

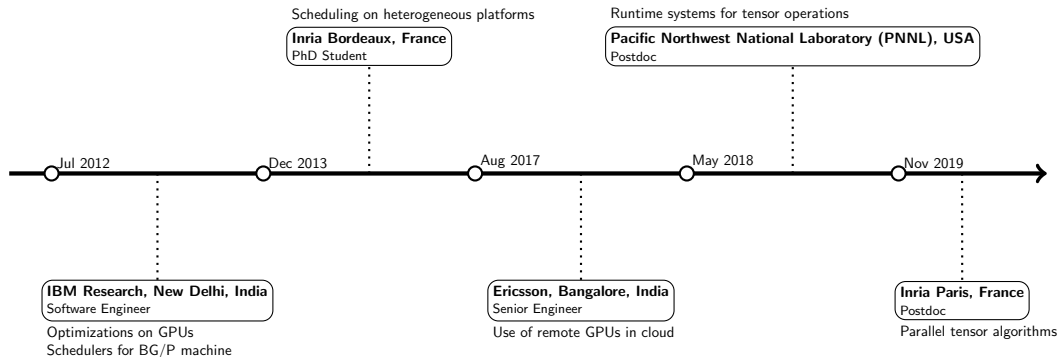
# Scalable Tensor Algorithms for Modern Computing Systems

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CNRS LIP/LaBRI Applicant

March 15, 2022

# Resume in timeline

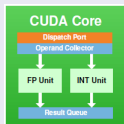


## Advisors/Close collaborators

- PhD supervisors at Inria Bordeaux, France: Olivier Beaumont, Lionel Eyraud-Dubois, Samuel Thibault, Emmanuel Agullo
- Postdoc supervisors/Close collaborators: Marcin Zalewski (PNNL, USA), Sriram Krishnamoorthy (PNNL, USA), Laura Grigori (Inria Paris, France), Grey Ballard (Wake Forest University, USA)

# Past research experience

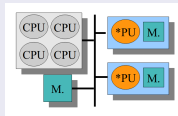
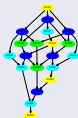
## GPU algorithms



IBM Research, India, 2013

■ Stencil computations

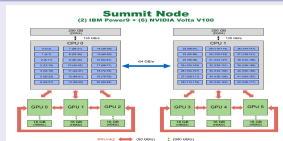
## Scheduling on heterogeneous platforms



PhD thesis, Inria Bordeaux, France, 2017

■ Dense linear algebra computations

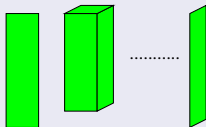
## Fast molecular simulations



PNNL, USA, 2019

■ ■ ■ Tensor computations, TAMM library

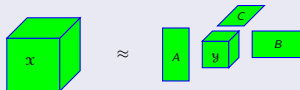
## Parallel tensor approximations



Inria Paris, France, 2019

■ ■ ■ Tensor-train decomposition

## Communication optimal algorithms



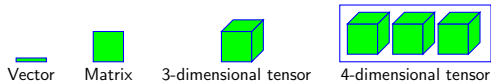
Inria Paris, France, 2019

■ ■ ■ Multiple Tensor-times-matrix computations (to obtain  $y$ )

Expertise: **Tensor computations**, **Parallel algorithms**, **Communication costs**, **Low-rank approximations**

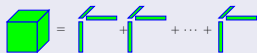
# Tensors and their uses

- **Neuroscience:** Neuron  $\times$  Time  $\times$  Trial
- **Media:** User  $\times$  Movie  $\times$  Time
- **Ecommerce:** User  $\times$  Product  $\times$  Time
- **Social-Network:** Person  $\times$  Person  $\times$  Time  $\times$  Type



- High dimensional tensors: Neural network, Molecular simulation, Quantum computing
- People work with low dimensional structure (decomposition) of the tensors

## Canonical decomposition



## Tucker decomposition



## Tensor-train decomposition



# Importance of communication

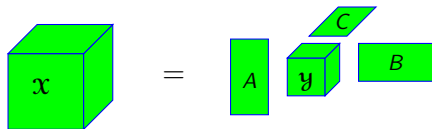
- Gaps between computation and communication costs growing exponentially

