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A Distributed-Memory Generalized Sparse Tensor Decomposition

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Motivation: decomposition of large-scale tensors

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- Generalized canonical polyadic (GCP) tensor decomposition
  - D. Hong, T. Kolda, J. Duersch, *SIAM Review,* 2019
  - Finds low-rank approximation of sparse tensors
  - Uses general loss function to better represent variety of tensor data
- Implementations available
  - TensorToolbox (Bader and Kolda) – Matlab
  - GenTen (Phipps and Kolda) – multicore CPU and GPU (via Kokkos)
- Very large tensors can exceed available memory in single-node systems
- SIAM CSE19: Scalable, distributed-memory, MPI-based implementation of CP-ALS using the Trilinos solver framework
- Today: Distributed memory, MPI-based implementation of GCP building from Trilinos/CP-ALS implementation

Canonical Polyadic (CP) Tensor Decomposition

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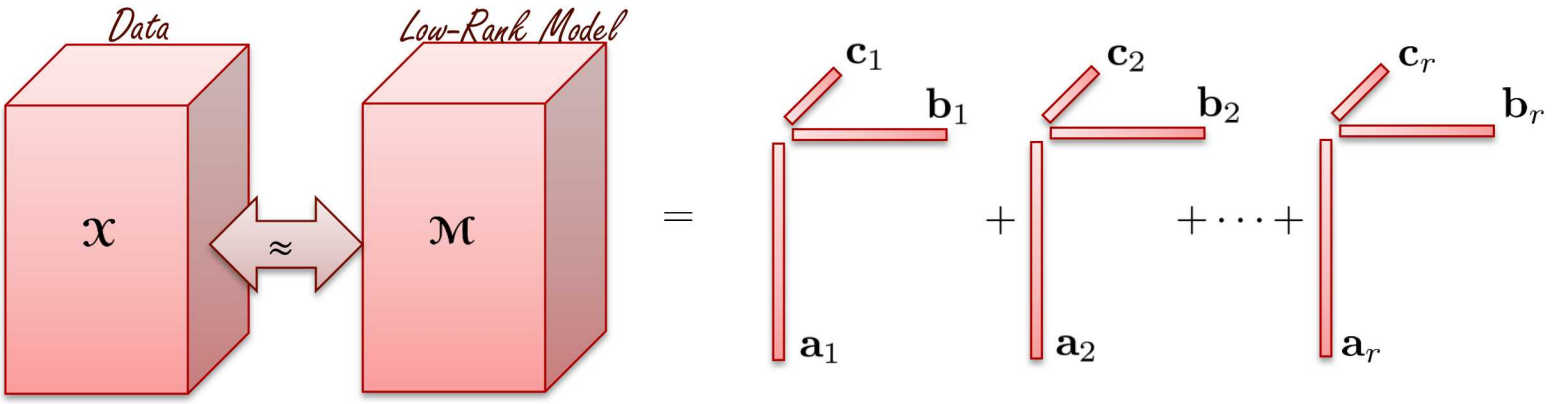
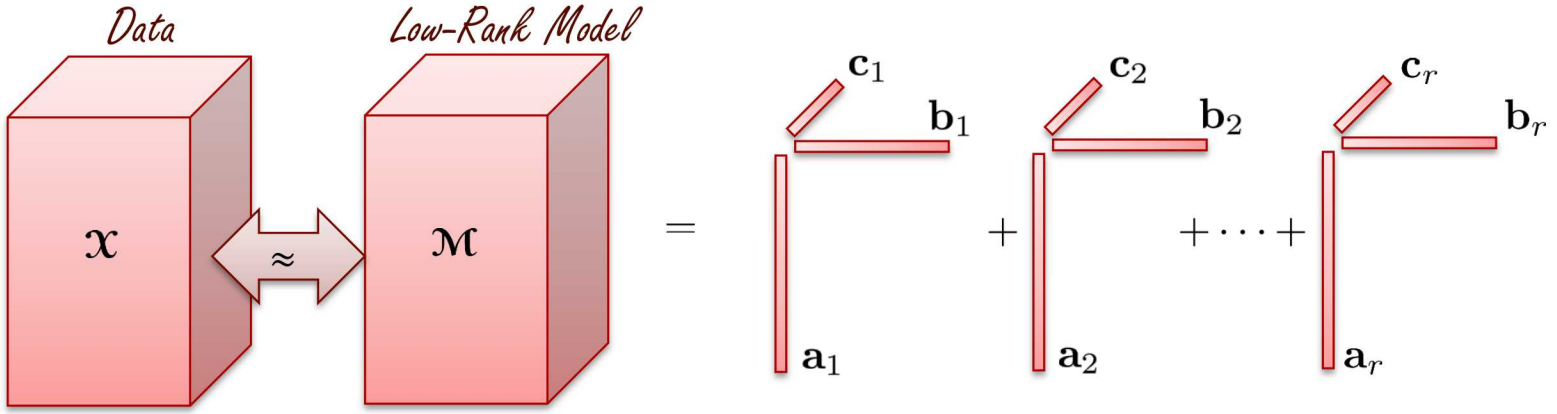
- CANDECOMP / PARAFAC (CP) decomposition
- F. Hitchcock (1927); J.D. Carroll & J-J Chang (1970); R. Harshman (1970)
- Seek low-rank approximation of tensor data



$$\underbrace{\mathcal{X} \approx \mathcal{M}}_{m \times n \times p} = \sum_{\alpha=1}^{r} \mathbf{a}_\alpha \circ \mathbf{b}_\alpha \circ \mathbf{c}_\alpha = [\![\underbrace{\mathbf{A}}_{m \times r}, \overbrace{\mathbf{B}}^{n \times r}, \underbrace{\mathbf{C}}_{p \times r}]\!]$$

