Scalable Tensor Algorithms for Modern Computing Systems

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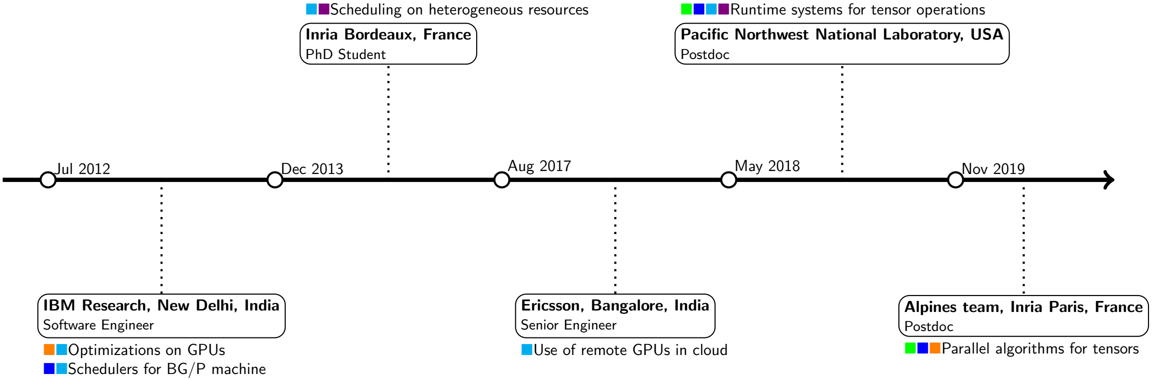
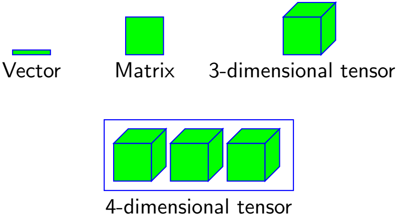
Resume

Interests: Tensors, Scalable Algorithms, Scheduling, Runtime Systems, Performance Optimizations



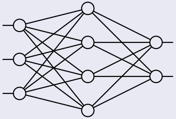
Tensors are used in Several Domains

- **Neuroscience**: Neuron × Time × Trial
- **Transportation**: Pickup × Dropoff × Time
- **Media**: User x Movie x Time
- **Ecommerce**: User x Product x Time
- **Cyber-Traffic**: IP x IP x Port x Time
- **Social-Network**: Person x Person x Time x Interaction-Type



High Dimensional Tensors

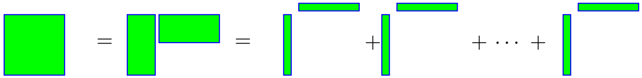
- **Neural Network**:



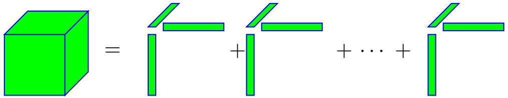
- **Molecular Simulation**: To represent wave functions
- **Quantum Computing**: To represent qubit states

Tensor Computations

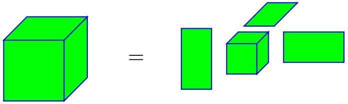
- Memory and computation requirements are exponential in the number of dimensions
  - A simulation involving just 100 spatial orbitals manipulates a huge tensor with 4^{100} elements
- People work with low dimensional structure (decomposition) of the tensors
  - A tensor is represented with smaller objects
  - Improves memory and computation requirements
- Most tensor decompositions rely on Singular Value Decomposition (SVD) of matrices
  - SVD represents a matrix as the sum of rank one matrices, $A = U\Sigma V^T = \sum_i \Sigma(i;i) U_i V_i^T$



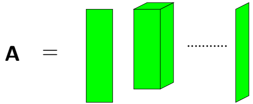
- Canonical decomposition (Also known as Canonical Polyadic or CANDECOMP/PARAFAC)



- Tucker decomposition



- Tensor Train decomposition (equivalently known as Matrix Product States)



Tensor notation: bold letters denote tensors, i.e., $\mathbf{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ is a d-dimensional tensor.

