# Parallel Communication Lower Bounds and Algorithms for Computations with Random Matrices


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# Communication lower bounds for a computation on $P$ processors

minimum amount of communication required to perform the computation in parallel

## Should avoid such settings

- If all operations are performed on a single processor, then no communication is required
- If data is duplicated on all processors, then communication may not be necessary

## Our assumptions

- Load balanced computation: each processor performs equal amount of operations
- There is one copy of data in the system

- There exist one processor that has at most $1/P$th amount of overall data – we examine the required data transfers for this processor to establish the lower bound

# Communication costs

- Communication cost: latency cost (number of messages) and bandwidth cost (volume of data transfers)
- Focus on bandwidth costs – it dominates when messages are large

## Communication cost of an algorithm

- Cost along the critical path – the path along which the communication (bandwidth) cost is maximum

# Focus on $A\Omega$ and $\Omega^T A\Omega$ computations

## $B = A\Omega$ computation

- $A \in \mathbb{R}^{n_1 \times n_2}$ and $\Omega$ is a $n_2 \times r$ random matrix
- Fundamental to all randomized linear algebra techniques including randomized SVD

## $B = A\Omega$ and $C = \Omega^T A\Omega$ computations together

- $A$ is a $n \times n$ matrix and $\Omega$ is a $n \times r$ random matrix
- Useful for Nyström approximation, $\widetilde{\mathrm{A}} = (\mathrm{A}\Omega)(\Omega^T \mathrm{A}\Omega)^\dagger(\mathrm{A}\Omega)^T$

$r$ is (much) less than the contracted dimension ($r \leq n_2$ and $r \leq n$).

# Table of Contents

# Table of Contents

# Classical matrix multiplication bound

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

Let $k = \min(n_1, n_2, n_3) \leq \ell = median(n_1, n_2, n_3) \leq m = \max(n_1, n_2, n_3)$.

- $\phi_A, \phi_B, \phi_C$: number of elements accessed by a processor in arrays $A$, $B$, $C$
- Minimum number of elements accessed in the critical path $= \phi_A + \phi_B + \phi_C$

| $P$ | $1$ to $\frac{m}{\ell}$ | $\frac{m}{\ell}$ to $\frac{\ell m}{k^2}$ | beyond $\frac{\ell m}{k^2}$ |
|---|---|---|---|
| $\phi_A + \phi_B + \phi_C =$ | $k\ell + \frac{km+\ell m}{P}$ | $2(\frac{k^2\ell m}{P})^{1/2} + \frac{\ell m}{P}$ | $3(\frac{k\ell m}{P})^{2/3}$ |

- Communication lower bound $= \phi_A + \phi_B + \phi_C - \frac{n_1 n_2 + n_2 n_3 + n_1 n_3}{P}$

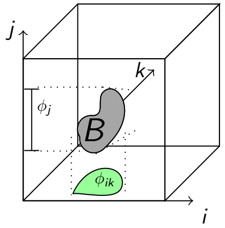
Can we improve this bound when one matrix is randomly generated?

# Table of Contents

# Approach to obtain communication lower bounds

A special case of Hölder-Brascamp-Lieb (HBL) inequality:

- For the 3d object $B$, $\phi_i \phi_{jk} \geq Volume(B)$
- $\phi_j$, $\phi_{ik}$: projections of $B$ on $j$-axis and $i-k$ plane
- Also implies that: $\phi_{ij}\phi_{ik} \geq Volume(B)$ and $\phi_{jk}\phi_{ik} \geq Volume(B)$




## Constraints for load balanced computation

- $B = A\Omega$ with $A \in \mathbb{R}^{n_1 \times n_2}$, $B \in \mathbb{R}^{n_1 \times r}$, and $\Omega$ is a random matrix

$$\text{for } i = 1{:}n_1, \text{ for } k = 1{:}n_2, \text{ for } j = 1{:}r$$
$$B[i][j] += A[i][k] * \Omega[k][j]$$

- $\phi_A, \phi_B$ : projection sizes of computation on arrays $A$, $B$
- From the HBL inequality: $\phi_A \phi_B \geq$ number of multiplications per processor $= \frac{n_1 n_2 r}{P}$
- Extra constraints: $\frac{n_1 n_2}{P} \leq \phi_A \leq n_1 n_2$, $\frac{n_1 r}{P} \leq \phi_B \leq n_1 r$