Find CP decomposition by solving optimization problem

- Generalized CP (GCP) decomposition (Hong, Kolda, Duersch, 2018) takes user-defined loss function $f(x_{ijk}, m_{ijk})$



$$\mathcal{X} \approx \mathcal{M} = \sum_{\alpha=1}^{r} \mathbf{a}_\alpha \circ \mathbf{b}_\alpha \circ \mathbf{c}_\alpha = [\![\mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$$

$f(x, m)$ provided by user

Optimization Problem: $\min \|\mathcal{X} - \mathcal{M}\|^2 \equiv \sum_i \sum_j \sum_k f(x_{ijk}, m_{ijk})$

Generalized loss functions represent variety of tensor data

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- For example, CP-ALS (alternating least squares) uses Normal loss function; good for Gaussian data:

Optimization Problem: $\min \|\mathcal{X} - \mathcal{M}\|^2 \equiv \sum_i \sum_j \sum_k (x_{ijk} - m_{ijk})^2$

- Other loss functions better represent other types of data:
  - Binary data
  - Count data
  - Non-negative data

Previous work: Distributed-memory CP-ALS using Trilinos

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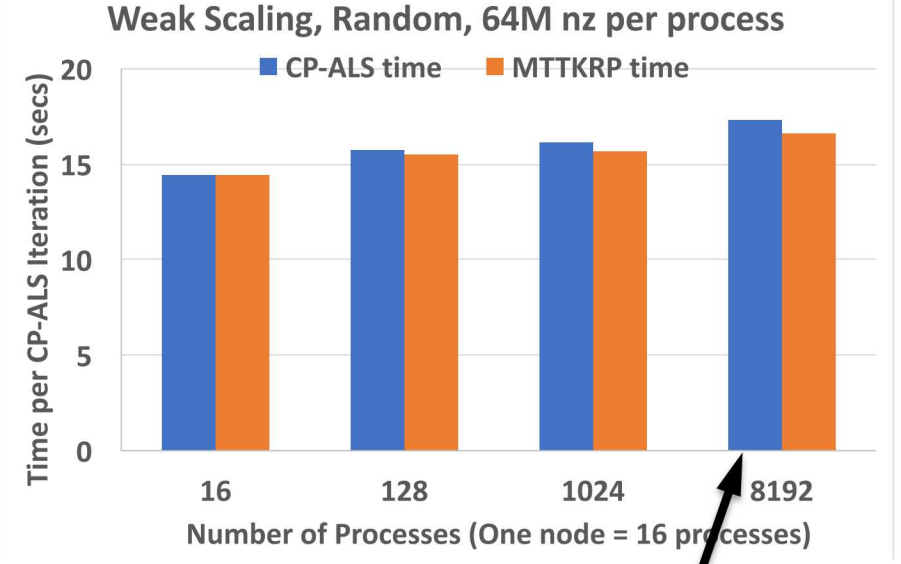
- Trilinos Solver Framework: Software for scientific applications with MPI+X parallelism
  - Linear algebra; linear, nonlinear, eigen solvers; discretization; meshing; load balancing; optimization
  - Built on Kokkos for on-node performance portability
- Tpetra parallel matrix, vector, communication classes
  - MultiVectors: dense storage, norms, etc. for factor matrices
  - Maps: parallel distribution of tensor and factor matrix
  - Import/Export: communication of factor matrix entries



***12.6 Terabyte** tensor on 8192 MPI processes (524 B nonzeros)*

MTTKRP uses Trilinos' SpMV communication pattern

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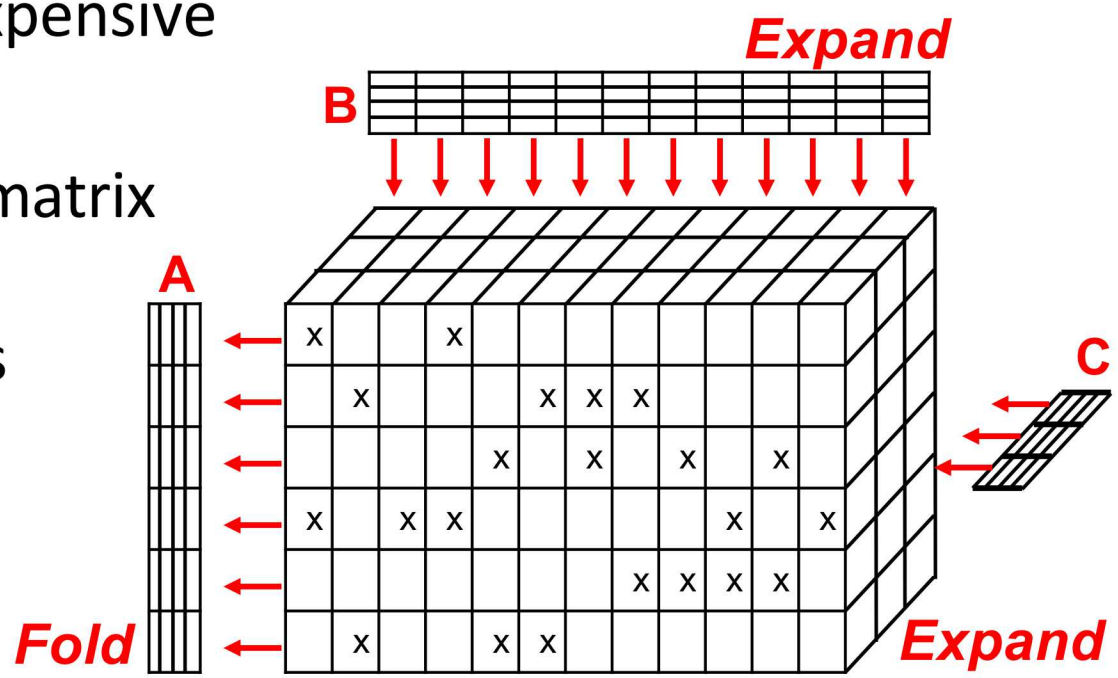
$$\mathbf{X}_{(1)}(\mathbf{C} \odot \mathbf{B}) \Rightarrow \sum_{ijk} x_{ijk}\, b_{jr}\, c_{kr}, r = 1, \ldots, R$$

