Illustration by Chris Brigman

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SAND2015-9290 C

Parallel Tucker Compression for Large-scale Scientific Data

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SIAM Conference on Applied Linear Algebra (AL15)
Atlanta, Georgia, USA
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U.S. DEPARTMENT OF ENERGY

A Celebration of Dianne P. O'Leary

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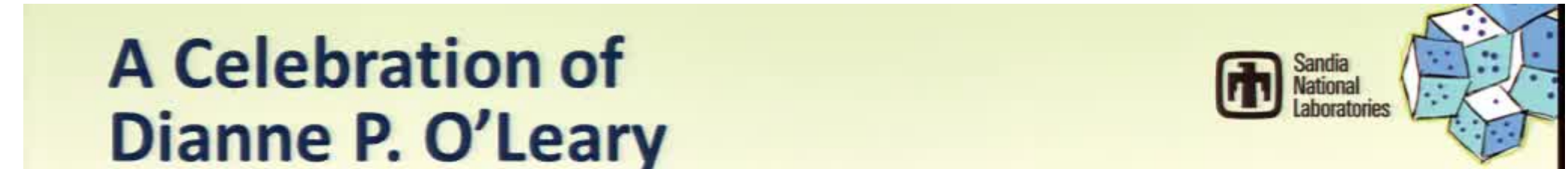

PhD Advisor, Mentor, Role Model, Colleague, Friend

Dianne, Parallel Computing, & Tensors!

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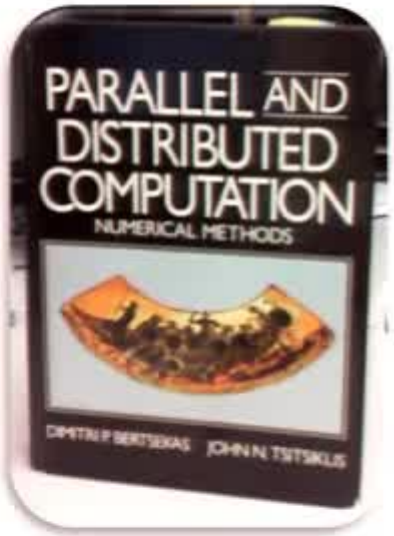
Unhappy student in Harland Glaz's scientific computing class. Didn't want Fortran and vector parallelization. Wanted C and MPI. He sent me to Dianne...

Reading class on parallel computing with this book:




```
From: oleary@cs.umd.edu (Dianne O'Leary)
To: kolda@msr.epm.ornl.gov
CC: oleary@cs.umd.edu
Subject: reference
Received: from prost.cs.umd.edu (prost.cs.umd.edu [128.8.128.57]) by
msr.EPM.ORNL.GOV (8.8.3/8.8.3) with ESMTP id KAA14047 for
<kolda@msr.epm.ornl.gov>; Thu, 19 Feb 1998 10:57:21 -0500 (EST)
Date: Thu, 19 Feb 1998 15:57:19 GMT
Content-Type: text/plain; charset=utf-8

Leibovici has an article in LAA 269 p. 307 on one way to
extend the svd to 3-d and higher.  I wonder if the sdd has
a similar extension?

Dianne
```

As a postdoc, the email that started me on tensors!

A Tensor is an N-Way Array

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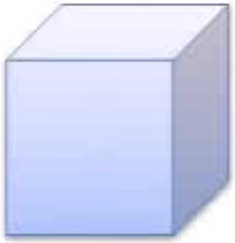
Vector
N = 1

x

Matrix
N = 2

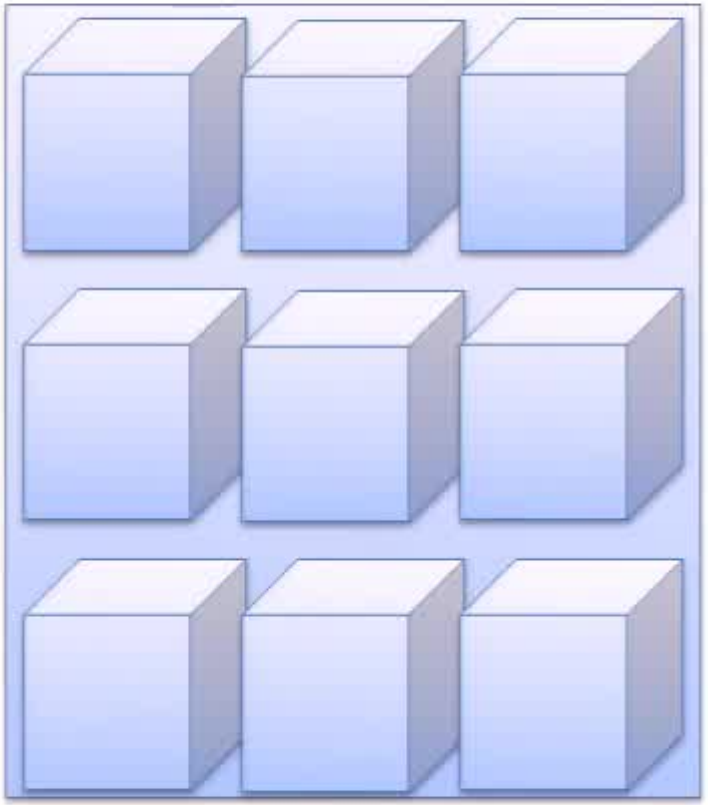
X

3rd-Order Tensor
N = 3



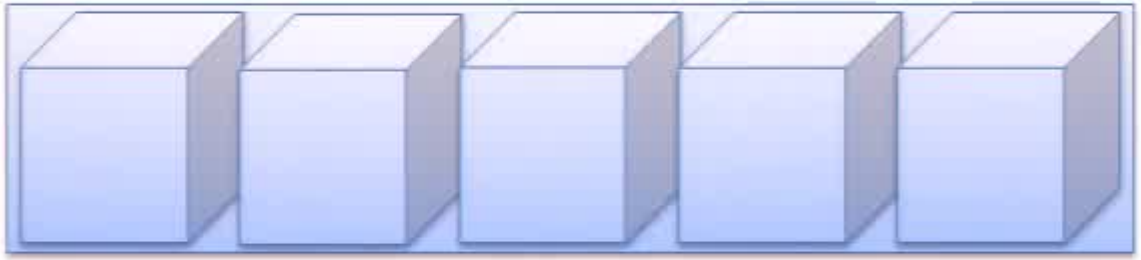
$\mathcal{X}$

5th-Order Tensor
N = 5



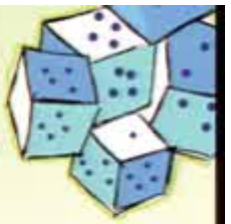
$\mathcal{X}$

4th-Order Tensor
N = 4



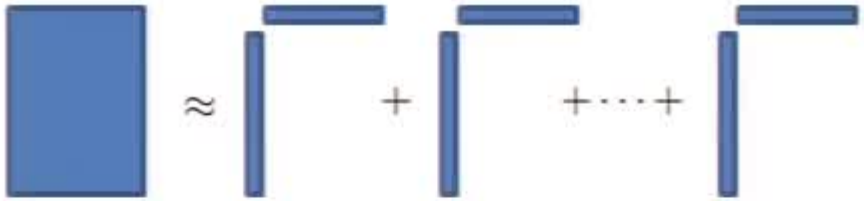
$\mathcal{X}$

Tensor Decompositions are the New Matrix Decompositions

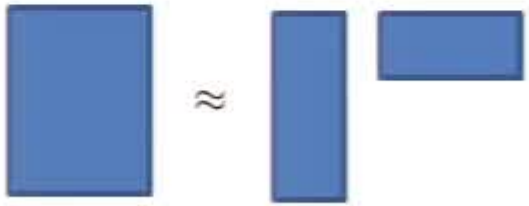


Singular value decomposition (SVD), eigendecomposition (EVD), nonnegative matrix factorization (NMF), sparse SVD, etc.