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

Source: Getting up to speed: The future of supercomputing

**Goal** : Scalable and communication optimal algorithms for tensor computations

# Higher-order SVD (HOSVD) to compute Tucker decomposition



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## Algorithm 1 3-dimensional HOSVD Algorithm( $\mathcal{X}$ )

---

- 1: Obtain factor matrices  $A, B$  and  $C$  from the matrix representations of the input tensor  $\mathcal{X}$
  - 2:  $\mathcal{Y} = \mathcal{X} \times_1 A^T \times_2 B^T \times_3 C^T$
  - 3: Return  $\mathcal{Y}, A, B, C$
- 

- $\mathcal{X}, \mathcal{Y}$ : 3-dimensional input and output tensors (or arrays) &  $A, B, C$ : matrices
- $\times_i$ : tensor contraction along the  $i$ th dimension (similar to matrix multiplication)
- Multiple Tensor-Times-Matrix (Multi-TTM) computation:  $\mathcal{Y} = \mathcal{X} \times_1 A^T \times_2 B^T \times_3 C^T$

# Communication lower bounds and Communication optimal algorithms

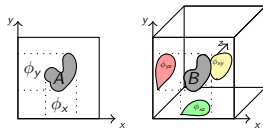
- 1 For Matrix Matrix Multiplications
- 2 For Multi-TTM Computations

## Settings

- $P$  number of processors
  - Each processor performs (asymptotically) equal amount of operations
  - One copy of data is in the system
    - $1/P$ th amount of inputs (before the computation) and output (after the computation) on each processor
  - Focus on bandwidth cost (volume of data transfers)
- 
- Submitted this work to SPAA 2022 conference
  - Joint work with L. Grigori, G. Ballard, K. Rouse, H. Al Daas

# Approach to obtain communication lower bounds

- Loomis-Whitney inequality: for  $d - 1$  dimensional projections
  - For the 2d object  $A$ ,  $\phi_x \phi_y \geq \text{Area}(A)$
  - For the 3d object  $B$ ,  $(\phi_{xy} \phi_{yz} \phi_{xz})^{\frac{1}{2}} \geq \text{Volume}(B)$
- Hölder-Brascamp-Lieb (HBL) inequality – generalization for arbitrary dimensional projections
  - Provide exponent for each projection



## Constraints for parallel load balanced matrix matrix multiplication

- $C = AB$  with  $A \in \mathbb{R}^{n_1 \times n_2}$ ,  $B \in \mathbb{R}^{n_2 \times n_3}$ , and  $C \in \mathbb{R}^{n_1 \times n_3}$

for  $i = 1:n_1$ , for  $k = 1:n_2$ , for  $j = 1:n_3$

$$C[i][j] += A[i][k] * B[k][j]$$

- $\phi_A, \phi_B, \phi_C$ : projections of computations on arrays  $A, B, C$
- From Loomis-Whitney/HBL inequality:  $\phi_A^{\frac{1}{2}} \phi_B^{\frac{1}{2}} \phi_C^{\frac{1}{2}} \geq \text{number of multiplications per processor} = \frac{n_1 n_2 n_3}{P}$
- Our contributions:  $\frac{n_1 n_2}{P} \leq \phi_A \leq n_1 n_2$ ,  $\frac{n_2 n_3}{P} \leq \phi_B \leq n_2 n_3$ ,  $\frac{n_1 n_3}{P} \leq \phi_C \leq n_1 n_3$



# Optimization problem and Communication lower bounds

Minimize  $\phi_A + \phi_B + \phi_C$  s.t.

$$\phi_A^{\frac{1}{2}} \phi_B^{\frac{1}{2}} \phi_C^{\frac{1}{2}} \geq \frac{n_1 n_2 n_3}{P}$$