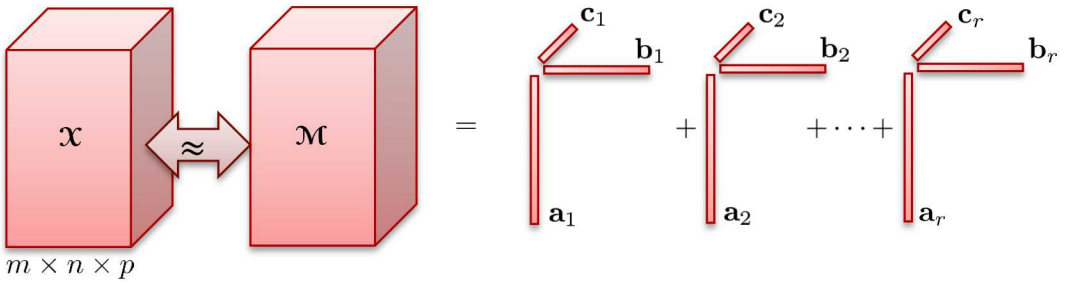
For each local tensor nonzero x_{ijk} …

…use R entries of factor matrices B and C to compute R contributions to MTTKRP

- Matricized Tensor Times Khatri-Rao Product (MTTKRP) is most expensive part of CP-ALS computation
- Expand: Sends input factor matrix entries to processors with corresponding tensor entries
- Fold: accumulates local contributions into output factor matrix



MTTKRP is key kernel of GCP direct optimization



Goal is to minimize: $F(\mathbf{A},\mathbf{B},\mathbf{C}) \equiv \sum_{ijk} f(x,m)$

Repeat until converged…

$$[\mathbf{A},\mathbf{B},\mathbf{C}] \leftarrow [\mathbf{A},\mathbf{B},\mathbf{C}] - \alpha[\frac{\partial F}{\partial \mathbf{A}}, \frac{\partial F}{\partial \mathbf{B}}, \frac{\partial F}{\partial \mathbf{C}}]$$

Gradients

$$\frac{\partial F}{\partial \mathbf{A}} = f'(\mathbf{X}_{(1)}, \mathbf{M}_{(1)})(\mathbf{C} \odot \mathbf{B})$$

$$\frac{\partial F}{\partial \mathbf{B}} = f'(\mathbf{X}_{(2)}, \mathbf{M}_{(2)})(\mathbf{C} \odot \mathbf{A})$$

$$\frac{\partial F}{\partial \mathbf{C}} = f'(\mathbf{X}_{(3)}, \mathbf{M}_{(3)})(\mathbf{B} \odot \mathbf{A})$$

Gradient tensor f' is the derivative of loss function f with respect to m, evaluated elementwise

MTTKRP using gradient tensor

Solve GCP Optimization via Stochastic Gradient Descent

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- Sample ***both*** tensor nonzeros and tensor zeros
  - Stratified sampling (sampling without replacement)
    Ensure an entry (nonzero or zero) is sampled at most once per iteration
  - Semi-stratified sampling (sampling with replacement)
    Allow duplicate samples of an entry
- Sampling to compute loss for convergence test
  - Sample <10% of tensor entries

$$\hat{F} \equiv \sum_{x_{ijk} \neq 0} \frac{\eta}{p} f\left(x_{ijk}, m_{ijk}\right) + \sum_{x_{ijk}=0} \frac{\zeta}{q} f\left(x_{ijk}, m_{ijk}\right)$$

  - η/p = number of nonzeros in tensor / number of nonzero samples
  - ζ/q = number of zeros in tensor / number of zero samples
- Sampling to compute stochastic gradients
  - Sample <1% of tensor entries in each iteration

Processor bounding boxes simplify sampling in distributed memory

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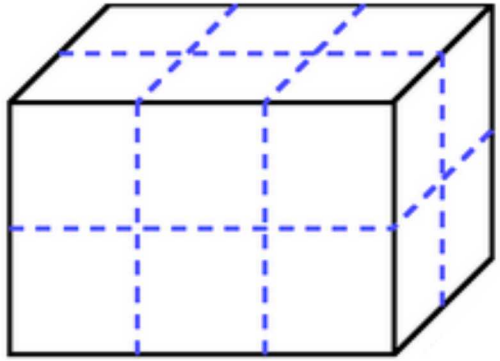

p x q x r = 3 x 2 x 2 processor layout

- Assume block-based distribution of tensor
  - Bounding boxes do not overlap
  - Bounding boxes cover entire index space of tensor
  - Each processor knows bounding box of its block
- Processors sample within their bounding boxes
  - Enables efficient searching for duplicate samples in stratified sampling
  - Maintains aligned communication pattern for expand/fold
- For *s* samples globally, select *s/np* indices on each of *np* processors (for load balance)
- Sample nonzeros proportionally to number of nonzeros in box (to prevent skew)
- Note: CP-ALS does not require bounding boxes; can use arbitrary tensor distributions