Previous/Ongoing Work

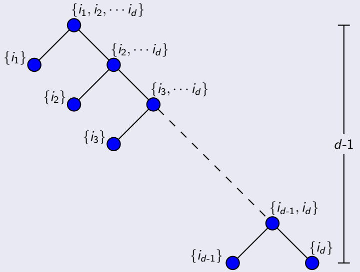
1. Parallel Tensor Train Algorithms

2. Scheduling on Heterogeneous Systems
   - Scheduling of Dense Linear Algebra Kernels
   - Communication Computation Overlap

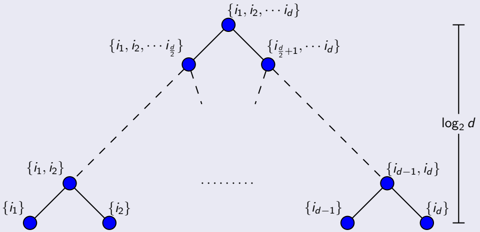
Tensor Train algorithms and Separation of dimensions

- A sequential algorithm to compute Tensor Train decomposition exists [Oseledets, 2011]

Sequential algorithm



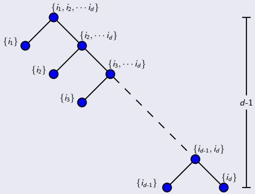
For better parallelization



- Can obtain better parallelism by expressing the operation in a balanced binary tree shape
  - Proposed a parallel algorithm based on this idea (joint work with L. Grigori, Inria Paris)

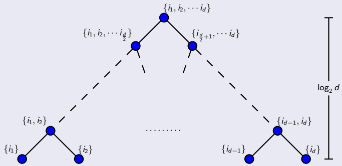
Tensor Train approximation algorithms

Sequential algorithm [Oseledets, 2011]



- Unfolding matrix: matricized representation of the tensor
- Perform truncated SVD of unfolding matrix A, $A = U\Sigma V^T + E_A$
- Work with ΣV^T on the right subtree

Our parallel algorithm



- Perform truncated SVD of unfolding matrix A, $A = U\Sigma V^T + E_A$
- Find diagonal matrices X, Y, and S, such that $\Sigma = XSY$
- Call left (resp. right) subtree with UX (resp. YV^T)

Approach 1: $X = I,\ Y = \Sigma,\ S = I$
Approach 2: $X = Y = \Sigma^{\frac{1}{2}},\ S = I$
Approach 3: $X = Y = \Sigma,\ S = \Sigma^{-1}$

Comparison of our approaches

- A 12-dimensional tensor with 4^{12} elements (generated with a popular low rank function)
- prescribed accuracy $= 10^{-6}$
- Compr: compression ratio, NE: number of elements, AA: approximation accuracy

Metric	Sequential Algo	Parallel Algo		
		Approach 1	Approach 2	Approach 3
Compr	99.993	99.817	99.799	99.993
NE	1212	30632	33772	1212
AA	2.271e-07	3.629e-08	2.820e-08	2.265e-07

SVD is expensive

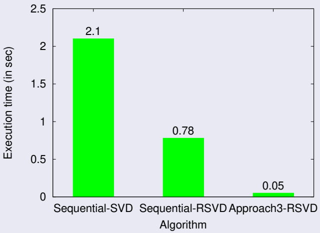
- Good alternatives to SVD: QR factorization with column pivoting (QRCP), randomized SVD (RSVD)

Approach	Rank	Compr	NE	Sequential-AA	Approach3-AA
SVD	5	99.994	992	6.079e-06	6.079e-06
QRCP+SVD				1.016e-05	1.384e-05
RSVD				6.079e-06	6.079e-06
SVD	6	99.992	1376	1.323e-07	1.340e-07
QRCP+SVD				3.555e-07	5.737e-07
RSVD				1.322e-07	1.322e-07

Performance Comparison

Single core performance

- Number of computations for both RSVD algorithms $= \mathcal{O}(n^d)$
- Approach3-SVD is very slow
- Approach3-RSVD is much faster

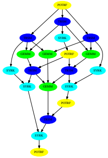


Parallel performance counts along the critical path on P processors

Algorithm	# Computations	Communications	# Messages
Sequential-RSVD	$\mathcal{O}(\frac{n^d}{P})$	$\mathcal{O}(\frac{n^{d-1}}{\sqrt{P}} \log P)$	$\mathcal{O}(d \log P)$
Parallel-RSVD	$\mathcal{O}(\frac{n^d}{P})$	$\mathcal{O}(\frac{n^{\frac{d}{2}}}{\sqrt{P}} \log P)$	$\mathcal{O}(\log d \log P)$