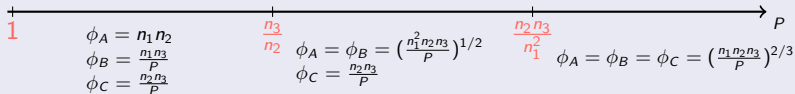
$$\frac{n_1 n_2}{P} \leq \phi_A \leq n_1 n_2$$

$$\frac{n_2 n_3}{P} \leq \phi_B \leq n_2 n_3$$

$$\frac{n_1 n_3}{P} \leq \phi_C \leq n_1 n_3$$

Amount of array accesses =  $\phi_A + \phi_B + \phi_C$

- Estimate the solution and prove optimality using all Karush–Kuhn–Tucker conditions are satisfied
- For  $n_1 \leq n_2 \leq n_3$ ,



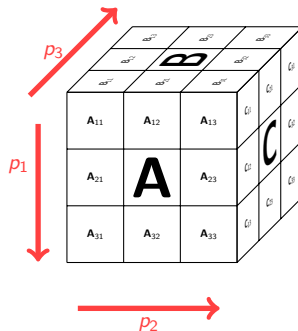
- Communication lower bound =  $\phi_A + \phi_B + \phi_C$  – data owned by the processor =  $\phi_A + \phi_B + \phi_C - \frac{n_1 n_2 + n_2 n_3 + n_1 n_3}{P}$

# Design of communication optimal algorithms for $C = AB$

## Arrangements of 8 processors



- $P$  is organized into  $p_1 \times p_2 \times p_3$  logical grid
- Select  $p_1, p_2$  and  $p_3$  based on the communication lower bounds
- Gather  $A$  on the set of processors along each slice of  $p_3$
- Gather  $B$  on the set of processors along each slice of  $p_1$
- Perform local computation
- Perform reduce operation along  $p_2$  to obtain  $C$



# 3-dimensional Multi-TTM ( $\mathcal{Y} = \mathcal{X} \times_1 \mathbf{A}^{(1)\top} \times_2 \mathbf{A}^{(2)\top} \times_3 \mathbf{A}^{(3)\top}$ )

- TTM-in-Sequence approach (used in Tucker-MPI)
  - $\mathcal{Y} = \left( \left( \mathcal{X} \times_1 \mathbf{A}^{(1)\top} \right) \times_2 \mathbf{A}^{(2)\top} \right) \times_3 \mathbf{A}^{(3)\top}$

All-at-Once definition with  $\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$ ,  $\mathcal{Y} \in \mathbb{R}^{r_1 \times r_2 \times r_3}$ ,  $\mathbf{A}^{(k)} \in \mathbb{R}^{n_k \times r_k}$  (our contribution)

for  $n'_1 = 1:n_1$ , for  $n'_2 = 1:n_2$ , for  $n'_3 = 1:n_3$

for  $r'_1 = 1:r_1$ , for  $r'_2 = 1:r_2$ , for  $r'_3 = 1:r_3$

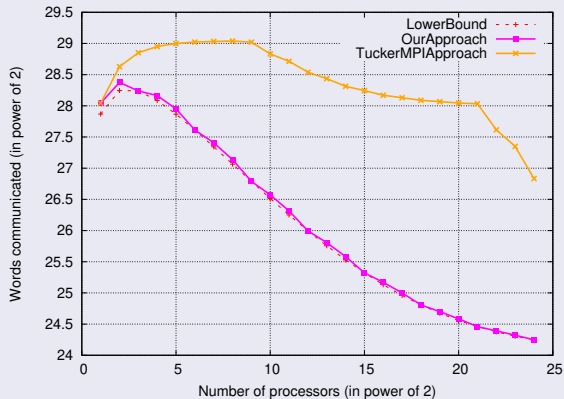
$\mathcal{Y}(r'_1, r'_2, r'_3) = \mathcal{Y}(r'_1, r'_2, r'_3)$

$+ \left( \mathcal{X}(n'_1, n'_2, n'_3) * \mathbf{A}^{(1)}(n'_1, r'_1) * \mathbf{A}^{(2)}(n'_2, r'_2) * \mathbf{A}^{(3)}(n'_3, r'_3) \right)$