Uniform boxes prevent skew in sampling

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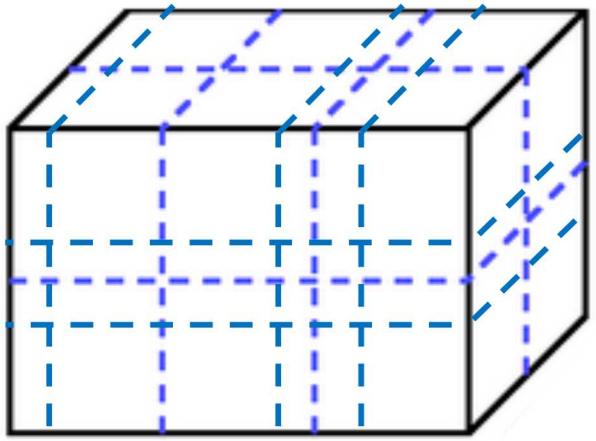
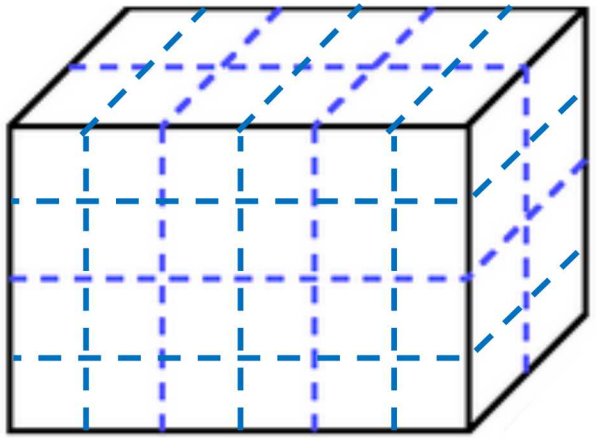
- Medium grain distribution:
  - Each box has equal number of nonzeros, unequal number of zeros – great for CP-ALS
  - For uniform sampling, sample equal number of nonzeros in each box
  - For load balance, sample equal number of zeros in each box
  - Can over/under sample zeros in each box



Tensor distributions with p x q x r = 6 x 4 x 2 processor layout

- Uniform boxes:
  - Equal number of indices (nonzero + zero) per box
  - Within a box, sample proportionally to number of nonzeros and zeros in the box



Error computation is adapted to bounding boxes

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$$\hat{F} \equiv \sum_{x_{ijk} \neq 0} \frac{\eta}{p} f\left(x_{ijk}, m_{ijk}\right) + \sum_{x_{ijk}=0} \frac{\zeta}{q} f\left(x_{ijk}, m_{ijk}\right)$$

- η/p = # of nonzeros in tensor / # of nonzero samples
- ζ/q = # of zeros in tensor / # of zero samples

- Replace η, ζ, p, q with on-processor values from bounding boxes
  - Local number of nonzeros, zeros, samples
- If zeros and nonzeros are perfectly balanced across processors, ratios don't change from global values
- If imbalanced, account for density of sampling within a processor

Solve GCP Optimization via Stochastic Gradient Descent (ADAM)

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"ADAM: a method for stochastic optimization," D. Kingma & J. Ba, ICLR 2015

STOCHASTIC GRADIENT DESCENT

Randomly initialize $\mathbf{A}, \mathbf{B}, \mathbf{C}$

Estimate loss $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

While not converged

$F_{old} = \hat{F}$

For τ iterations

Compute stochastic gradients $\mathbf{G}_A = \frac{\partial F}{\partial A}$; $\mathbf{G}_B$; $\mathbf{G}_C$

Compute $\mathbf{A}, \mathbf{B}, \mathbf{C}$ using $\mathbf{G}_A, \mathbf{G}_B, \mathbf{G}_C$ and step size

Estimate loss function $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

If $\hat{F} > Fold$, backup and reduce step size

Return $\mathbf{A}, \mathbf{B}, \mathbf{C}$

Solve GCP Optimization via Stochastic Gradient Descent (ADAM)

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Estimate loss function $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

If $\hat{F} > Fold$, backup and reduce step size

Return $\mathbf{A}, \mathbf{B}, \mathbf{C}$

Use fixed stratified sampling to estimate loss (<10% of tensor indices); construct sampled tensor only once

Solve GCP Optimization via Stochastic Gradient Descent (ADAM)

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STOCHASTIC GRADIENT DESCENT

Randomly initialize $\mathbf{A}, \mathbf{B}, \mathbf{C}$

Estimate loss $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

While not converged

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For τ iterations

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Estimate loss function $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

If $\hat{F} > Fold$, backup and reduce step size

Return $\mathbf{A}, \mathbf{B}, \mathbf{C}$

COMPUTE STOCHASTIC GRADIENTS

Sample nonzero and zero indices $\{ijk\}$

Construct gradient tensor $\boldsymbol{\mathcal{Y}}$ with

$y_{ijk} = \frac{\partial f}{\partial m}(x_{ijk}, m_{ijk})$ for samples $\{ijk\}$

$$\mathbf{G}_A = \frac{\partial F}{\partial A} = \text{MTTKRP}(\boldsymbol{\mathcal{Y}}, \boldsymbol{B}, \boldsymbol{C})$$

$$\mathbf{G}_B = \frac{\partial F}{\partial B} = \text{MTTKRP}(\boldsymbol{\mathcal{Y}}, \boldsymbol{C}, \boldsymbol{A})$$

$$\mathbf{G}_C = \frac{\partial F}{\partial C} = \text{MTTKRP}(\boldsymbol{\mathcal{Y}}, \boldsymbol{A}, \boldsymbol{B})$$

Solve GCP Optimization via Stochastic Gradient Descent (ADAM)

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Use stratified or semi-stratified sampling (<1% of tensor indices)

STOCHASTIC GRADIENT DESCENT

Randomly initialize $\mathbf{A}, \mathbf{B}, \mathbf{C}$

Estimate loss $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

While not converged

$F_{old} = \hat{F}$

For τ iterations

Compute stochastic gradients $\mathbf{G}_A = \frac{\partial F}{\partial A}$; $\mathbf{G}_B$; $\mathbf{G}_C$

Compute $\mathbf{A}, \mathbf{B}, \mathbf{C}$ using $\mathbf{G}_A, \mathbf{G}_B, \mathbf{G}_C$ and step size

Estimate loss function $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

If $\hat{F} > Fold$, backup and reduce step size

Return $\mathbf{A}, \mathbf{B}, \mathbf{C}$

COMPUTE STOCHASTIC GRADIENTS

Sample nonzero and zero indices $\{ijk\}$

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$$y_{ijk} = \frac{\partial f}{\partial m}(x_{ijk}, m_{ijk}) \text{ for samples } \{ijk\}$$