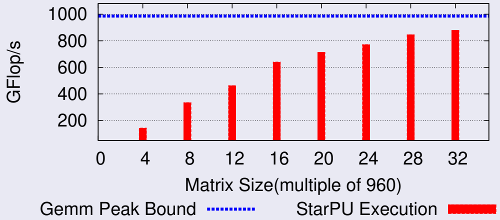
Scheduling on Heterogeneous Systems

- Heterogeneous systems are common in High Performance Computing (HPC) (147 out of 500 in TOP500 list)
- Task based runtimes are a popular approach to exploit these systems



- Task based runtimes: StarPU, OmpSS, Legion, PaRSEC
- Application is represented as a graph of tasks (computations)
- E.g., Cholesky graph for 4×4 tile matrix

StarPU scheduler performance



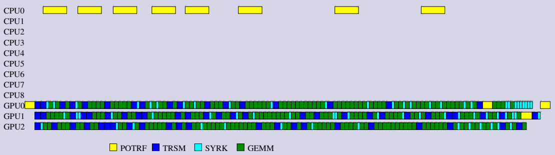
- A platform with 9 CPUs and 3 GPUs
- Scheduler is based on popular heft strategy

- Goal: Enhance performance bounds and propose better scheduling strategies

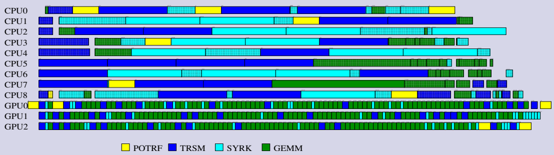
Joint work with E. Agullo, O. Beaumont, L. Eyraud-Dubois, and S. Thibault during my PhD at Inria Bordeaux

Our strategy and Performance comparison

Trace for 12 X 12 tile matrix of Cholesky factorization



StarPU scheduling strategy, performance = 686 GFlop/s

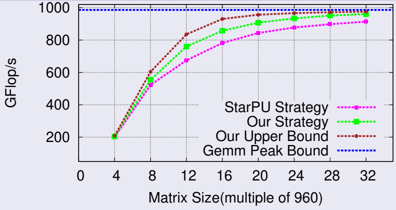


Our strategy, performance = 760 GFlop/s

Theoretical guarantees of our strategy and performance comparison

- Each resource selects the best suited task
- A fast resource restarts the blocking task

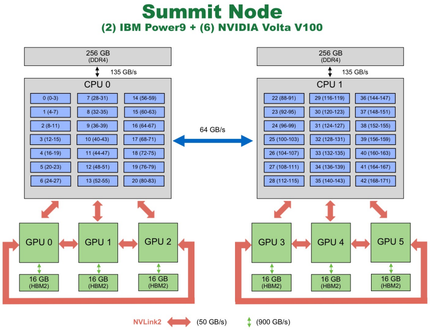
(#CPUs, #GPUs)	For a set of independent tasks: Approximation ratio	For a set of independent tasks: Worst case ex.
(1,1)	$\frac{1+\sqrt{5}}{2}$	$\frac{1+\sqrt{5}}{2}$
(m,n)	$2+\sqrt{2} \approx 3.41$	$2+\frac{2}{\sqrt{3}} \approx 3.15$

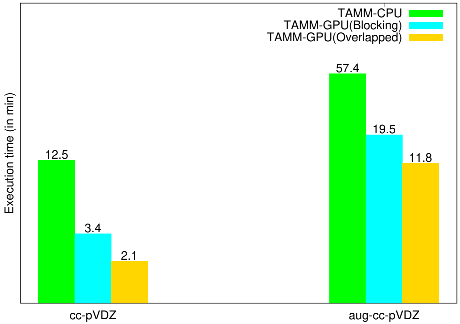


- Our upper bound is obtained by a linear program

Minimizing impact of communications on Summit supercomputer

- Maximizing the overlap of communications and computations
- Implemented proposed approaches in Tensor Algebra for Manybody Methods (TAMM) library
- Molecular chemistry application (CCSD), Ubiqtin molecule, cc-pVDZ (737 basis functions, 220 nodes), aug-cc-pVDZ (1243 basis functions, 256 nodes)





Joint work with S. Krishnamoorthy and M. Zalewski during my postdoc at PNNL, USA

Fig source: `https://www.olcf.ornl.gov`

Project: Scalable Tensor Algorithms for Modern Computing Systems

1. Design of Scalable Communication Optimal Algorithms for Tensors (Main Focus)
2. Extension of Existing Approaches/Algorithms (Short/Mid Term Research Plans)
3. Exploratory Topics (Mid/Long Term Research Plans)