- Applied our framework to compute lower bounds
- Designed similar communicational optimal algorithms (though 6-dimensional)

# Simulated performance comparison

$$n_1 = n_2 = n_3 = 2^{20}, r_1 = r_2 = r_3 = 2^8$$



- Typical scenarios in data compression problems
- Our approach communicates much less than the state-of-the-art approach (TuckerMPI)

# 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 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
- Same for manipulation operations of popular tensor representations
- Create a tensor library

# 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 as a tensor computation
  - Canonical rank of the tensor determines the complexity of the computation
  - 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
         $\mathcal{G}(i_1, i_2, j_2) = \mathcal{G}(i_1, i_2, j_2) + \mathcal{A}(i_1, i_2, i_3) * B(i_3, j_2)$ 
      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 reduce the number of operations (first try)

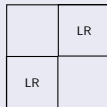
# Hierarchical matrix concepts to tensors

## Hierarchical matrices

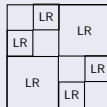
- Data sparse approximation of non-sparse matrices



Original Matrix



Step 1

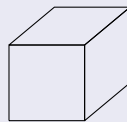


Step 2

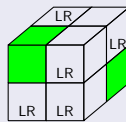
*LR*: low rank block

## 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



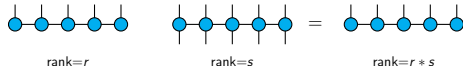
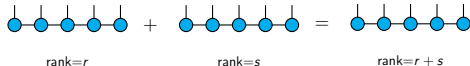
Step 1



# High dimensional tensor representations

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.

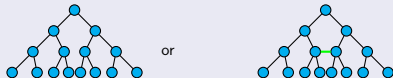
- Adding tensors and applying an operator in Tensor-train representation



- Requires a truncation process which iterates over cores one by one – not suitable to work in parallel

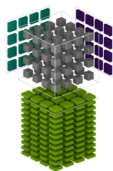
## New tensor representations – suitable for parallelization

- Look at new representations in tree format



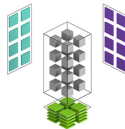
- Data will be stored at the leaf nodes

# Architecture aware algorithms and Training of tensorized neural networks



$$D = \begin{matrix} \text{FP16 or FP32} & \text{FP16} & \text{FP16} & \text{FP16 or FP32} \end{matrix} +$$

NVIDIA A100 Tensor Core FP64



- Recent Nvidia GPUs have tensor cores to accelerate AI computations
- Design parallel algorithms which take architecture details into account
- Design parallel methods to train tensorized neural networks

# Integration in the LIP/LaBRI laboratory

## My research plans

- **Main focus:** scalable and communication optimal tensor algorithms
- **Short term plans:** Strassen's concepts to tensors, hierarchical matrix concepts to tensors
- **Long term plans:** new tensor representations, parallel training of tensorized neural networks

## ROMA team (LIP laboratory)

- *Bora Ucar:* design of tensor compression and manipulation algorithms
- *Gregoire Pichon:* low-rank based methods
- *Anne Benoit, Loris Marchal, Yves Robert and Frederic Vivien:* scalability and scheduling aspects in the long term

## SATANAS team (LaBRI laboratory)

- *Olivier Beaumont and Lionel Eyraud-Dubois:* parallel training of tensorized neural networks
- *Mathieu Faverge:* low-rank based methods
- *Abdou Guermouche, Samuel Thibault:* exploitation of maximum potential of HPC systems in the long term

## Bringing additional skills

- High dimensional dense tensor computations, use of tensors in molecular simulations (for both teams)
- Communication lower bounds for linear algebra computations (for both teams)
- Scalable approaches for large HPC systems and GPU computations (only for the ROMA team)

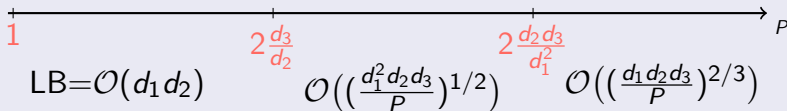
# Thank You!