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$$\mathbf{G}_B = \frac{\partial F}{\partial B} = \text{MTTKRP}(\mathcal{Y}, \boldsymbol{C}, \boldsymbol{A})$$

$$\mathbf{G}_C = \frac{\partial F}{\partial C} = \text{MTTKRP}(\mathcal{Y}, \boldsymbol{A}, \boldsymbol{B})$$

Distributed memory GCP Optimization via Stochastic Gradient Descent

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Sample within bounding boxes;
no communication needed

Communicate (expand)
A, B, C entries corresponding
to samples in $\mathcal{Y}$

Communicate (fold) in MTTKRP

COMPUTE STOCHASTIC GRADIENTS

Sample nonzero and zero indices $\{ijk\}$

Construct gradient tensor $\boldsymbol{\mathcal{Y}}$ with

$$y_{ijk} = \frac{\partial f}{\partial m}(x_{ijk}, m_{ijk}) \text{ for samples } \{ijk\}$$

$$\mathbf{G}_A = \frac{\partial F}{\partial A} = \text{MTTKRP}(\boldsymbol{\mathcal{Y}}, \boldsymbol{B}, \boldsymbol{C})$$

$$\mathbf{G}_B = \frac{\partial F}{\partial B} = \text{MTTKRP}(\boldsymbol{\mathcal{Y}}, \boldsymbol{C}, \boldsymbol{A})$$

$$\mathbf{G}_C = \frac{\partial F}{\partial C} = \text{MTTKRP}(\boldsymbol{\mathcal{Y}}, \boldsymbol{A}, \boldsymbol{B})$$

Majority of communication is in computing stochastic gradients

Distributed memory GCP Optimization via Stochastic Gradient Descent

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STOCHASTIC GRADIENT DESCENT

Randomly initialize $\mathbf{A}, \mathbf{B}, \mathbf{C}$

Estimate loss $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

While not converged

$F_{old} = \hat{F}$

For τ iterations

Compute stochastic gradients $\mathbf{G}_A = \frac{\partial F}{\partial A}$; $\mathbf{G}_B$; $\mathbf{G}_C$

Compute $\mathbf{A}, \mathbf{B}, \mathbf{C}$ using $\mathbf{G}_A, \mathbf{G}_B, \mathbf{G}_C$ and step size

Estimate loss function $\hat{F} = \sum_{\{ijk\}} f(x_{ijk}, m_{ijk})$

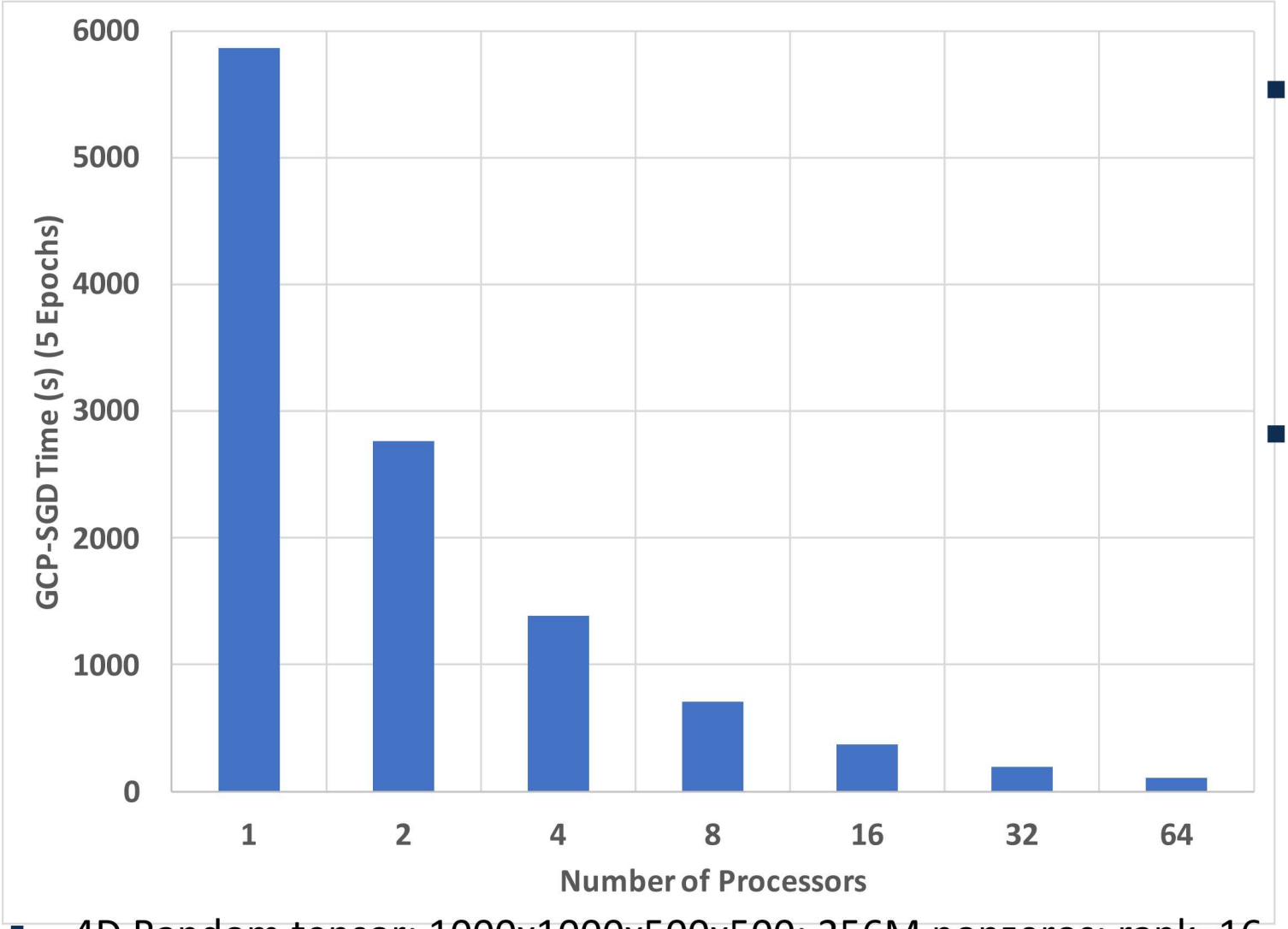
If $\hat{F} > Fold$, backup and reduce step size