Scalable communication optimal algorithms for tensors

- Analyze existing algorithms
- Determine communication lower bounds
- Propose communication optimal algorithms
- Implement the proposed algorithms

Main focus

Extension of existing approaches

- Strassen's concepts to tensors
- Concepts of hierarchical matrices to tensors
- Separation order of dimensions in tensor train

Short/Mid term plans

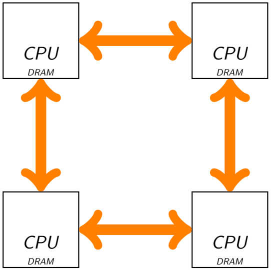
Exploratory topics

- New tensor representations
- Architecture aware algorithms
- Randomization in tensors
- Factorizations of tensors

Mid/Long term plans

Communication and its importance in HPC

- Running time of an algorithm depends on
  - Computations
    - Number of operations * time-per-operation
  - Data movement
    - Volume of communication / Network-bandwidth
    - Number of messages * Network-latency



- Gaps growing exponentially with time (Source: Getting up to speed: The future of supercomputing)

	time-per-operation	Network-bandwidth	Network-latency
Annual improvements	59 %	26 %	15 %

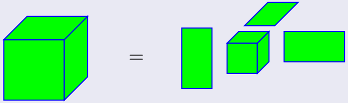
- Avoid communication to save time (and energy)

Scalabale algorithms for popular tensor operations

- Determine the communication lower bounds for tensor decompositions
- Analyse the popular decomposition algorithms and communications performed by them
- Propose new scalable communication optimal algorithms
  - If possible design tiles/tasks based algorithms
- Implement the proposed algorithms
  - Handle performance issues for homogeneous systems
    - Load balancing
    - Memory aware approaches
    - scheduling strategies
- Same for manipulation operations of popular tensor representations
- Extend implementation for heterogeneous systems (start with Nvidia GPUs based heterogeneous systems)
- Create a tensor library

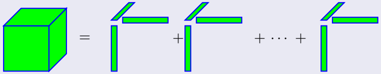
Popular tensor decompositions

Tucker decomposition



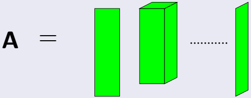
- Determine communication lower bounds for this operation
- Analyse communications performed by state of the art algorithms
- Propose and implement new scalable communication algorithms

Canonical decomposition



- No deterministic algorithm to find the decomposition
- Analyse one iteration of the popular existing algorithms
- Propose and implement scalable algorithms for one iteration

Tensor Train decomposition



- Determine communication lower bounds for this operation
- Analyse communication performed by popular algorithm
- Propose and implement new scalable communication algorithms

Proving communication lower bounds for parallel computations

How people did it for linear algebra operations?

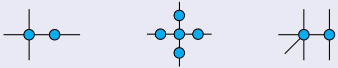
- People obtain results for matrix multiplication operations
- Same lower bound apply to almost all direct linear linear algebra operations using reduction [Ballard et. al., 09] , for instance, bound for LU factorization

$$\begin{pmatrix} I & & -B \\ A & I & \\ & & I \end{pmatrix} = \begin{pmatrix} I & & \\ A & I & \\ & & I \end{pmatrix} \begin{pmatrix} I & & -B \\ & I & AB \\ & & I \end{pmatrix}$$

Approach to compute lower bounds for tensor computations

Notation: Tensors are denoted by solid shapes and number of lines denote the dimensions of the tensors. Connecting two lines implies summation (or contraction) over the connected dimensions.

- Obtain bounds for basic tensor operations: Tensor times matrix (TTM), Multiple tensor times matrix (Multi-TTM), Tensor contraction

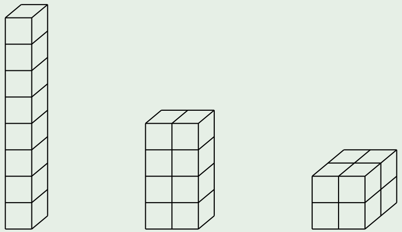


- Express decompositions and manipulations in terms of these basis operations

Communication lower bounds on P processors

- Recently started to work with L. Grigori (Inria Paris, France) and G. Ballard (Wake Forest University, USA)
- Revisited communication lower bounds for matrix multiplications
  - Expressed existing approaches in suitable forms for tensors
  - Lower bounds also instruct arrangement of processors in optimal algorithms
  - Improved the constants in the existing ranges of P (Demmel et.al [IPDPS 2013])

Arrangements of 8 processors



- Plan to continue this collaboration to compute lower bounds for tensor computations