# Backup Slides

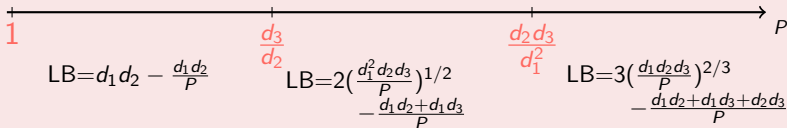
# Existing lower bounds for matrix matrix multiplication

- $C = AB$ , where  $A \in \mathbb{R}^{n_1 \times n_2}$ ,  $B \in \mathbb{R}^{n_2 \times n_3}$ , and  $C \in \mathbb{R}^{n_1 \times n_3}$
- Let  $d_1 = \min(n_1, n_2, n_3) \leq d_2 = \text{median}(n_1, n_2, n_3) \leq d_3 = \max(n_1, n_2, n_3)$

## Existing communication lower bounds (CARMA [IPDPS 2013])



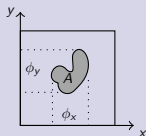
## Our communication lower bounds



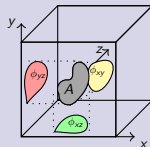
# Loomis-Whitney & Hölder-Brascamp-Lieb inequalities

## Size of $d - 1$ dimensional projections (Loomis-Whitney inequality)

- 2-dimensional object  $A$  and its 1-dimensional projections  $\phi_x, \phi_y$
- $\phi_x \phi_y \geq \text{Area}(A)$



- 3-dimensional object  $A$  and its 2-dimensional projections:  $\phi_{xy}, \phi_{yz}, \phi_{xz}$
- $(\phi_{xy} \phi_{yz} \phi_{xz})^{\frac{1}{3-1}} \geq \text{Volume}(A)$



## Hölder-Brascamp-Lieb (HBL) inequality – Generalization of Loomis-Whitney inequality

$$\Delta = \begin{matrix} & A & B & C \\ \begin{matrix} i \\ j \\ k \end{matrix} & \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix} \end{matrix}$$

for  $i = 1:n_1$ , for  $k = 1:n_2$ , for  $j = 1:n_3$

$$C[i][j] + = A[i][k] * B[k][j]$$

- Find  $\mathbf{x} = [x_1 \ x_2 \ x_3]^T$  such that  $\Delta \cdot \mathbf{x} \geq \mathbf{1}$ ,  $\mathbf{1}$  is vector of all ones
- $\phi_A, \phi_B, \phi_C$ : projections of computations on arrays  $A, B, C$
- HBL inequality:  $\phi_A^{x_1} \phi_B^{x_2} \phi_C^{x_3} \geq \text{Amount of computations}$
- To make inequality tight select  $\mathbf{x}$  such that  $\mathbf{1}^T \mathbf{x}$  is minimum  $\Rightarrow x_1 = x_2 = x_3 = \frac{1}{2}$

# Optimization problem and Communication lower bounds

- $\phi_A, \phi_B, \phi_C$  indicate the amount of array accesses

Minimize  $\phi_A + \phi_B + \phi_C$  s.t.

$$\phi_A^{\frac{1}{2}} \phi_B^{\frac{1}{2}} \phi_C^{\frac{1}{2}} \geq \frac{n_1 n_2 n_3}{P}$$

$$\frac{n_1 n_2}{P} \leq \phi_A \leq n_1 n_2$$

$$\frac{n_2 n_3}{P} \leq \phi_B \leq n_2 n_3$$

$$\frac{n_1 n_3}{P} \leq \phi_C \leq n_1 n_3$$

Generalized version ( $d_1 \leq d_2 \leq d_3$ )

Minimize  $\phi_1 + \phi_2 + \phi_3$  s.t.

$$\phi_1^{\frac{1}{2}} \phi_2^{\frac{1}{2}} \phi_3^{\frac{1}{2}} \geq \frac{d_1 d_2 d_3}{P}$$