Return $\mathbf{A}, \mathbf{B}, \mathbf{C}$

Communicate (expand) A, B, C for fixed samples; Allreduce

Distribute G_A, G_B, G_C in same way as A, B, C; *no communication needed here*

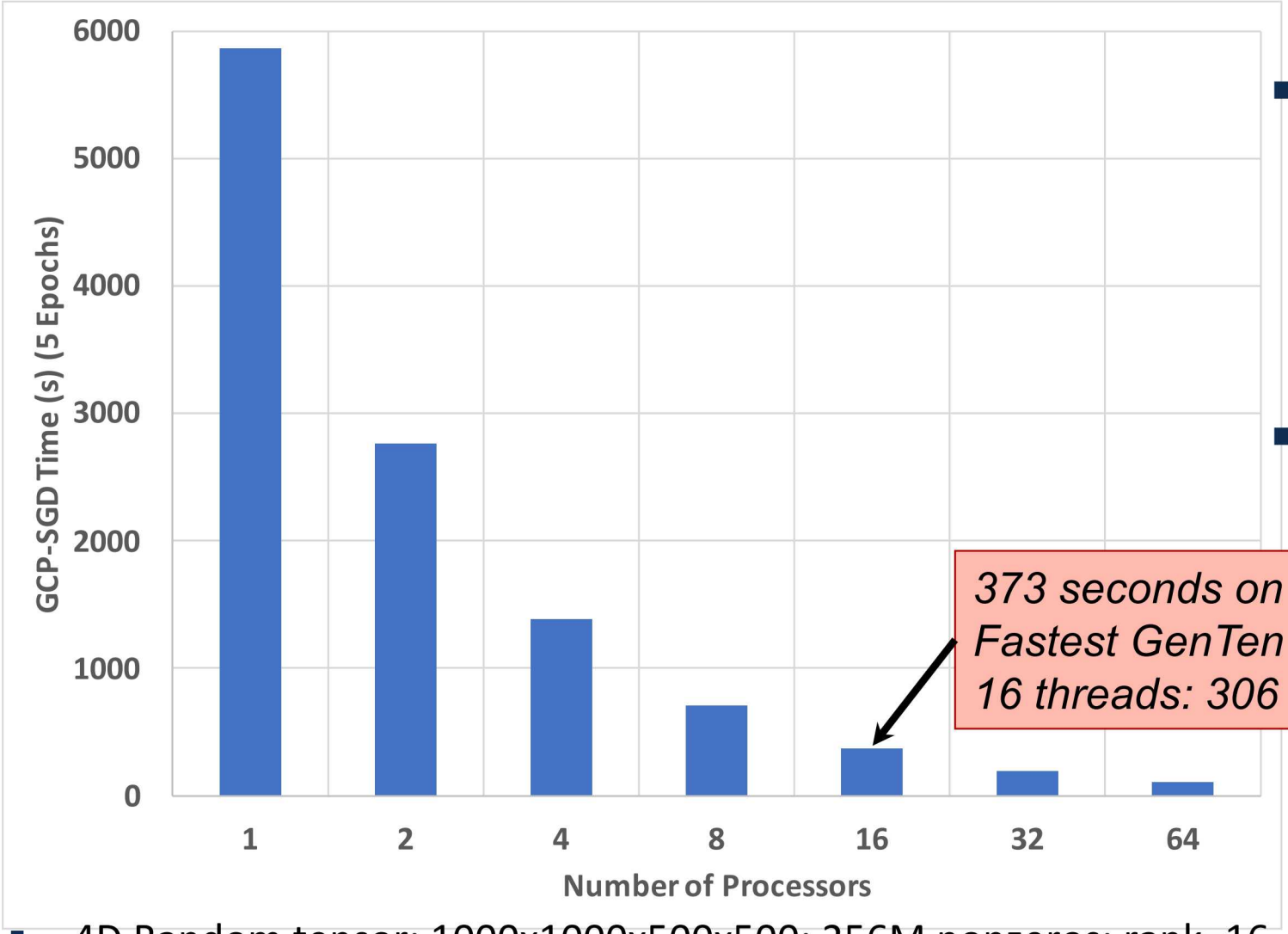
Best-case strong scaling is good



- Best case: perfect balance, alignment; small factor matrices
- 52.7x speedup on 64 processors

- 4D Random tensor: 1000x1000x500x500; 256M nonzeros; rank=16
- 5M samples in Fixed tensor; 1.5M samples in Stoc Grad tensor
- SkyBridge cluster (2.6 GHz Intel Sandy Bridge with Infiniband)