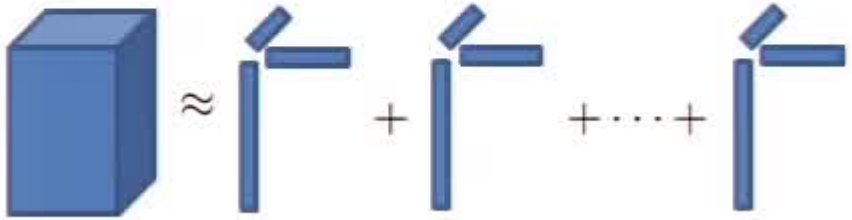
Viewpoint 1: Sum of outer products, useful for interpretation



Viewpoint 2: High-variance subspaces, useful for compression

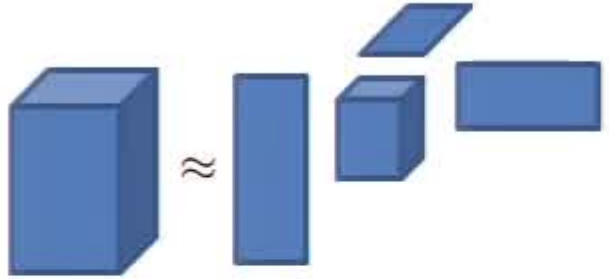


CP Model: Sum of d-way outer products, useful for interpretation



CANDECOMP, PARAFAC, Canonical Polyadic, CP

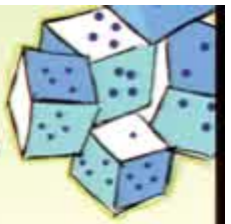
Tucker Model: Project onto high-variance subspaces to reduce dimensionality



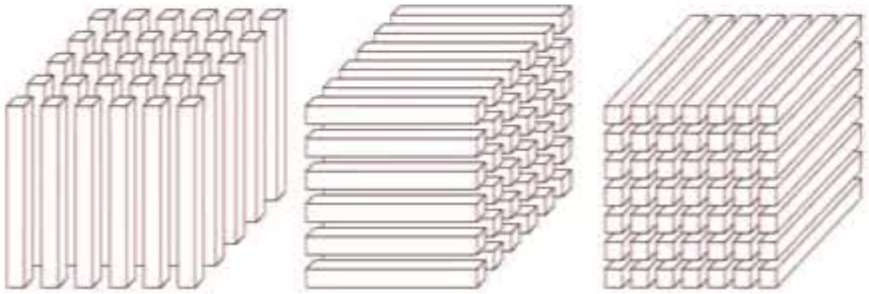
HOSVD, Best Rank-(R1,R2,...,RN) decomposition

Other models for compression include hierarchical Tucker and tensor train.

Tensor Fibers, Mode-n Unfolding, and Mode-n Multiplication



Tensor "mode-n fibers" analogous to matrix rows and columns



Mode-1 Fibers Mode-2 Fibers Mode-3 Fibers

$\mathbf{X}_{(n)}$ denotes mode-n unfolding, arranges mode-n fibers as matrix columns

$$\mathcal{X} = \left[\begin{array}{cc|cc} 1 & 3 & 5 & 7 \\ 2 & 4 & 6 & 8 \end{array}\right]$$

$$\mathbf{X}_{(1)} = \begin{bmatrix} 1 & 3 & 5 & 7 \\ 2 & 4 & 6 & 8 \end{bmatrix}$$

$$\mathbf{X}_{(2)} = \begin{bmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{bmatrix}$$

$$\mathbf{X}_{(3)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix}$$

$$n\text{-rank}(\mathcal{X}) = \text{col-rank}(\mathbf{X}_{(n)})$$

Tensor-times-matrix (TTM) in mode-n multiplies mode-n fibers times matrix

$$I_1 \times \cdots \times I_n \times \cdots \times I_N \qquad K \times I_n$$

$$\mathcal{Y} = \mathcal{X} \times_n \mathbf{U}$$

$$I_1 \times \cdots \times K \times \cdots \times I_N$$

Equivalent to matrix operation:

$$K \times \hat{I}_n \rightarrow \mathbf{Y}_{(n)} = \mathbf{U}\mathbf{X}_{(n)} \leftarrow I_n \times \hat{I}_n, \quad K \times I_n$$

$$I = \prod I_n, \quad \hat{I}_n = I/I_n$$

Optimization Problem

$$\min_{\hat{\mathcal{X}}} \sum_{i_1 \ldots i_N} (x_{i_1 \ldots i_N} - \hat{x}_{i_1 \ldots i_N})^2 \text{ subject to } \hat{\mathcal{X}} = \mathcal{G} \times \{ \mathbf{U}^{(n)} \}$$

Homework: (1) At an optimum, it must be the case that

$$\mathcal{G} = \mathcal{X} \times \{ \mathbf{U}^{(n)\mathsf{T}} \}$$

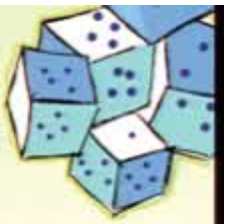
(2) The minimization problem above can be written as

$$\max_{\{ \mathbf{U}^{(n)} \}} \sum_{i_1 \ldots i_N} g^2_{i_1 \ldots i_N} \text{ subject to } \mathcal{G} = \mathcal{X} \times \{ \mathbf{U}^{(n)\mathsf{T}} \}$$

$$\mathbf{U}^{(n)} = \arg\max_{\mathbf{U}} \| \mathbf{U}^{\mathsf{T}} \mathbf{Y}_{(n)} \|_F^2 \text{ subject to } \mathcal{Y} = \mathcal{X} \times \{ \mathbf{U}^{(m)\mathsf{T}} \}_{m \neq n}$$

Solution to (*) is to choose $\mathbf{U}^{(n)}$ to be the R_n leading left singular vectors of $\mathbf{Y}_{(n)}$.

Sequentially Truncated HOSVD improves further



procedure ST-HOSVD($\mathcal{X}$, ϵ)

$\mathcal{Y} \leftarrow \mathcal{X}$

for $n = 1, \ldots, N$ **do**

$\mathbf{S}^{(n)} \leftarrow \mathbf{Y}_{(n)} \mathbf{Y}_{(n)}^{\mathsf{T}}$

$R_n \leftarrow$ min R such that $\sum_{r>R} \lambda_r(\mathbf{S}^{(n)}) \leq \epsilon^2 \|\mathcal{X}\|^2 / N$