# Optimization problem and communication lower bounds

$$\textit{Minimize } \phi_A + \phi_B \quad \text{s.t.}$$
$$\phi_A \phi_B \geq \frac{n_1 n_2 r}{P}$$
$$\frac{n_1 n_2}{P} \leq \phi_A \leq n_1 n_2$$
$$\frac{n_1 r}{P} \leq \phi_B \leq n_1 r$$

## Amount of non-random array accesses $= \phi_A + \phi_B$

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

$1 \qquad n_1 \qquad \frac{n_1 n_2}{r} \qquad P$

$1$ to $n_1$: $\phi_A^* = \frac{n_1 n_2}{P}$, $\phi_B^* = \frac{n_1 r}{P}$

$n_1$ to $\frac{n_1 n_2}{r}$: $\phi_A^* = \frac{n_1 n_2}{P}$, $\phi_B^* = r$

$\frac{n_1 n_2}{r}$ to $P$: $\phi_A^* = \phi_B^* = \left(\frac{n_1 n_2 r}{P}\right)^{1/2}$

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

# Table of Contents

# A naive way to minimize communication cost for $B = A\Omega$

$$\begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix} = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} \cdot \Omega$$

Structure of the algorithm for each processor $i$:

- owns $A_i$ row block ($1/P$ th portion of $A$), generates random matrix $\Omega$, and performs $B_i = A_i \cdot \Omega$

When $P$ is small, communication cost of the algorithm is 0 (Optimal).

What about when $P$ is large?

# Matrix multiplication with a random matrix

**Require:** $\Pi$ is a $p_1 \times p_2 \times p_3$ grid of processors, $|\Pi| = P$.

**Require:** A is evenly divided into a $p_1 \times p_2$ grid of rectangular blocks of dimension $n_1/p_1 \times n_2/p_2$, and each block $\mathrm{A}_{ij}$ is evenly divided across a set of $p_3$ processors. $\mathrm{A}_{ij}^{(k)}$ is owned by processor rank $(i, j, k)$.

**Ensure:** $\mathrm{B} = \mathrm{A}\Omega$, B is evenly divided across a $p_1 \times p_3$ grid of blocks, and each block $\mathrm{B}_{ik}$ is evenly divided across a set of $p_2$ processors. $\mathrm{B}_{ik}^{(j)}$ is owned by processor rank $(i, j, k)$.

1: **function** $\mathrm{B}_{ik}^{(j)} = \textsc{RandMatMul}(\mathrm{A}_{ij}^{(k)}, \Pi)$
2: $\quad (i, j, k) = \textsc{MyRank}(\Pi)$
3: $\quad \mathrm{A}_{ij} = \textsc{All-Gather}(\mathrm{A}_{ij}^{(k)}, \Pi_{ij*})$ ▷ Gather the required data of input matrix A
4: $\quad \Omega_{jk} = \textsc{GenRandom}(n_2/p_2, r/p_3)$ ▷ Generate the required random submatrix
5: $\quad \bar{\mathrm{B}}_{ik} = \mathrm{A}_{ij} \cdot \Omega_{jk}$ ▷ Perform local matrix multiplication
6: $\quad \mathrm{B}_{ik}^{(j)} = \textsc{Reduce-Scatter}(\bar{\mathrm{B}}_{ik}, \Pi_{i*k})$ ▷ Sum results to compute $\mathrm{B}_{ik}^{(j)}$
7: **end function**

Communication cost is optimal when $p_1$, $p_2$ & $p_3$ are chosen based on lower bounds.

# Table of Contents

# Nyström approximation

Let $\mathrm{A} \in \mathbb{R}^{n\times n}$ be a symmetric positive definite matrix and $\Omega \in \mathbb{R}^{n\times r}$ be a random matrix.