Best-case strong scaling is good



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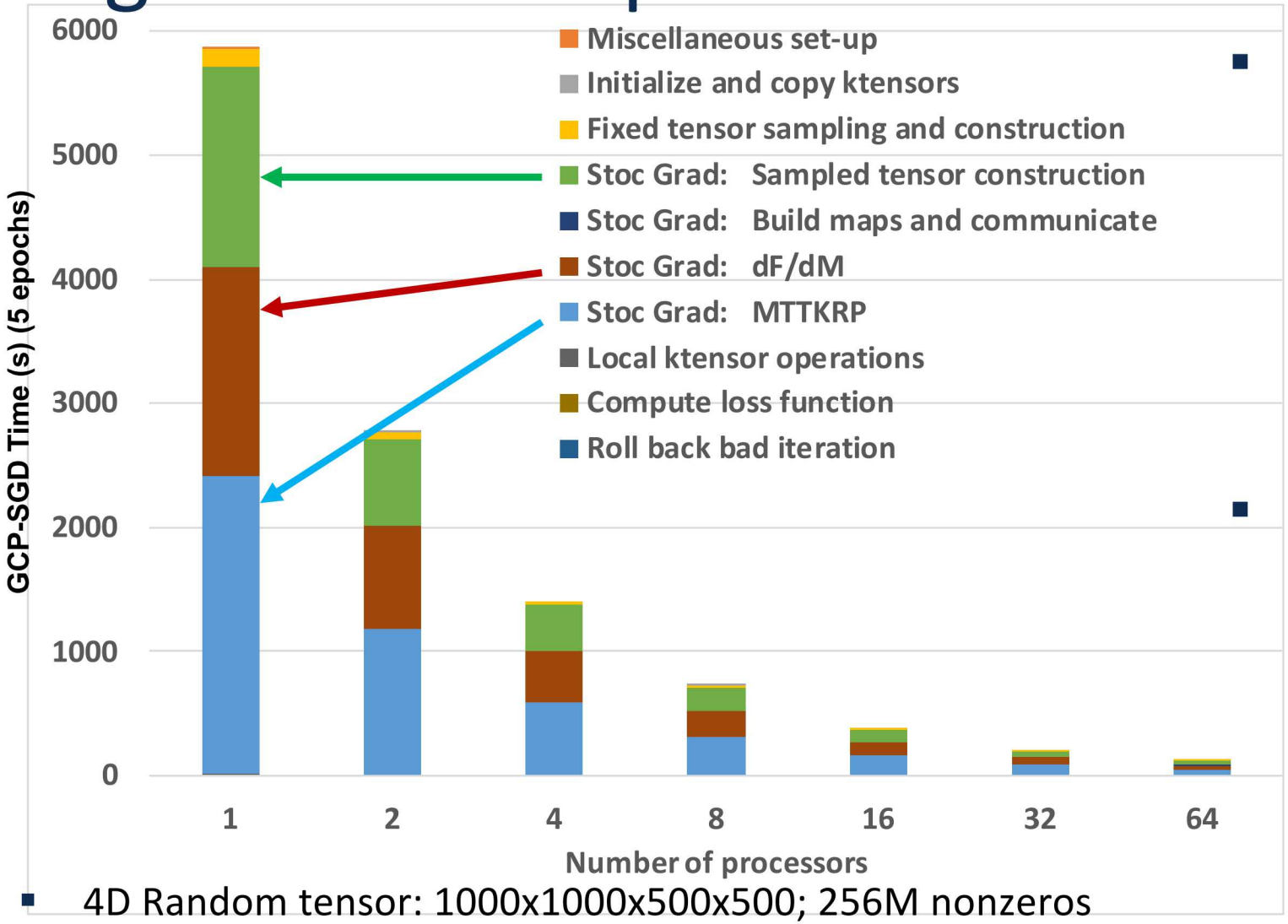
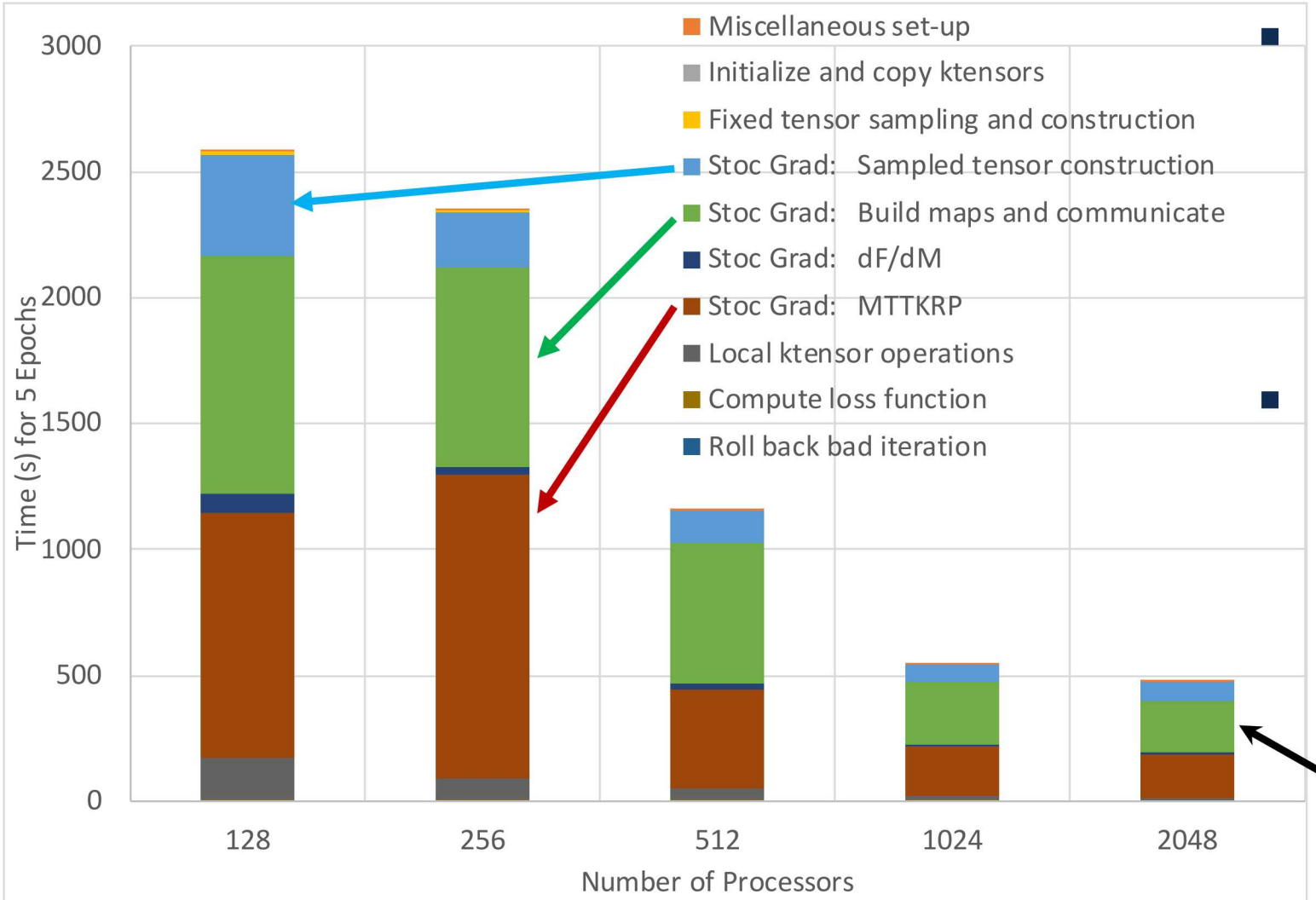
Most time spent in stochastic gradient computation