$\mathbf{U}^{(n)} \leftarrow$ leading R_n eigenvectors of $\mathbf{S}^{(n)}$

$\mathcal{Y} \leftarrow \mathcal{Y} \times_n \mathbf{U}^{(n)\mathsf{T}}$

end for

$\mathcal{G} \leftarrow \mathcal{Y}$

return $(\mathcal{G}, \{\mathbf{U}^{(n)}\})$

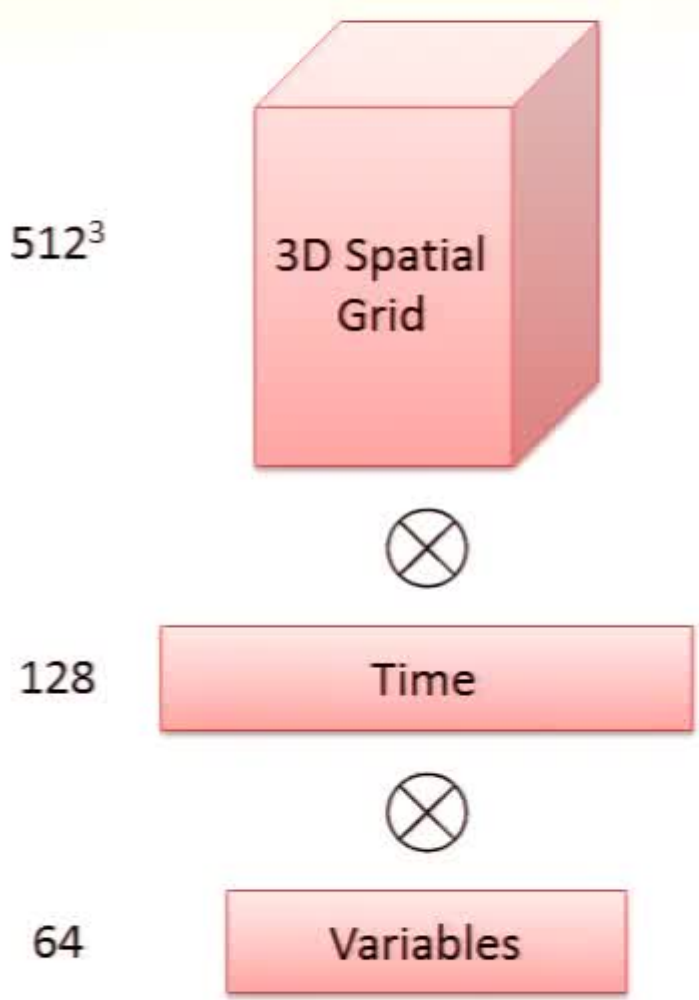
end procedure

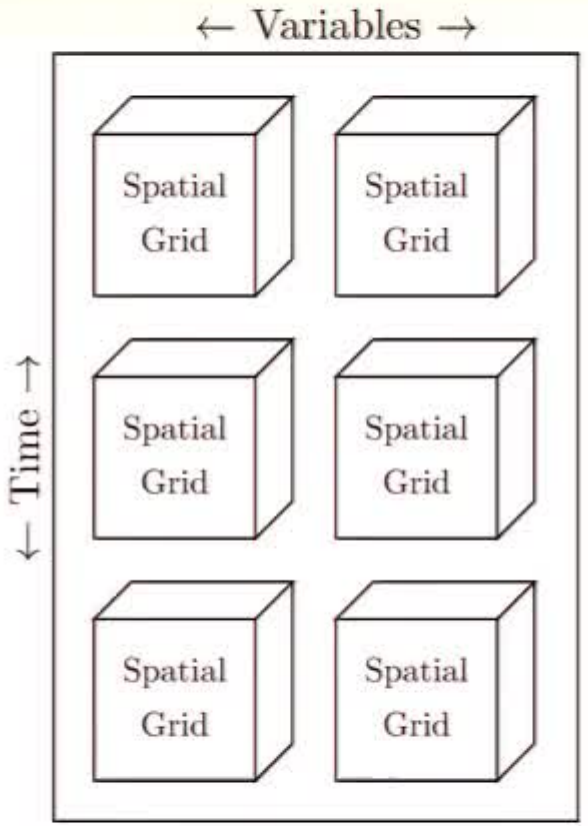
Smaller at each step.

$$\|\mathcal{X} - \hat{\mathcal{X}}\|^2 = \sum_{n=1}^{N} \left(\sum_{i=R_n+1}^{I_n} \lambda_i(\mathbf{S}^{(n)}) \right) \leq \epsilon^2 \|\mathcal{X}\|^2$$

Vannieuwenhoven, Vandebril, and Meerbergen (2012)

Tensors in Scientific Applications are Huge, Need Parallel Methods

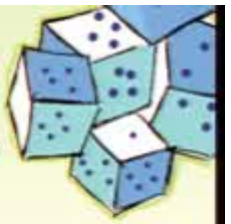




2^{40} elements

8TB (double precision)

Key Kernels in ST-HOSVD are TTM and Gram



procedure ST-HOSVD($\mathcal{X}$, ϵ)
  $\mathcal{Y} \leftarrow \mathcal{X}$
  for $n = 1, \ldots, N$ **do**
Gram $\mathbf{S}^{(n)} \leftarrow \mathbf{Y}_{(n)}\mathbf{Y}_{(n)}^{\mathsf{T}}$
    $R_n \leftarrow \min R$ such that $\sum_{r>R} \lambda_r(\mathbf{S}^{(n)}) \leq \epsilon^2 \|\mathcal{X}\|^2/N$
    $\mathbf{U}^{(n)} \leftarrow$ leading R_n eigenvectors of $\mathbf{S}^{(n)}$
TTM $\mathcal{Y} \leftarrow \mathcal{Y} \times_n \mathbf{U}^{(n)\mathsf{T}}$
  end for
  $\mathcal{G} \leftarrow \mathcal{Y}$
  return $(\mathcal{G}, \{\mathbf{U}^{(n)}\})$
end procedure

Unfolded Tensor Distribution

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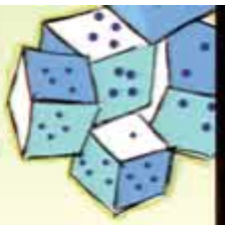


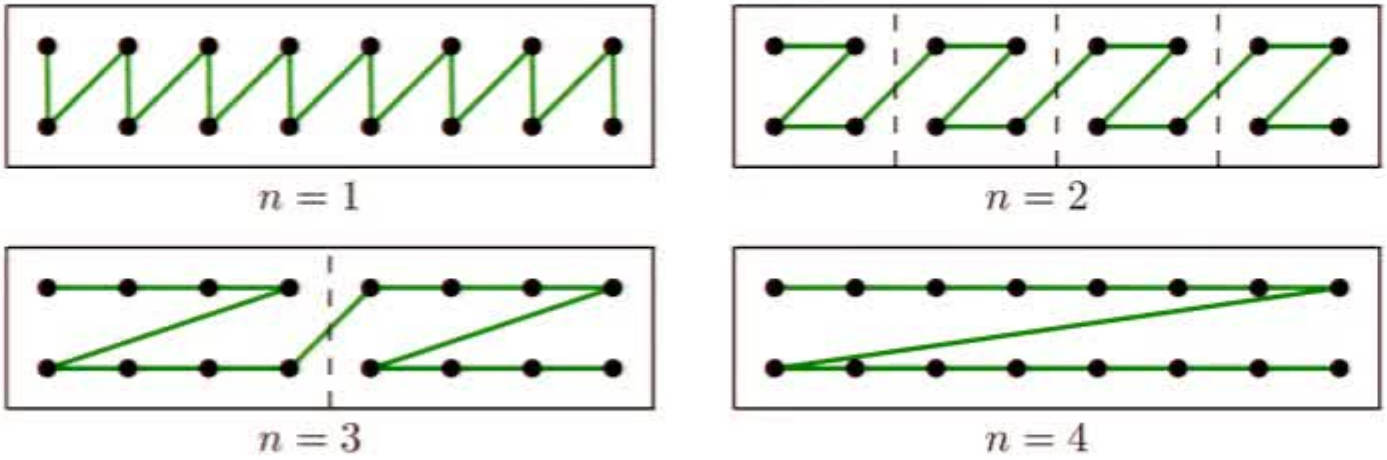
Global Tensor Size: $J_1 \times J_2 \times \cdots \times J_N, \quad J = \prod J_n, \quad \hat{J}_n = J/J_n$