- Nyström approximation of A, $\widetilde{\mathrm{A}} = (\mathrm{A}\Omega)(\Omega^T \mathrm{A}\Omega)^\dagger(\mathrm{A}\Omega)^T$
- Requires to compute both $\mathrm{A}\Omega$ and $\Omega^T \mathrm{A}\Omega$

## Constraints for load balanced computation

$$\mathrm{B} = \mathrm{A}\Omega, \quad \mathrm{C} = \Omega^T \mathrm{B}$$

- $\phi_A, \phi_B, \phi_C$ : projection sizes of computations on arrays $A$, $B$, $C$
- Each processor performs $1/P$th portion of each computation
- From the HBL inequality: $\phi_A\phi_B \geq \frac{n^2 r}{P}$, $\phi_B\phi_C \geq \frac{nr^2}{P}$
- Extra constraints: $\frac{n^2}{P} \leq \phi_A \leq n^2$, $\frac{nr}{P} \leq \phi_B \leq nr$, $\frac{r^2}{P} \leq \phi_C \leq r^2$

# Optimization problem and communication lower bounds

$$\textit{Minimize } \phi_A + \phi_B + \phi_C \text{ s.t.}$$

$$\phi_A\phi_B \geq \frac{n^2 r}{P} \phi_B\phi_C \geq \frac{nr^2}{P}$$

$$\frac{n^2}{P} \leq \phi_A \leq n^2, \frac{nr}{P} \leq \phi_B \leq nr, \frac{r^2}{P} \leq \phi_C \leq r^2$$

## Amount of non-random array accesses $= \phi_A + \phi_B + \phi_C$

- Estimate the solution and prove optimality using all Karush–Kuhn–Tucker conditions are satisfied
- For $n \geq r$,

$1$ — $r$ — $n$ — $\frac{n(n+r)}{r}$ — $P$

Between $1$ and $r$: $\phi_A^* = \frac{n^2}{P}$, $\phi_B^* = \frac{nr}{P}$, $\phi_C^* = \frac{r^2}{P}$

Between $r$ and $n$: $\phi_A^* = \frac{n^2}{P}$, $\phi_B^* = \frac{nr}{P}$, $\phi_C^* = r$

Between $n$ and $\frac{n(n+r)}{r}$: $\phi_A^* = \frac{n^2}{P}$, $\phi_B^* = r$, $\phi_C^* = \frac{nr}{P}$

Between $\frac{n(n+r)}{r}$ and $P$: $\phi_A^* = n\left(\frac{nr}{(n+r)P}\right)^{1/2}$, $\phi_B^* = \left(\frac{nr(n+r)}{P}\right)^{1/2}$, $\phi_C^* = r\left(\frac{nr}{(n+r)P}\right)^{1/2}$

- Communication lower bound $= \phi_A + \phi_B + \phi_C -$ data owned by the processor
$$= \phi_A + \phi_B + \phi_C - \frac{n^2+nr+r^2}{P}$$

# Table of Contents

# Parallel algorithms for $B = A\Omega$ and $C = \Omega^T B$

**Require:** $\Pi$ is a $p_1 \times p_2 \times p_3$ processor grid, $\Psi$ is a $q_1 \times q_2 \times q_3$ processor grid, and $|\Pi| = |\Psi| = P$.
**Require:** A is evenly divided into a $p_1 \times p_2$ grid of rectangular blocks, and each block $A_{ij}$ is evenly divided across a set of $p_3$ processors with $A_{ij}^{(k)}$ is owned by processor rank $(i, j, k)$ in $\Pi$.
**Ensure:** $B = A\Omega$, B is evenly divided across a $q_1 \times q_3$ grid of blocks, and each block $B_{i'k'}$ is evenly divided across a set of $q_2$ processors with $B_{i'k'}^{(j')}$ is owned by processor rank $(i', j', k')$ in $\Psi$.
**Ensure:** $C = \Omega^T B$, C is evenly divided across a $q_2 \times q_3$ grid of blocks, and each block $C_{j'k'}$ is evenly divided across a set of $q_1$ processors with $C_{j'k'}^{(i')}$ is owned by processor rank $(i', j', k')$ in $\Psi$.

```
1: function (B_{i'k'}^{(j')}, C_{j'k'}^{(i')}) = RandCompNys(A_{ij}^{(k)}, Π, Ψ)
2:     (i, j, k) = MyRank(Π)
3:     Perform B = AΩ in p1 × p2 × p3 grid of processors
4:     //Change distribution of B so that it is suitable for q1 × q2 × q3 grid
5:     (i', j', k') = MyRank(Ψ)
6:     if for any i, p_i ≠ q_i then B_{i'k'}^{(j')} = Redistribute(B) end if
7:     Perform C = Ω^T B in q1 × q2 × q3 grid of processors
8: end function
```

