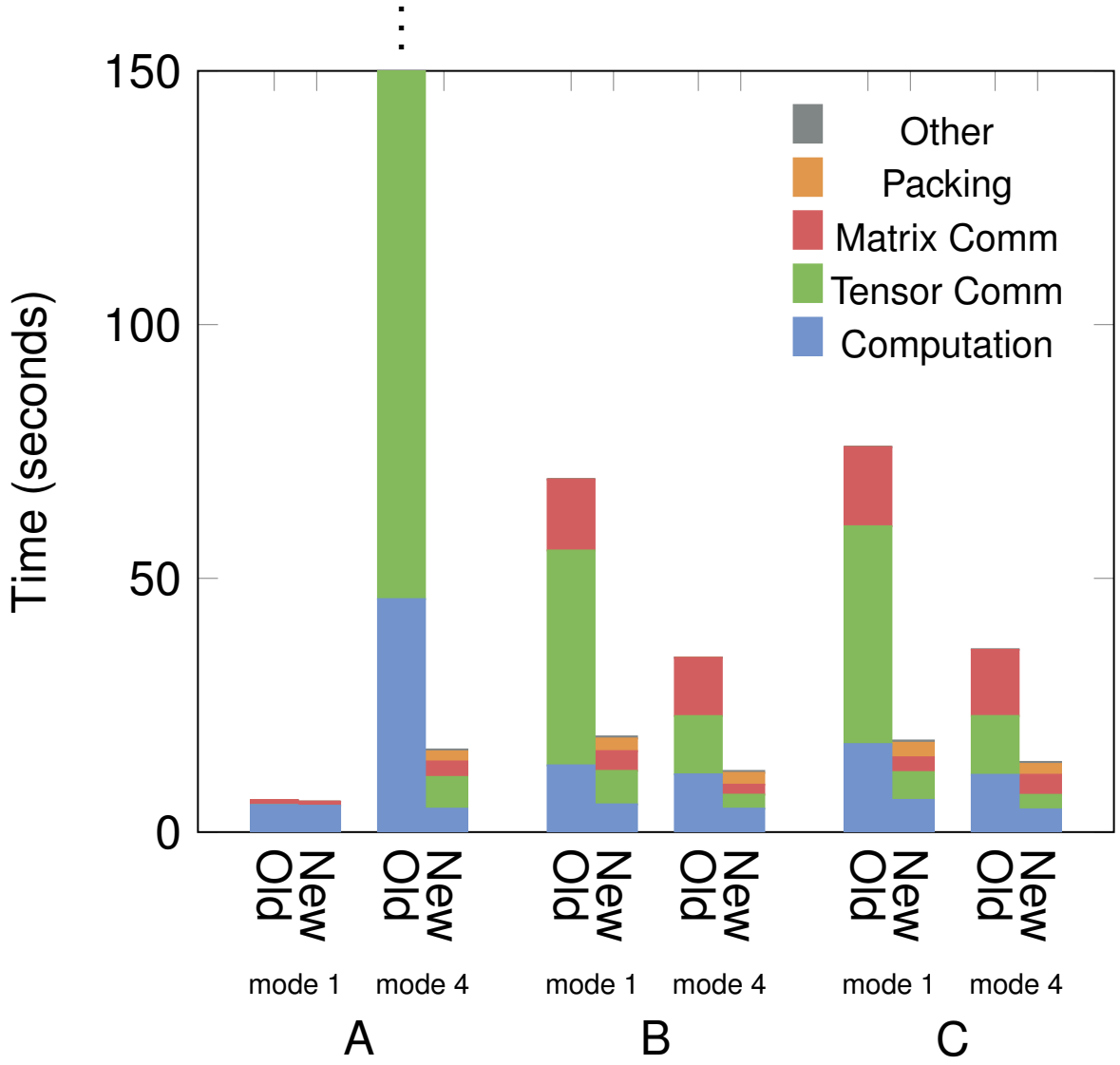
Two compression scenarios

- High: 1e-2 error, 20,000X comp.
- Low: 1e-4 error, 400X comp.