Processor Grid Size: $P_1 \times P_2 \times \cdots \times P_N, \quad P = \prod P_n, \quad \hat{P}_n = P/P_n$

Global Unfolded Tensor: $J_n \times \hat{J}_n$

Processor Grid: $P_n \times \hat{P}_n$

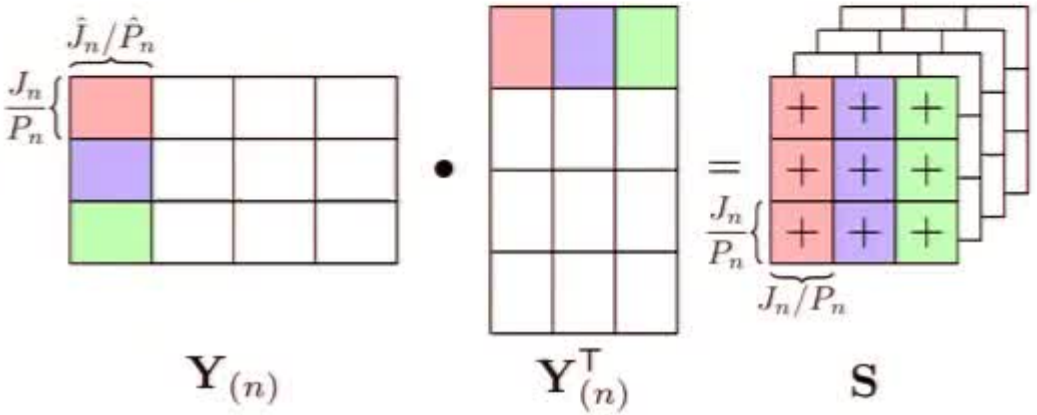
Local Layout: 2 x 2 x 2 x 2



Parallel Gram

$$\mathbf{S} = \mathbf{Y}_{(n)}\mathbf{Y}_{(n)}^{\mathsf{T}}$$

procedure GRAM($\mathcal{Y}$,n)
  myProcID $\leftarrow (p_1, p_2, \ldots, p_N)$
  myProcCol $\leftarrow (p_1, \ldots, p_{n-1}, *, p_{n+1}, \ldots, p_N)$
  myProcRow $\leftarrow (*, \ldots, *, p_k, *, \ldots, *)$
  $\mathbf{V}^{[p_n]} \leftarrow \bar{\mathbf{Y}}_{(n)}\bar{\mathbf{Y}}_{(n)}^{\mathsf{T}}$
  for $i = 1$ to $P_n - 1$ **do**
    $j \leftarrow (p_n - i) \mod P_n$
    $k \leftarrow (p_n + i) \mod P_n$
    Send $\bar{\mathcal{Y}}$ to process $(p_1, \ldots, p_{n-1}, j, \ldots, p_N)$
    Receive $\mathcal{W}$ from process $(p_1, \ldots, p_{n-1}, k, \ldots, p_N)$
    $\mathbf{V}^{[k]} \leftarrow \bar{\mathbf{Y}}_{(n)}\mathbf{W}_{(n)}^{\mathsf{T}}$
  end for
  $\bar{\mathbf{S}}$ = All-Reduce($\mathbf{V}$, myProcRow)
  return $\bar{\mathbf{S}}$
end procedure



$$C_{\text{GRAM}} = \gamma 2J_nJ/P + 2(P_n - 1)(\alpha + \beta J/P) + 2\alpha \log \hat{P}_n + 2\beta(\hat{P}_n - 1)J_n^2/P$$

$$M_{\text{GRAM}} = J/P + J/P + J_n^2/P_n + J_n^2/P_n$$

Application Results: Compression versus Accuracy

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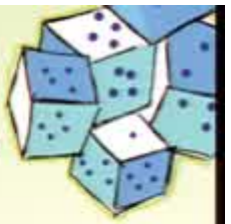
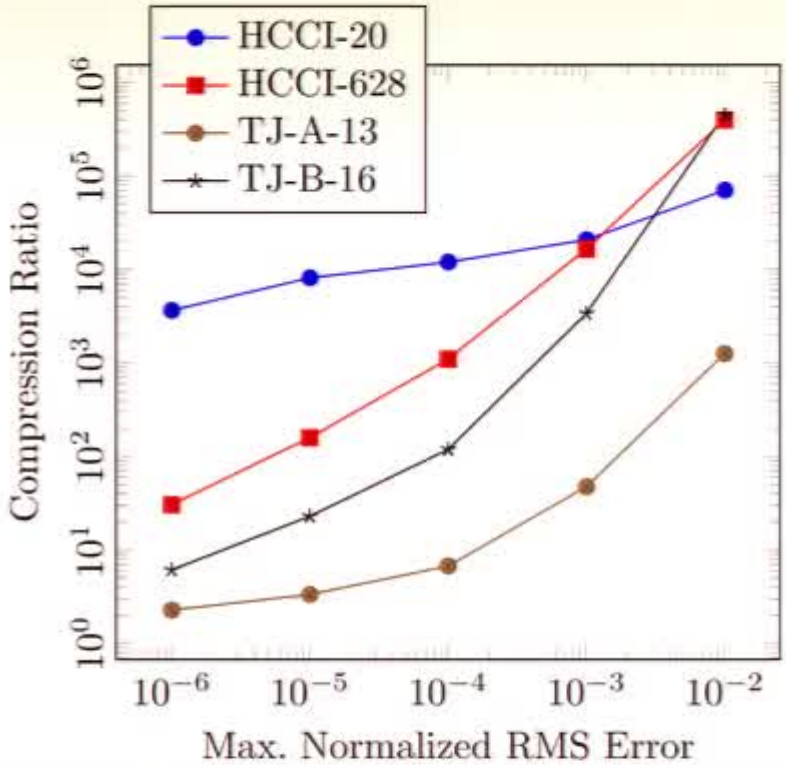


Ranks depend on error:

$$\|\mathcal{X} - \hat{\mathcal{X}}\| \leq \sqrt{\sum_{n=1}^{N} \left(\sum_{i=R_n+1}^{I_n} \lambda_i(\mathbf{S}^{(n)}) \right)} \leq \epsilon \|\mathcal{X}\|$$

Compression ratio:

$$C = \prod_{k=1}^{N} I_n \Big/ \left(\prod_{k=1}^{N} R_n + \sum_{k=1}^{N} I_n R_n \right).$$



Simulation of an autoignitive premixture of air and ethanol in Homogeneous Charge Compression Ignition

HCCI-628: 672 x 672 x 33 x 628, 72 GB

Temporally-evolving planar slot jet flame with DME (dimethyl ether) as the fuel

TJ-A-13: 300 x 500 x 240 x 35 x 13, 122 GB

TJ-B-16: 460 x 700 x 360 x 35 x 16, 512 GB

Thanks to Hemanth Kolla and Ankit Bhagatwala for combustion application data, from Sandia's S3D direct numerical simulation code