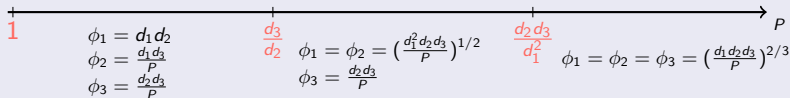
$$\frac{d_1 d_2}{P} \leq \phi_1 \leq d_1 d_2$$

$$\frac{d_1 d_3}{P} \leq \phi_2 \leq d_1 d_3$$

$$\frac{d_2 d_3}{P} \leq \phi_3 \leq d_2 d_3$$

Amount of accesses  $= \phi_1 + \phi_2 + \phi_3$

- Estimate the solution and prove optimality using all Karush–Kuhn–Tucker conditions are satisfied



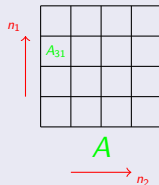
- Communication lower bound  $= \phi_1 + \phi_2 + \phi_3 - \text{data owned by the processor} = \phi_1 + \phi_2 + \phi_3 - \frac{d_1 d_2 + d_2 d_3 + d_1 d_3}{P}$



# Design of Communication Optimal Algorithms

Data Distribution ( $P$  is organized into a  $p_1 \times p_2 \times p_3$  grid)

- $p_1, p_2$ , and  $p_3$  evenly distribute  $n_1, n_2$ , and  $n_3$
- Each processor has  $\frac{1}{p}$ th amount of input and output variables
- $A_{31} = A(2\frac{n_1}{p_1} + 1 : 3\frac{n_1}{p_1}, 1 : \frac{n_2}{p_2})$  is evenly distributed among  $(3, 1, *)$  processors
- $B_{12} = B(1 : \frac{n_2}{p_2}, \frac{n_3}{p_3} + 1 : 2\frac{n_3}{p_3})$  is evenly distributed among  $(*, 1, 2)$  processors



## Algorithm 2 $C = AB$ Matrix Multiplication Algorithm

- 1:  $(p'_1, p'_2, p'_3)$  is my processor id
- 2: //All-gather input matrices  $A$  and  $B$
- 3:  $A_{p'_1 p'_2} = \text{All-Gather}(A, (p'_1, p'_2, *))$
- 4:  $B_{p'_2 p'_3} = \text{All-Gather}(B, (*, p'_2, p'_3))$
- 5:  $T = \text{Local-Matrix-Multiplication}(A_{p'_1 p'_2}, B_{p'_2 p'_3})$  // Local matrix multiplication in a temporary
- 6:  $\text{Reduce-Scatter}(C_{p'_1 p'_3}, T, (p'_1, *, p'_3))$  // Reduce-scatter the output

# 3-dimensional Multi-TTM ( $\mathcal{Y} = \mathcal{X} \times_1 \mathbf{A}^{(1)\top} \times_2 \mathbf{A}^{(2)\top} \times_3 \mathbf{A}^{(3)\top}$ )

## All-at-Once 3-dimensional Multi-TTM Computation

for  $n'_1 = 1:n_1$ , for  $n'_2 = 1:n_2$ , for  $n'_3 = 1:n_3$

for  $r'_1 = 1:r_1$ , for  $r'_2 = 1:r_2$ , for  $r'_3 = 1:r_3$

$\mathcal{Y}(r'_1, r'_2, r'_3) = \mathcal{Y}(r'_1, r'_2, r'_3)$

$+ \left( \mathcal{X}(n'_1, n'_2, n'_3) * \mathbf{A}^{(1)}(n'_1, r'_1) * \mathbf{A}^{(2)}(n'_2, r'_2) * \mathbf{A}^{(3)}(n'_3, r'_3) \right)$

$$\Delta = \begin{bmatrix} \mathbf{I}_{3 \times 3} & \mathbf{1}_3 & \mathbf{0}_3 \\ \mathbf{I}_{3 \times 3} & \mathbf{0}_3 & \mathbf{1}_3 \end{bmatrix}$$