Three processor grids

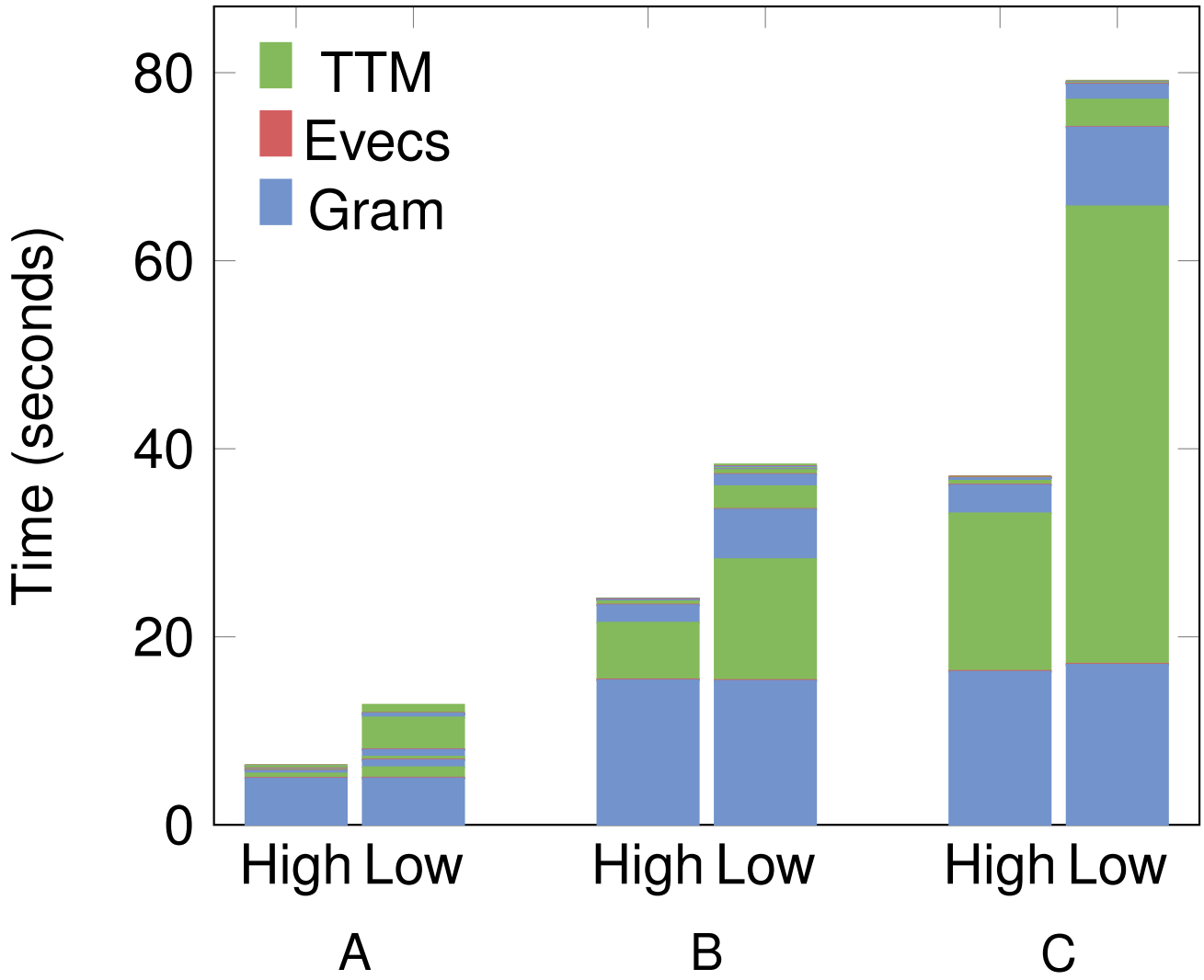
- A: $1 \times 1 \times 40 \times 1 \times 100$
- B: $10 \times 8 \times 5 \times 1 \times 10$
- C: $40 \times 10 \times 1 \times 1 \times 10$