$\epsilon = 10^{-5}$

Dataset	Reduced Size	Max. Elem. Error	Comp. Ratio
HCCI-1	(16, 16, 4, 1)	3.6e-5	573
HCCI-20	(20, 18, 6, 5)	2.0e-4	7083
HCCI-628	(192, 183, 16, 104)	1.2e-3	139
TJ-A-1	(257, 139, 186, 20, 1)	1.7e-3	9
TJ-A-13	(300, 209, 240, 25, 13)	3.2e-3	3

Sample Results for one Species in HCCI: Error is Negligible

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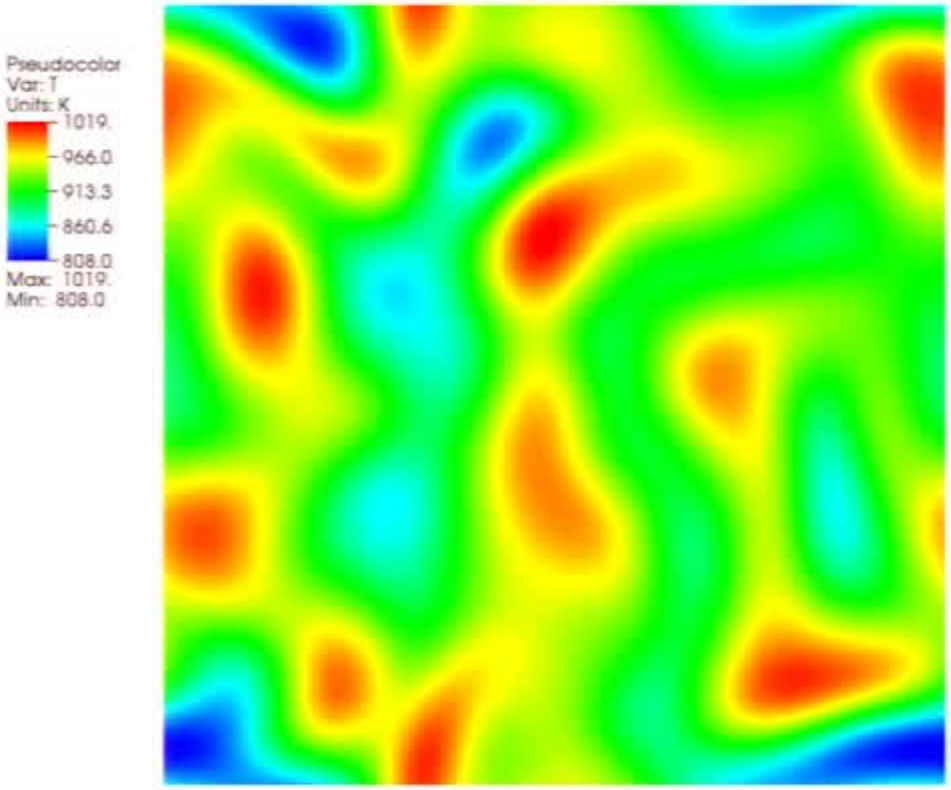
Compression: 586

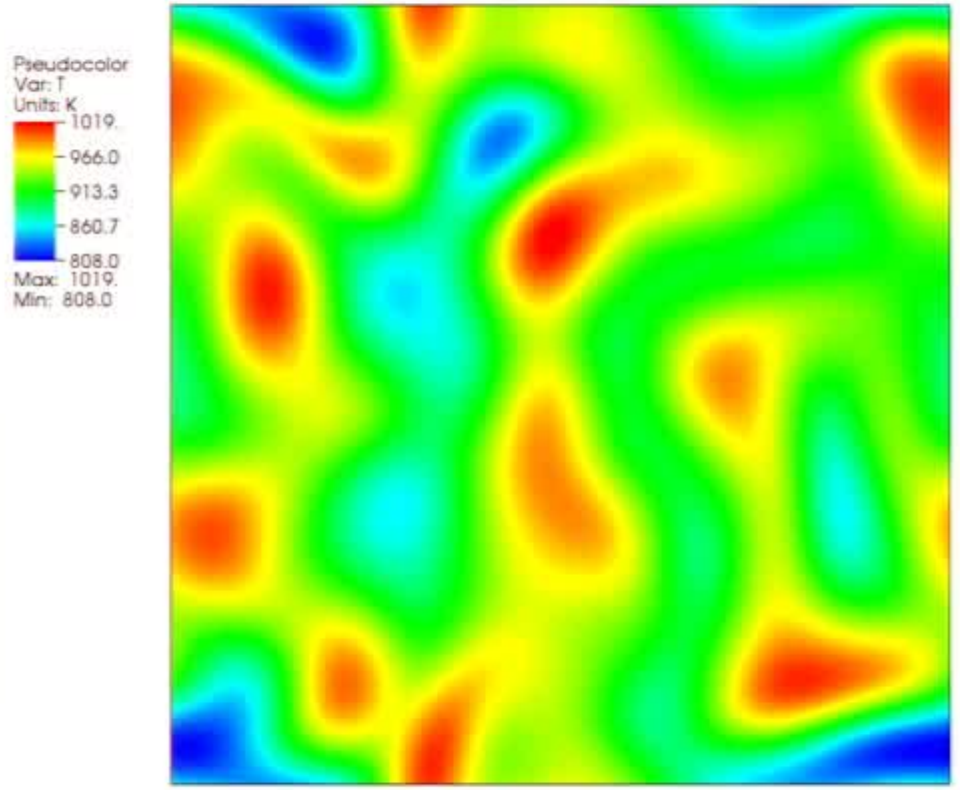
Original $\mathcal{X}$

672 x 672 x 33 x 8



Recovered $\hat{\mathcal{X}}$

48 x 48 x 20 x 3



910MB $\Rightarrow$ 1.5MB

$$\frac{||\mathcal{X} - \hat{\mathcal{X}}||}{||\mathcal{X}||} = 3.08 \times 10^{-8}$$

Sample Results for "Derived" Quantity: Error is Negligible

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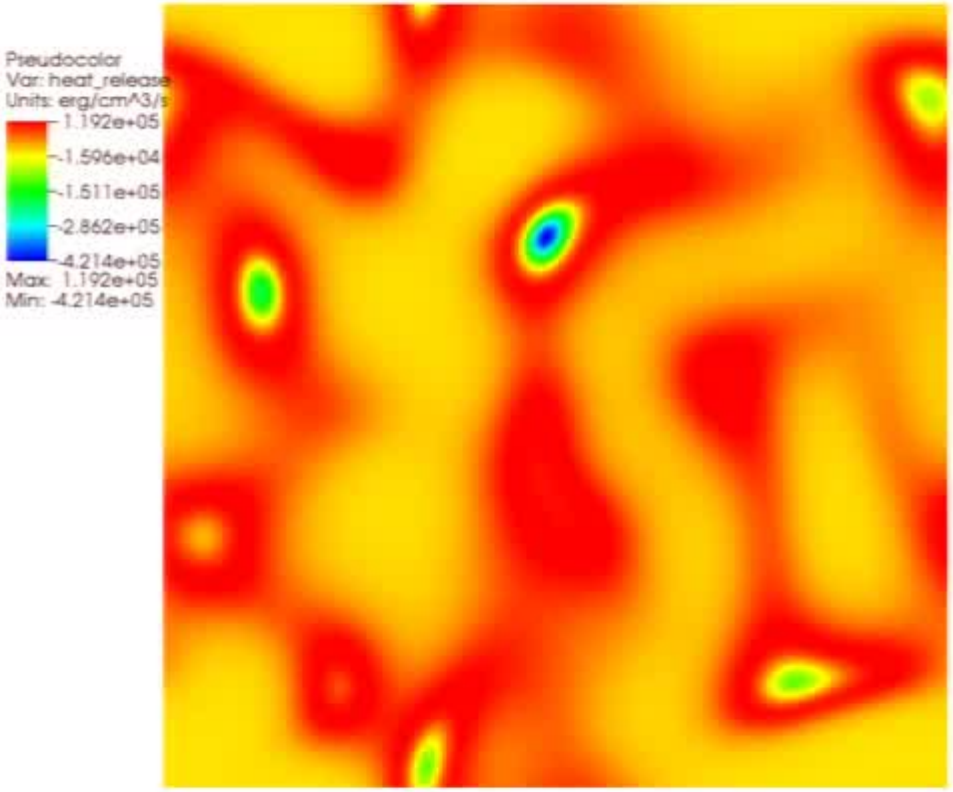
Compression: 586