Research Project

1. Design of Scalable Communication Optimal Algorithms for Tensors (Main Focus)
2. Extension of Existing Approaches/Algorithms (Short/Mid Term Research Plans)
3. Exploratory Topics (Mid/Long Term Research Plans)

Strassen's concepts to tensors

Matrix multiplication of $n \times n$ square matrices

- Complexity of traditional matrix multiplication is $\mathcal{O}(n^3)$
- Strassen's matrix multiplication
  - Expressed matrix multiplication operation as a tensor operation
  - Canonical rank of the tensor determines the complexity of the operation
  - Complexity is $\mathcal{O}(n^{2.81})$
- Plan to extend Strassen's concepts to tensor contractions

Contraction of a 3-dimensional tensor with a matrix

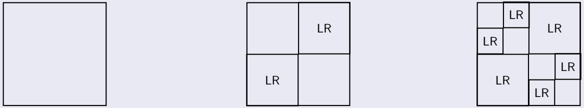
for $i_1 = 1 : n$ **do**
  for $i_2 = 1 : n$ **do**
    for $i_3 = 1 : n$ **do**
      for $j_2 = 1 : n$ **do**
        $\mathbf{G}(i_1, i_2, j_2) = \mathbf{G}(i_1, i_2, j_2) + \mathbf{A}(i_1, i_2, i_3) * B(i_3, j_2)$
      end for
    end for
  end for
end for

- Total $\mathcal{O}(n^4)$ operations
- Apply Strassen's algorithm for each i_1, total $\mathcal{O}(n^{3.81})$ operations
- Expressing as a canonical decomposition of $8 \times 8 \times 4$ tensor can further reduces the number of operations

Hierarchical Matrix concepts to Tensors

Hierarchical Matrices

- Data sparse approximation of non-sparse matrices

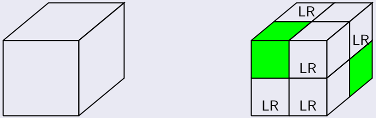


Original Matrix Step 1 Step 2

LR: low rank block

Tensors

- $f(i,j,k) = \frac{1}{|i-j|+|j-k|+|k-i|}$
- Value is small if difference of any pair is large
- Formalize and evaluate this approach for tensors



Original Tensor Step 1

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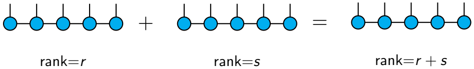
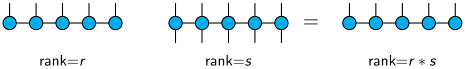
Tensor Representations for High Dimensional Tensors

- Tensor Train is the popular representation to work with high dimensional tensors
- Adding tensors and aplying an operator in this representation

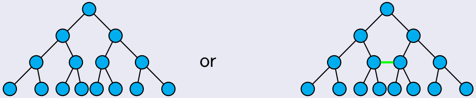




- Requires a truncation process which iterates over cores one by one
- This representation is not much suited to work in parallel

New Tensor Representations

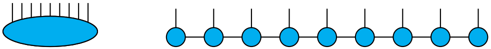
- Look at new representations in tree format – suitable for parallelization



  - Data will be stored at the leaf nodes
  - Interal nodes will help to manipulate tensors in parallel

Randomization in Tensor Computations

- Randomized SVD and UTV factorization are now well established
- Apply randomization to tensors
- Perform factorizations of tensors
  - For example: QR like factorization of a tensor



Integration in the ROMA team

Anne Benoit, Loris Marchal, Gregoire Pichon, Yves Robert, Bora Ucar, and Frederic Vivien

Team

- Parallel algorithms
- Scheduling strategies
- Memory aware algorithms
- Sparse tensor computations
- Low rank compression algorithms

Expertise of the team

Scalable communication optimal algorithms for tensors

- Analyze existing algorithms
- Determine communication lower bounds
- Propose communication optimal algorithms
- Implement the proposed algorithms

Main focus

Extension of existing approaches

- Strassen's concepts to tensors
- Concepts of hierarchical matrices to tensors
- Separation order of dimensions in tensor train

Short/Mid term plans

Exploratory topics

- New tensor representations
- Architecture aware algorithms
- Randomization in tensors
- Factorizations of tensors

Mid/Long term plans

Bringing additional skills in the team

- High dimensional dense tensor computations
- Communication lower bounds for linear algebra computations
- Scalable approaches for large HPC systems
- Use of tensors in quantum and molecular simulations