- Many kernels scaling well
  - Sampled tensor construction
  - MTTKRP
  - Derivative computation
- Costs for building maps and communicating are small but grow with number of processors

- 4D Random tensor: 1000x1000x500x500; 256M nonzeros
- 5M samples in Fixed tensor; 1.5M samples in Stoc Grad tensor
- SkyBridge cluster (2.6 GHz Intel Sandy Bridge with Infiniband)

More variability seen in real tensors

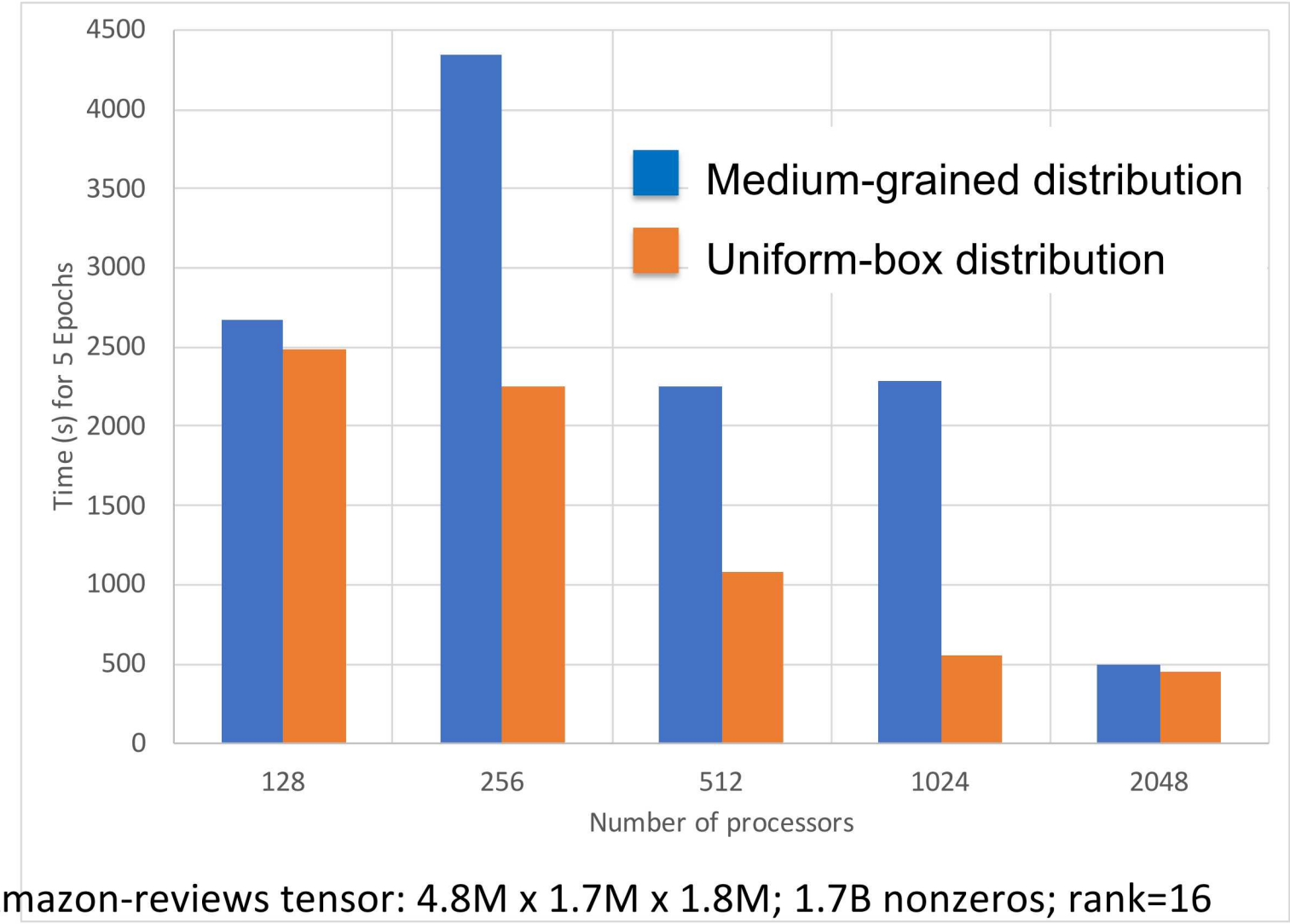


- Benefit from more processors; tensor too large for single shared-memory node
- Building maps, communicating are more expensive

With 2048 procs, ~4K samples/proc

- 3D Amazon-reviews tensor: 4.8M x 1.7M x 1.8M; 1.7B nonzeros; rank=16
- 83M samples in Fixed tensor; 8.3M samples in Stoc Grad tensor
- SkyBridge cluster (2.6 GHz Intel Sandy Bridge with Infiniband)

Uniform-box distribution benefits performance



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Conclusions and Future Work

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- Distributed memory implementation of GCP-SGD is scalable and feasible for decomposition of very large tensors
  - Bounding box of processor's indices aids in efficient distributed-memory sampling
  - Trilinos' Tpetra data structures manage communication and factor matrix operations
  - Small sample sizes challenge strong scaling
- Next step: integration of on-node parallelism
  - Use capabilities in GenTen (Phipps, Kolda), such as on-node MTTKRP
- MPI-based code soon to be released on gitlab.com: GentenMPI