Original $\mathcal{X}$

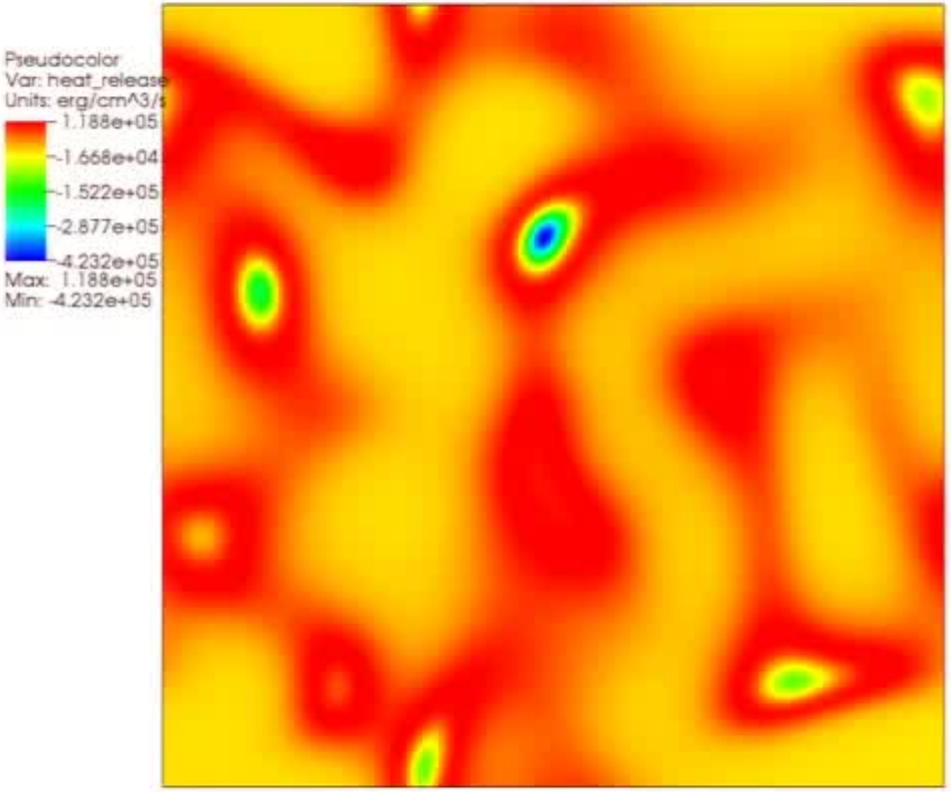
672 x 672 x 33 x 8



910MB ⇒ 1.5MB

Recovered $\hat{\mathcal{X}}$

48 x 48 x 20 x 3



$$\frac{||\mathcal{X} - \hat{\mathcal{X}}||}{||\mathcal{X}||} = 3.08 \times 10^{-8}$$

Sample Results for one Species in 3D HCCI: Error is Negligible

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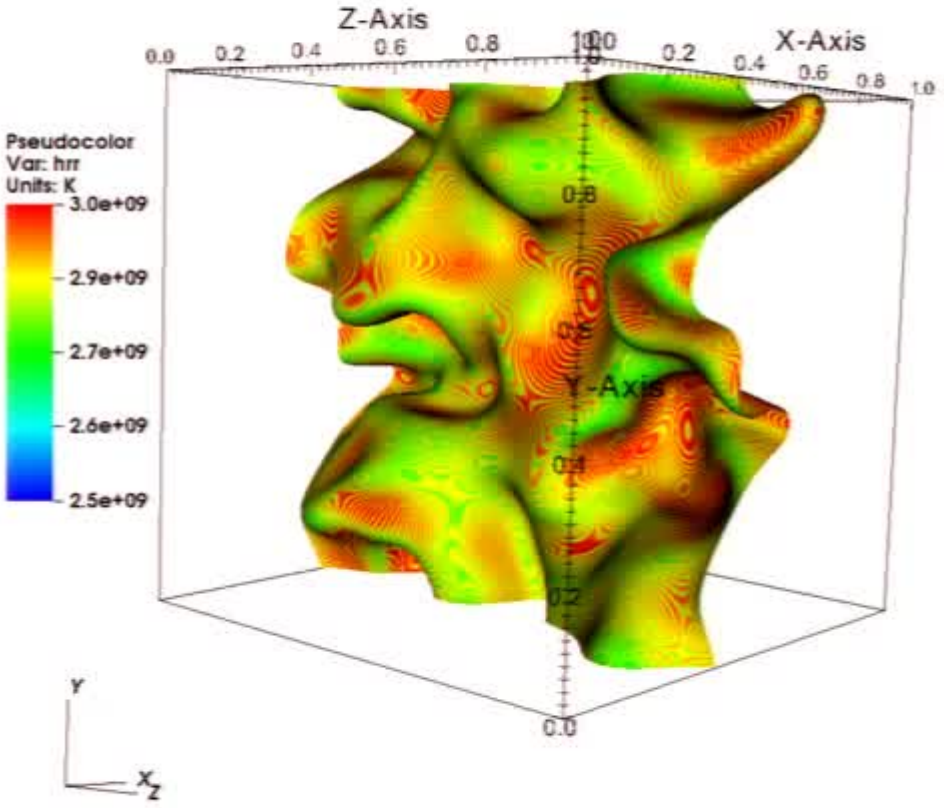
Original $\mathcal{X}$