Gram Algorithm Comparison

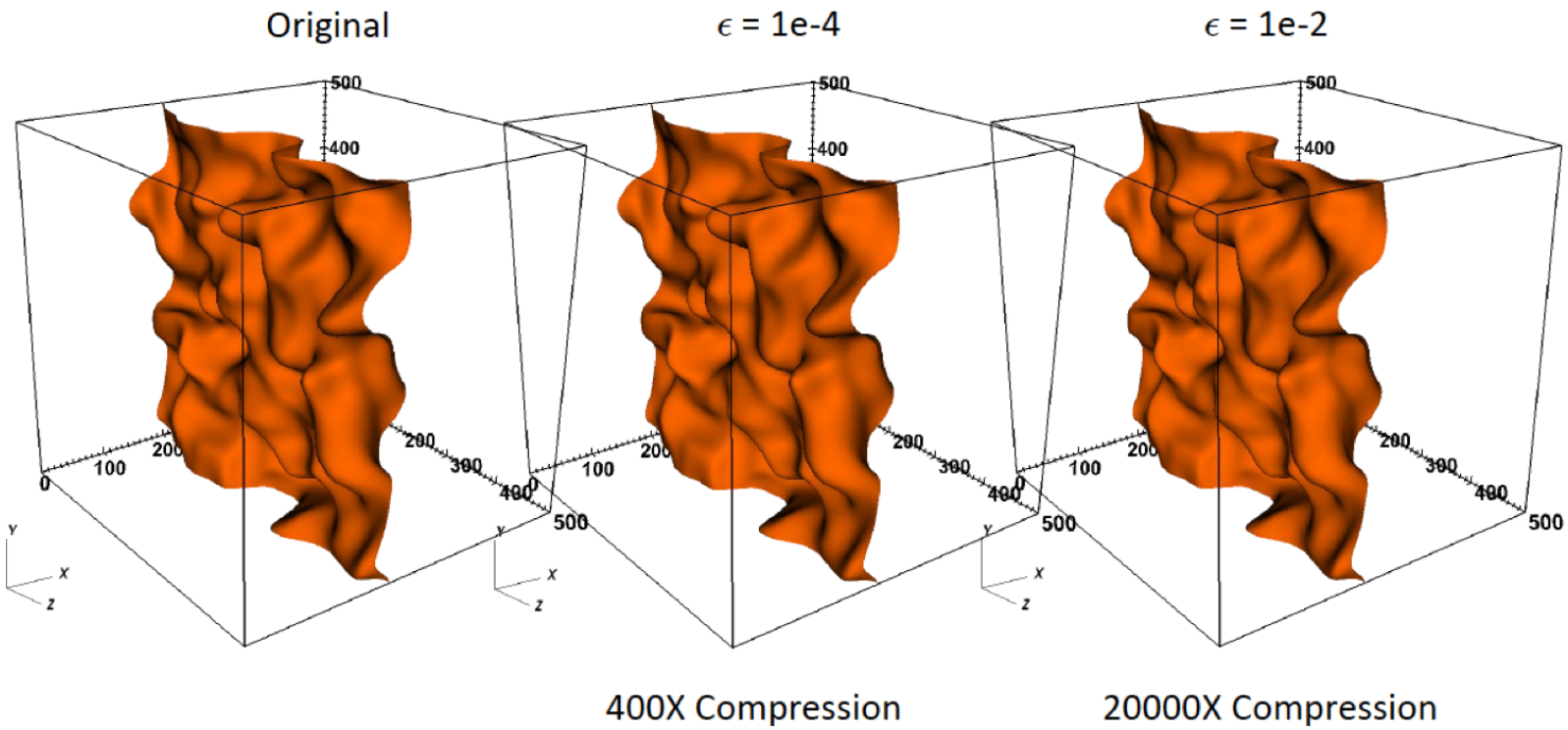


- Old algorithm from our previous work [ABK16]

Processor Grid Comparison



Flame Surface Reconstruction



Flame surface at single time step.
Using temperature variable (iso-value is 2/3 of max).

Software: TuckerMPI

`https://gitlab.com/tensors/TuckerMPI`

- Open source code for computing Tucker compression
- MPI/BLAS/LAPACK/C++11
- Designed for dense tensors

Summary

- CP and Tucker decompositions are useful and popular tools for multidimensional data analysis, can be applied to large datasets
- Parallel CP bottlenecked by MTTKRP
  - our algorithm's communication cost matches lower bound
  - we avoid redundant computation and communication across modes
- Parallel Tucker bottlenecked by SVD and TTM
  - need communication-efficient distributions and algorithms
  - we can tune the processor grid for efficiency
  - partial reconstruction for analysis can be done on laptop

For more details:

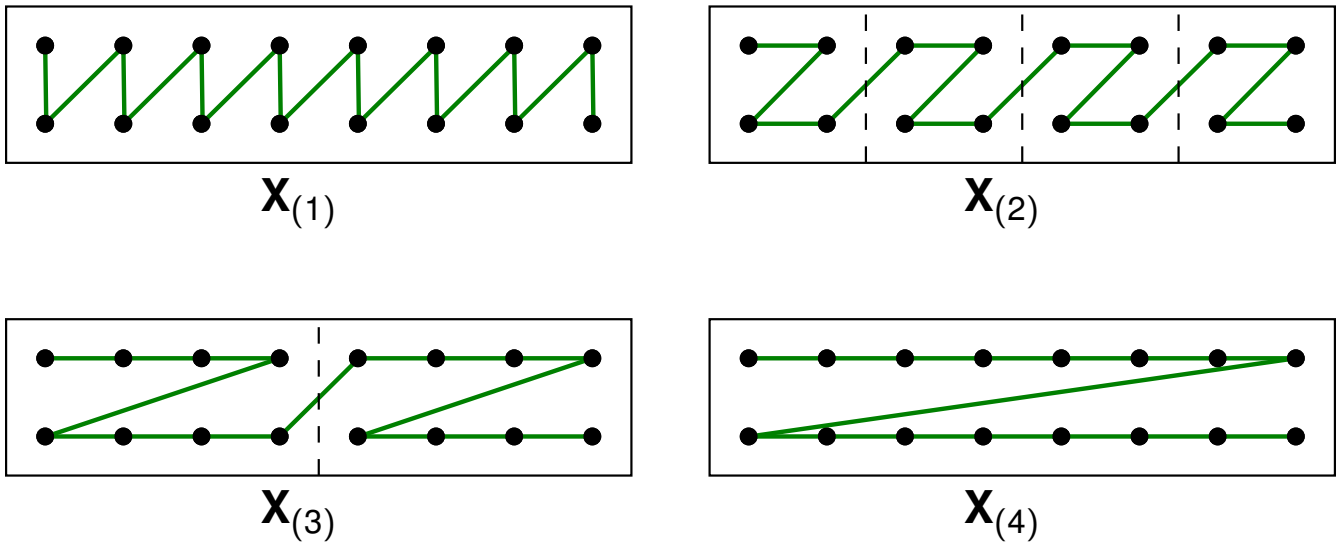
Parallel Nonnegative CP Decomposition of Dense Tensors
Grey Ballard, Koby Hayashi, and Ramakrishnan Kannan
International Conference on High Performance Computing 2018
`https://ieeexplore.ieee.org/document/8638076`
[BHK18]

TuckerMPI: Efficient Parallel Software for Tucker Decompositions of Dense Tensors
Grey Ballard, Alicia Klinvex, and Tamara G. Kolda
arXiv 2019
`https://arxiv.org/abs/1901.06043`
[BKK19]

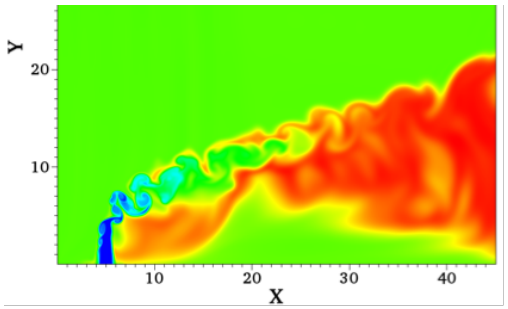
Local tensor data layout in memory

Local matricizations (with no data movement)
lead to matrices in funny layouts

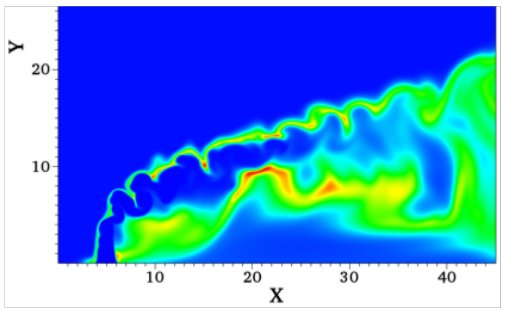
Example: $2 \times 2 \times 2 \times 2$ tensor's matricization layouts

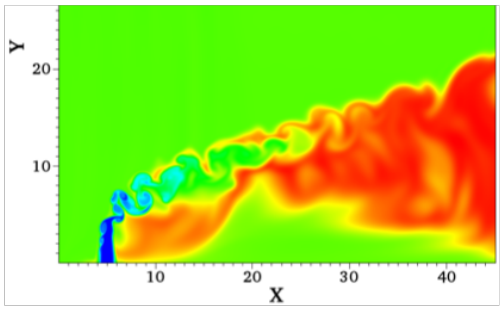


More eyeball norm comparisons (JICF)

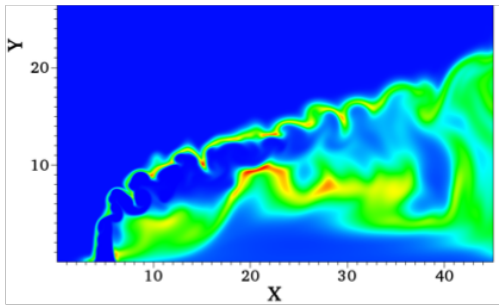


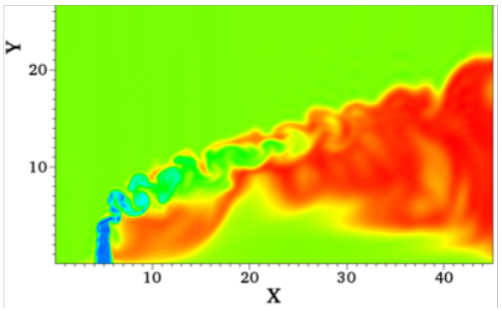
Original



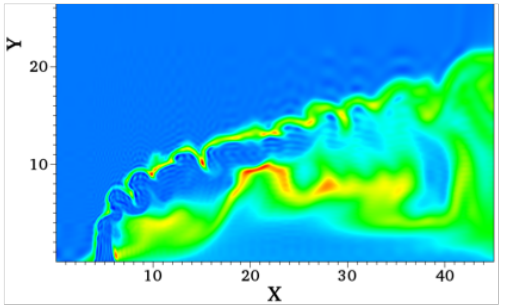


$\epsilon = 10^{-4}$
(110X)