- Total number of 4 – array operations =  $n_1 r_1 n_2 r_2 n_3 r_3$
- $\Delta$  is not full rank
  - Consider each vector  $\mathbf{x}$  such that  $\Delta \cdot \mathbf{x} = \mathbf{1}$ ,  $\mathbf{x}$  is of the form  $[a \ a \ a \ 1-a \ 1-a]^\top$  and  $0 \leq a \leq 1$
- $\phi_{\mathcal{X}}, \phi_{\mathcal{Y}}$ : tensor projections &  $\phi_1, \phi_2, \phi_3$ : matrix projections
- From HBL,  $\phi_{\mathcal{X}}^{1-a} \phi_{\mathcal{Y}}^{1-a} \phi_1^a \phi_2^a \phi_3^a \geq \text{Amount of computations}$

# Solving Optimization Problem to Compute Lower Bounds

- Select a processor which performs  $\frac{n_1 r_1 n_2 r_2 n_3 r_3}{P}$  amount of 4 – array operations
- After applying lower and upper bounds for each projection, we need to solve the following optimization problem

Minimize  $\phi_x + \phi_y + \phi_1 + \phi_2 + \phi_3$  s.t.

$$\phi_x^{1-a} \phi_y^{1-a} \phi_1^a \phi_2^a \phi_3^a \geq \frac{n_1 r_1 n_2 r_2 n_3 r_3}{P}$$

$$\frac{n_1 n_2 n_3}{P} \leq \phi_x \leq n_1 n_2 n_3$$

$$\frac{r_1 r_2 r_3}{P} \leq \phi_y \leq r_1 r_2 r_3$$

$$\frac{n_1 r_1}{P} \leq \phi_1 \leq n_1 r_1$$

$$\frac{n_2 r_2}{P} \leq \phi_2 \leq n_2 r_2$$

$$\frac{n_3 r_3}{P} \leq \phi_3 \leq n_3 r_3$$

# Divide the problem into two parts

## Matrix part

Minimize  $\phi_1 + \phi_2 + \phi_3$  s.t.

$$\phi_1 \phi_2 \phi_3 \geq \frac{n_1 r_1 n_2 r_2 n_3 r_3}{P}$$

$$\frac{n_1 r_1}{P} \leq \phi_1 \leq n_1 r_1$$

$$\frac{n_2 r_2}{P} \leq \phi_2 \leq n_2 r_2$$

$$\frac{n_3 r_3}{P} \leq \phi_3 \leq n_3 r_3$$

## Tensor part

Minimize  $\phi_x + \phi_y$  s.t.

$$\phi_x \phi_y \geq \frac{n_1 r_1 n_2 r_2 n_3 r_3}{P}$$

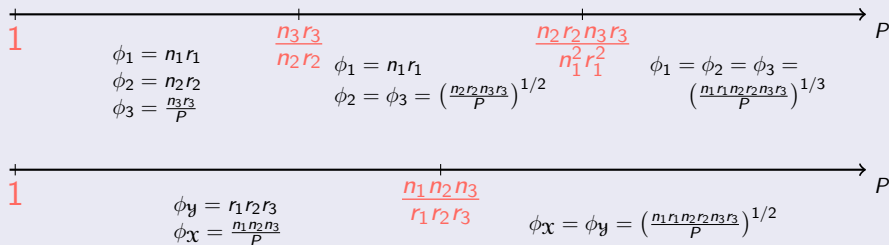
$$\frac{n_1 n_2 n_3}{P} \leq \phi_x \leq n_1 n_2 n_3$$

$$\frac{r_1 r_2 r_3}{P} \leq \phi_y \leq r_1 r_2 r_3$$

# Amount of Accesses and Lower bounds

- We assume  $n_1 r_1 \leq n_2 r_2 \leq n_3 r_3$  and  $r_1 r_2 r_3 \leq n_1 n_2 n_3$
- Estimate solutions for both parts using Lagrange multipliers ( optimality can be proven using KKT conditions)

Amount of accesses =  $\phi_x + \phi_y + \phi_1 + \phi_2 + \phi_3$



$$\text{Communication lower bound} = \phi_x + \phi_y + \phi_1 + \phi_2 + \phi_3 - \frac{n_1 n_2 n_3 + r_1 r_2 r_3 + n_1 r_1 + n_2 r_2 + n_3 r_3}{P}$$