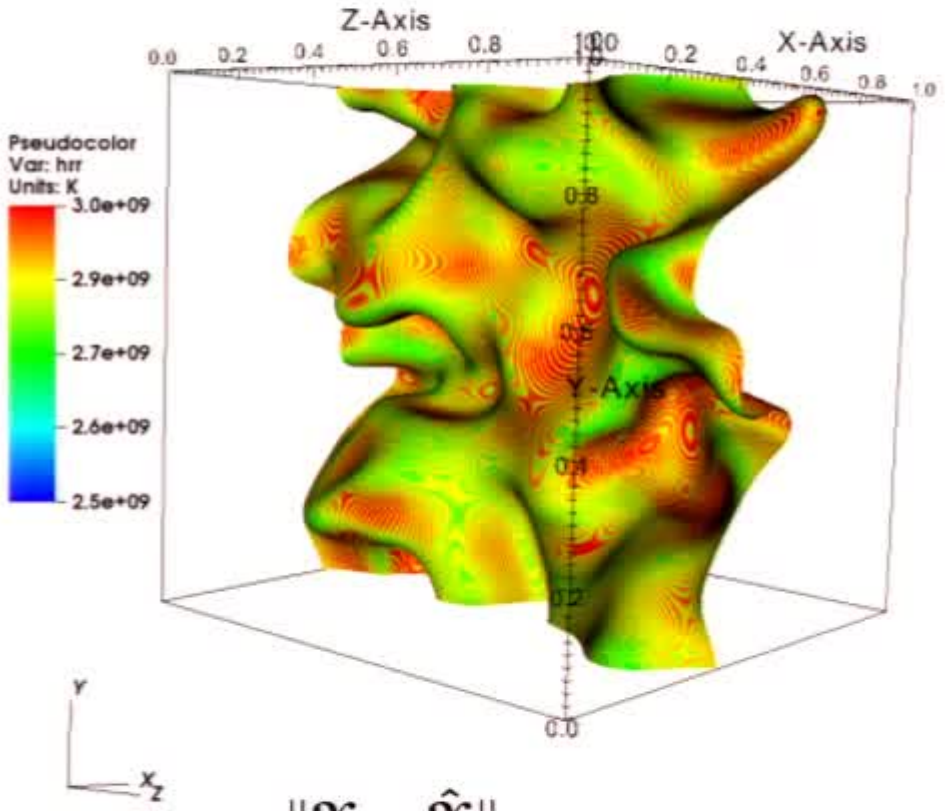
500 x 500 x 500 x 11 x 5

Compression: 1000

Recovered $\hat{\mathcal{X}}$

50 x 50 x 50 x 11 x 5





52 GB ⇒ 52 MB

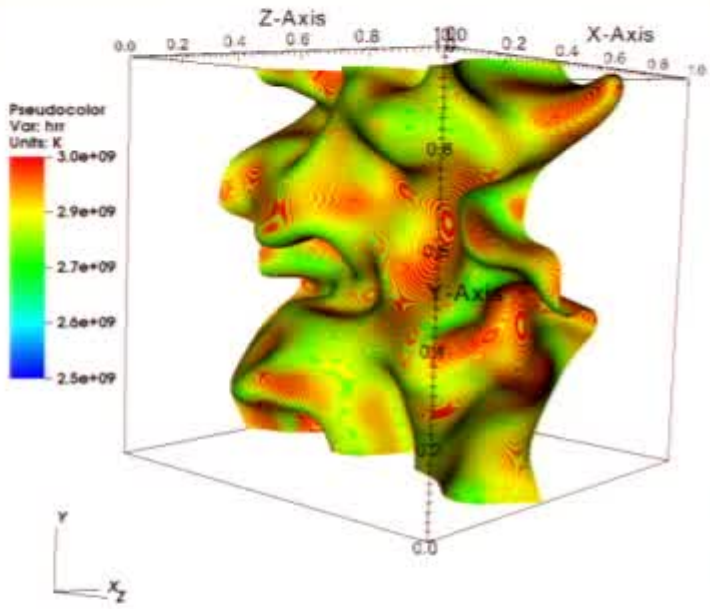
$$\frac{\|\mathcal{X} - \hat{\mathcal{X}}\|}{\|\mathcal{X}\|} = 3.3 \times 10^{-9}$$

Partial Reconstruction

Reconstruction requires as much space as the original data!

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

$I_1 \times I_2 \times I_3 \times I_4 \times I_5$



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

$$\bar{\mathcal{X}} = \mathcal{G} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{U}^{(3)} \times_4 \underbrace{\mathbf{U}^{(4)}\mathbf{e}_k}_{\text{Pick out } k\text{th species}} \times_5 \underbrace{\mathbf{U}^{(5)}\mathbf{e}_l}_{\text{Pick out } l\text{th time}}$$

$I_1 \times I_2 \times I_3 \times 1 \times 1$

Parameter Choices: Processor Grid Configuration & Mode Order

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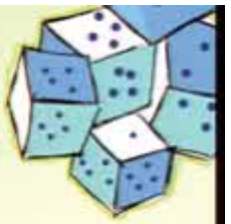
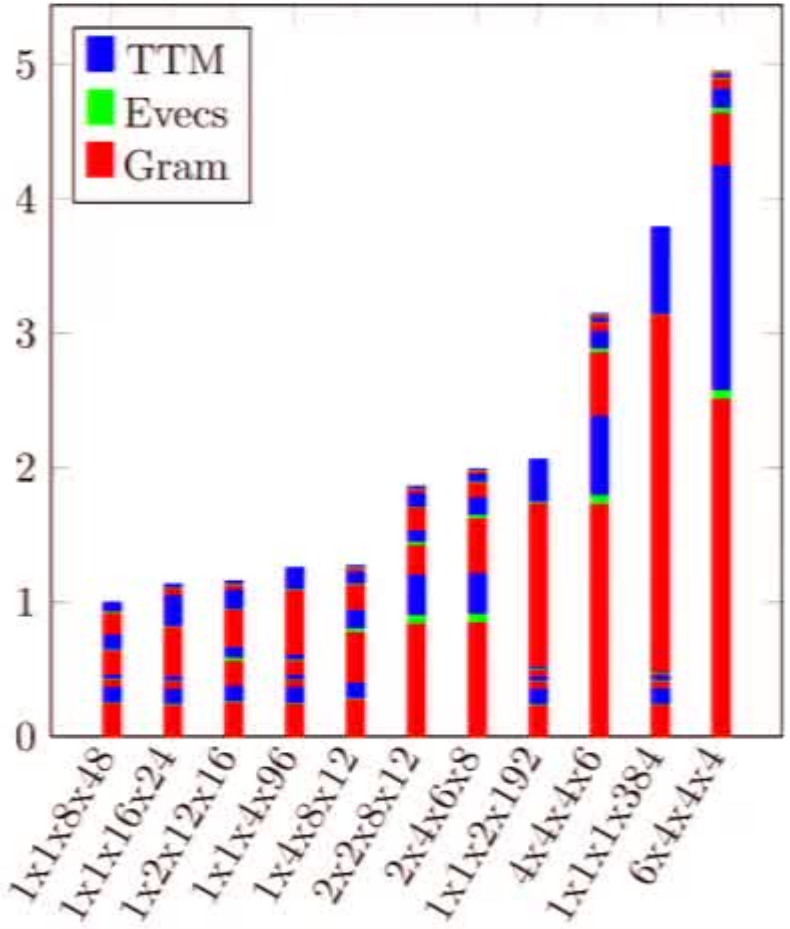