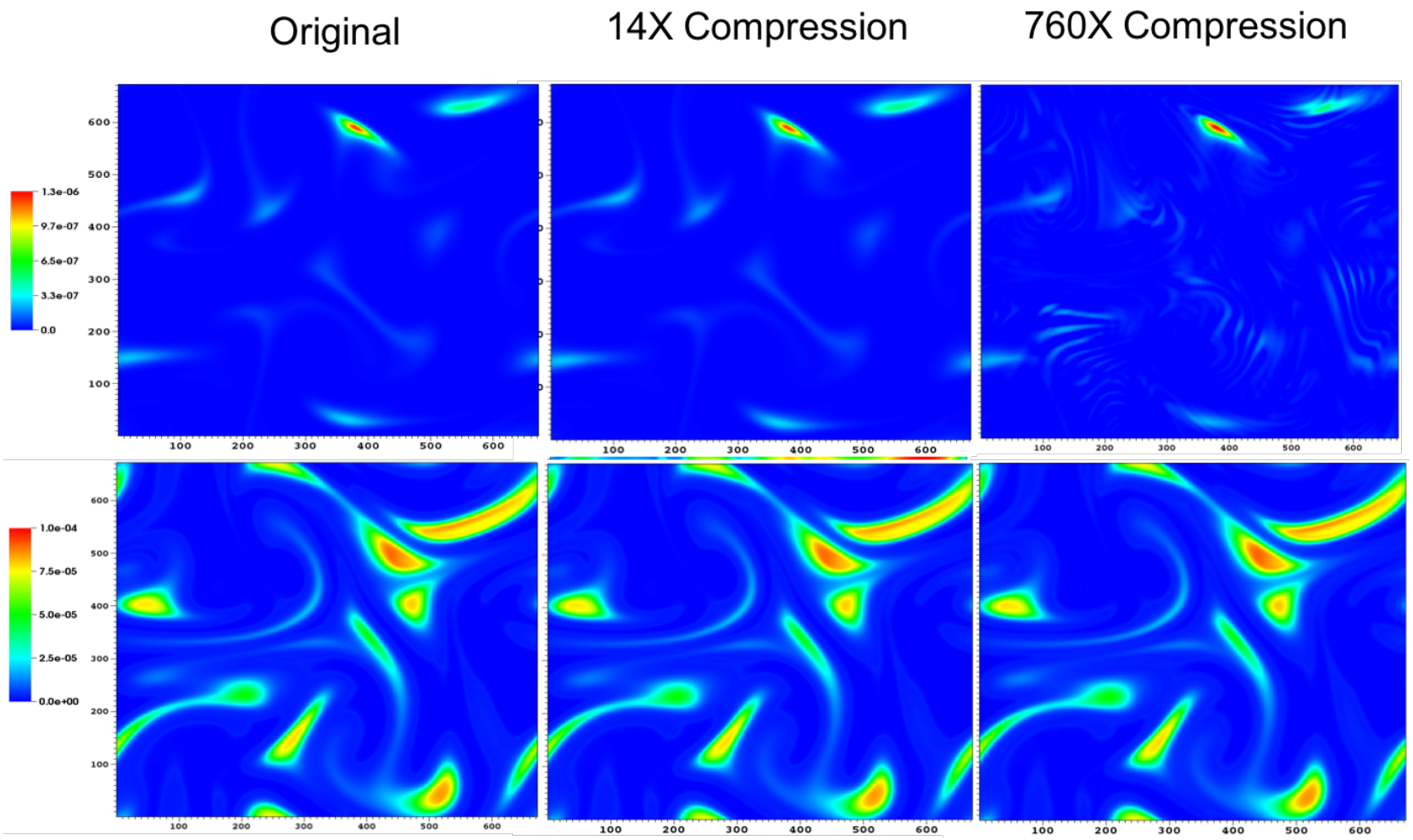




$\epsilon = 10^{-2}$
(40000X)

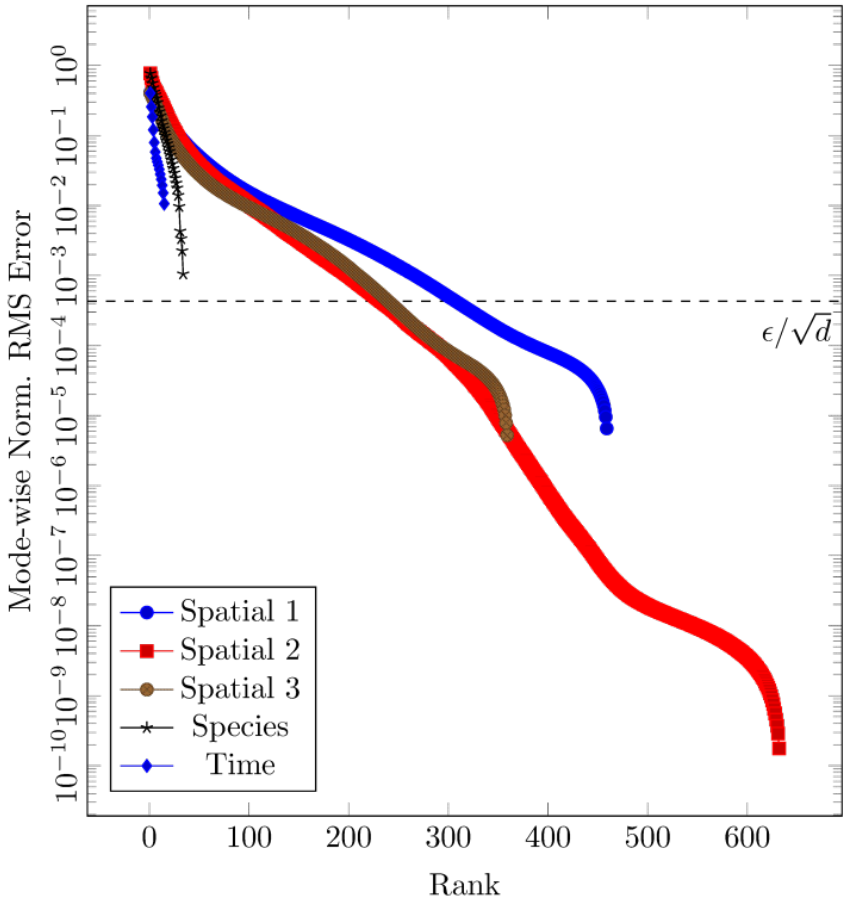


More eyeball norm comparisons (HCCI)

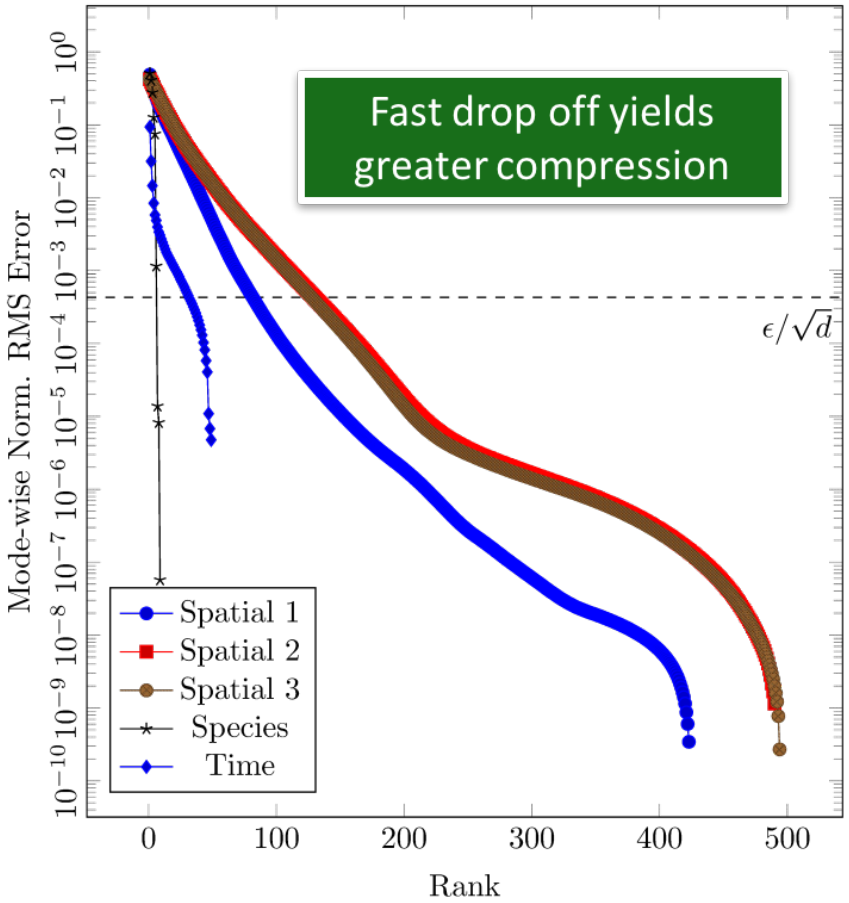


Compressibility depends on data (sing. value decay)