Processor Grid Configuration

I: 384 x 384 x 384 x 384

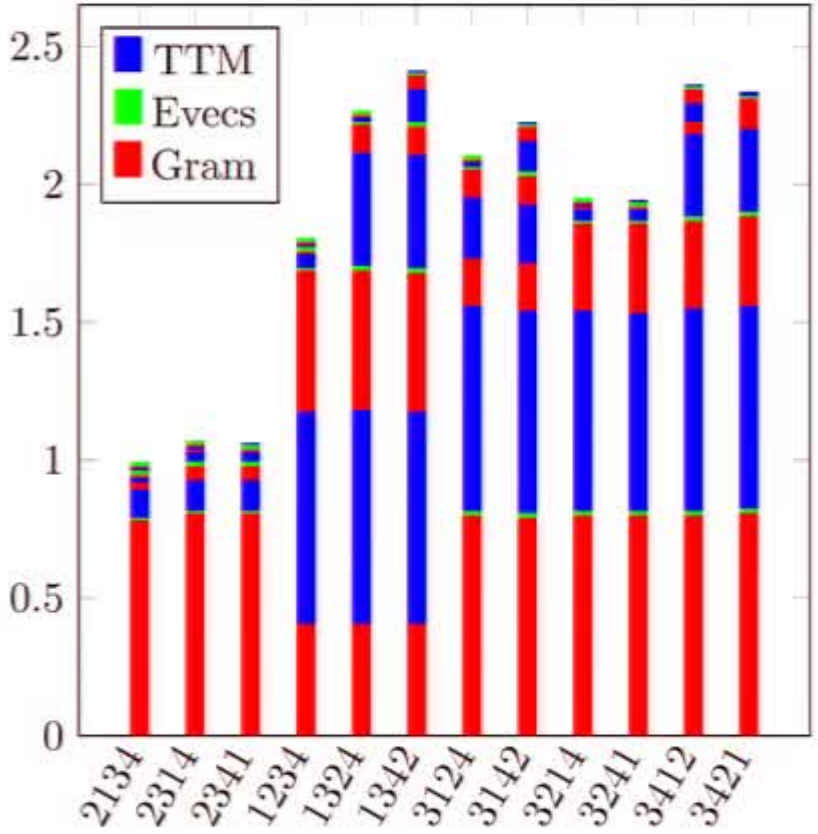
R: 96 x 96 x 96 x 96



Mode Order

I: 25 x 250 x 250 x 250

R: 10 x 10 x 100 x 100



Strong & Weak Scaling

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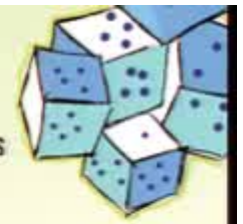


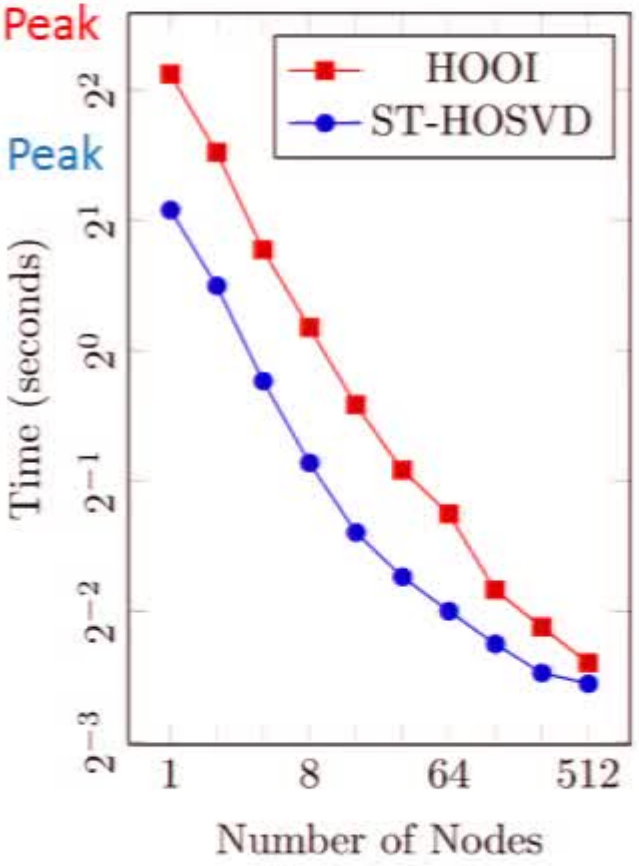
Strong Scaling with 24 x 2^k processors

I: 500 x 300 x 240 x 35

R: 42 x 115 x 81 x 19

40% Peak

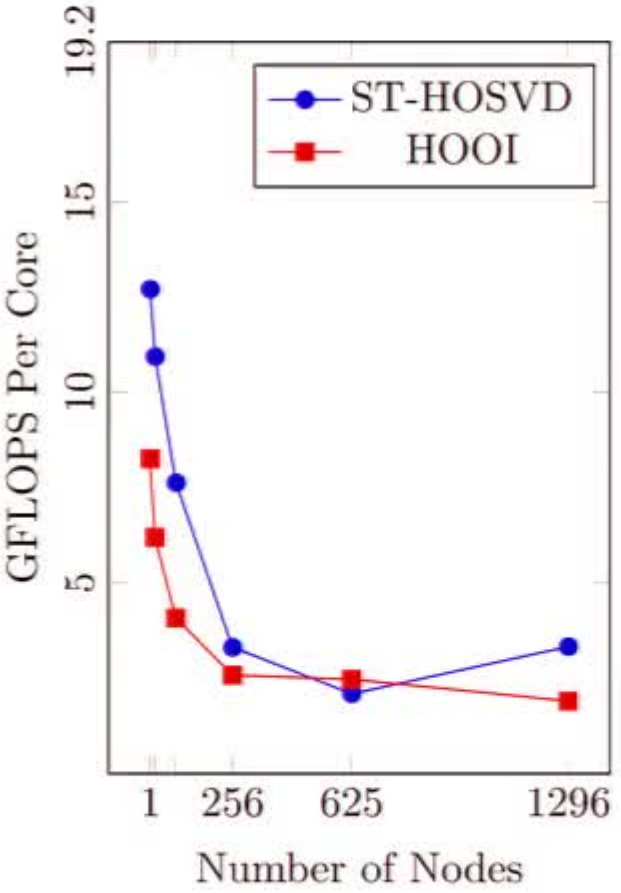
83% Peak



Weak Scaling with 24 x k^4 processors

I: $200k$ x $200k$ x $200k$ x $200k$

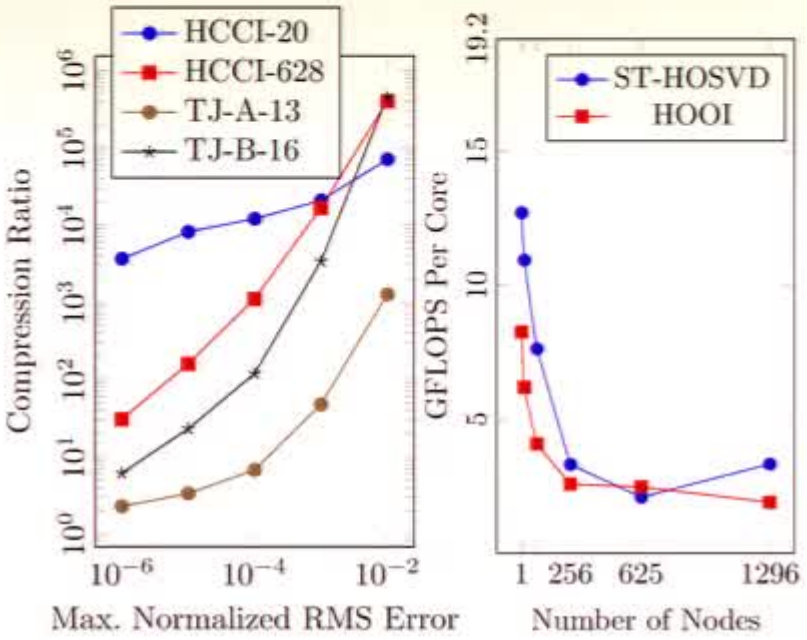
R: $20k$ x $20k$ x $20k$ x $20k$



70 secs
15 TB

Parallel Tucker Compression

- First-ever implementation of distributed-memory parallel Tucker decomposition
  - Avoids unnecessary data permutations
- Up to 10^5 compression on real-world data with minimal loss in accuracy
- Scales well – achieving 17% of peak on 1000s of processors
- Future work
  - Detailed application studies
  - Use QR instead of Gram



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W. Austin, G. Ballard, and T. G. Kolda, ***Parallel Tensor Compression for Large-Scale Scientific Data***, arXiv:1510.06689, October 2015, submitted for publication

In Memory of... Carla Martin

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