TJLR: 460 x 700 x 360 x 35 x 16



SP-50: 500 x 500 x 500 x 11 x 50

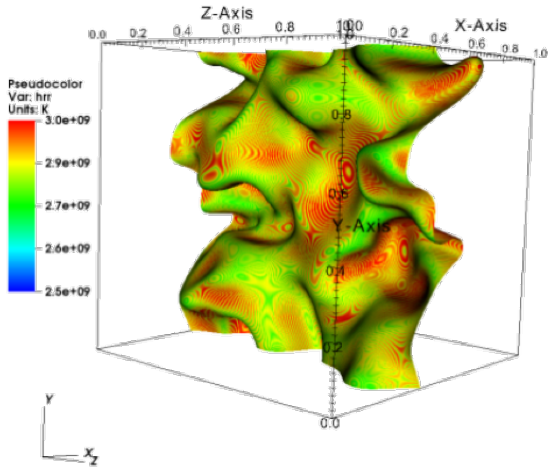


Partial reconstruction

Reconstruction requires as much space as the original data!

$$\hat{\mathcal{X}} = \mathcal{G} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{U}^{(3)} \times_4 \mathbf{U}^{(4)} \times_5 \mathbf{U}^{(5)}$$

$$N_1 \times N_2 \times N_3 \times N_4 \times N_5$$



But we can just reconstruct the portion that we need at the moment:

$$\bar{\mathcal{X}} = \mathcal{G} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{C}^{(3)}\mathbf{U}^{(3)} \times_4 \mathbf{C}^{(4)}\mathbf{U}^{(4)} \times_5 \mathbf{C}^{(5)}\mathbf{U}^{(5)}$$

$$N_1 \times N_2 \times \frac{N_3}{2} \times 1 \times 1$$

$$\mathbf{C}^{(3)} = \begin{bmatrix} 1/2 & 0 & \cdots & 0 \\ 1/2 & 0 & \cdots & 0 \\ 0 & 1/2 & \cdots & 0 \\ 0 & 1/2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix}$$

Downsample

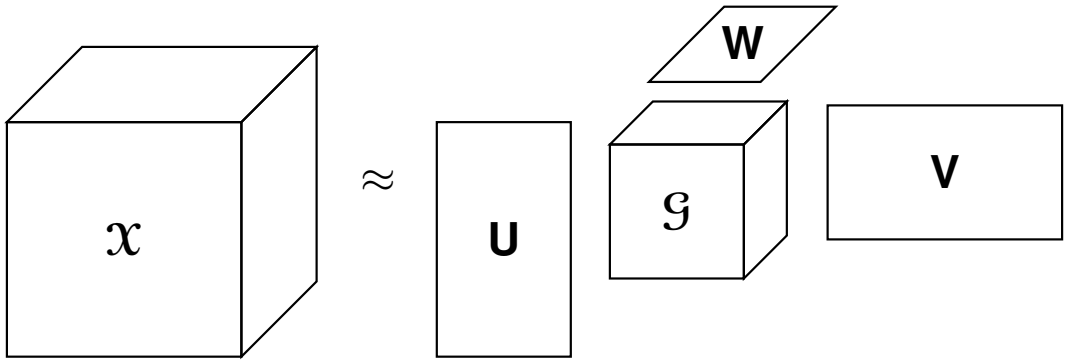
$$\mathbf{C}^{(4)} = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

Pick single variable

$$\mathbf{C}^{(5)} = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

Pick single time step

Tucker compression

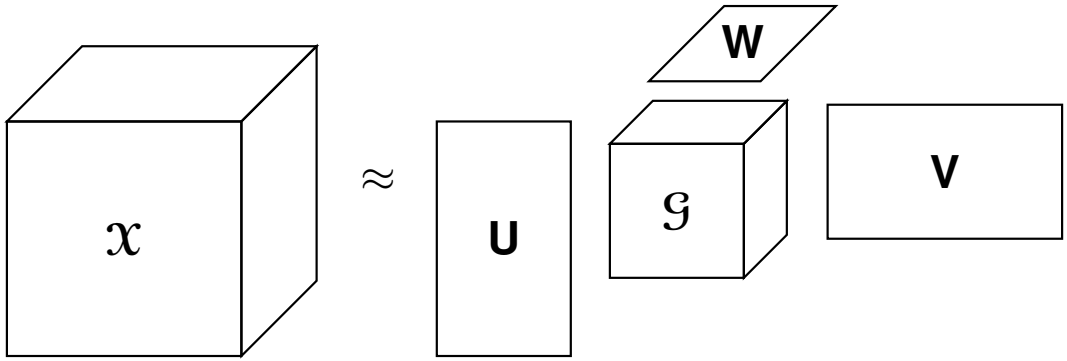


$$\underbrace{\mathcal{X}}_{I\times J\times K} \approx \underbrace{\mathcal{G}}_{P\times Q\times R} \times_1 \underbrace{\mathbf{U}}_{I\times P} \times_2 \underbrace{\mathbf{V}}_{J\times Q} \times_3 \underbrace{\mathbf{W}}_{K\times R}$$

Compression ratio

$$C = \frac{IJK}{PQR + IP + JQ + KR} \approx \frac{IJK}{PQR}$$

Tucker approximation error



$$x_{ijk} \approx \tilde{x}_{ijk} = \sum_{p,q,r} g_{pqr} u_{ip} v_{jq} w_{kr}$$

Approximation error

$$\frac{\left\|\mathcal{X} - \tilde{\mathcal{X}}\right\|}{\|\mathcal{X}\|} = \frac{\left(\sum_{i,j,k} \left(x_{ijk} - \sum_{p,q,r} g_{pqr} u_{ip} v_{jq} w_{kr}\right)^2\right)^{1/2}}{\left(\sum_{i,j,k} x_{ijk}^2\right)^{1/2}}$$

Strong scaling benchmark

Problem Setup

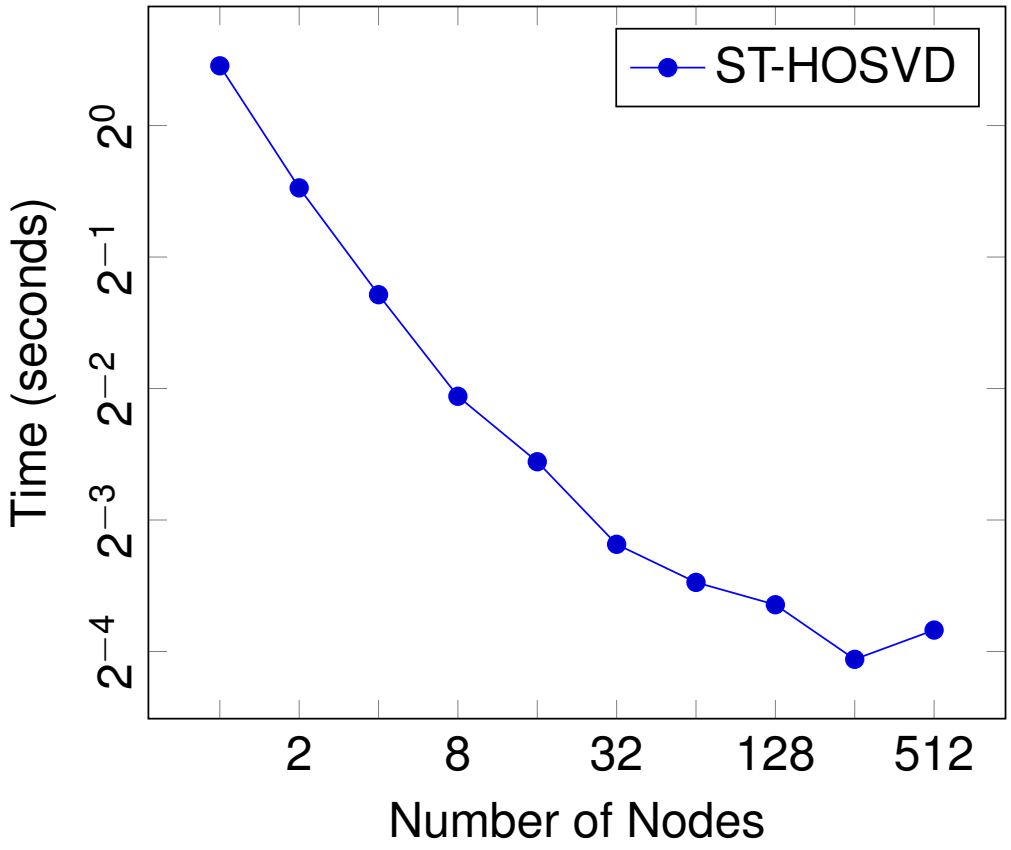
- $200 \times 200 \times 200 \times 200$ data tensor (12 GB)
- $20 \times 20 \times 20 \times 20$ core tensor
- $24 \cdot 2^k$ processors (cores)

Result

- small problem, but running time decreases with up to 6144 cores

Compute Platform

- Edison (NERSC), Cray XC30
- 24-core nodes



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