# Processor grid dimensions

- Not clear how to obtain processor grid dimensions that exactly match lower bounds ($p_i = q_i$ for $i = 0, 1, 2$)

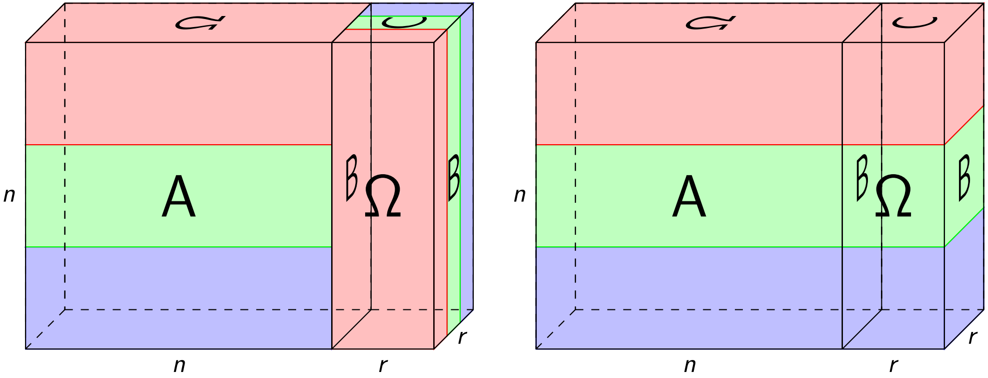
Approach 1 (*Redistribution* ):

- Perform $\mathrm{B} = \mathrm{A}\Omega$ in $p_1 \times p_2 \times p_3$ grid of processors and $\mathrm{C} = \Omega^{\mathsf{T}}\mathrm{B}$ in $q_1 \times q_2 \times q_3$ grid of processors
  - Communication cost is far from the lower bound by the sum of the communication cost of $B$ and the redistribution cost

Approach 2 (*No-Redistribution* ):

- $\mathrm{B} = \mathrm{A}\Omega$ is the dominating computation
  - Use the optimal processor grid of this computation to also perform $\mathrm{C} = \Omega^{\mathsf{T}}\mathrm{B}$

# *Redist*ribution vs *No-Redist*ribution on 3 processors




Total number of iteration points $= n^2 r + nr^2 = n(n+r)r$

# Table of Contents

# Experimental settings

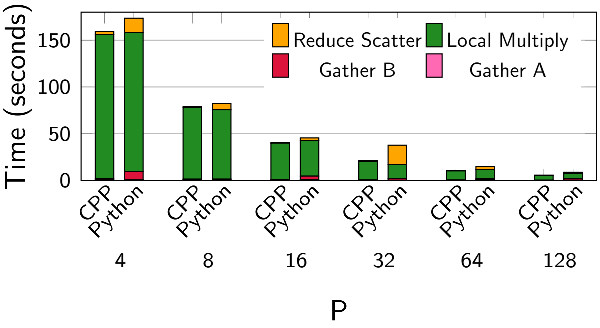
| NERSC Perlmutter GPU Partition | | |
|---|---|---|
| Processor | 1 × AMD EPYC 7763 per node | |
| # NUMA domains | 4 | |
| # Cores | 64 per node, 16 per NUMA domain | |
| # Hyperthreads | 2 per core, 32 per NUMA domain | |
| # GPUs | 4 × NVIDIA A100 per node | |
| Memory | 256 GB DDR4 per node, 40GB per GPU | |
| | **CPU-only** | **GPU** |
| Compiler | Intel C++ version 2024.1.0 | NVIDIA CUDA C++ version 24.5-1 |
| BLAS and PRNG | MKL 2024.1 | CUDA toolkit 12.4 |
| MPI | CRAY MPICH 8.1.30 (CUDA-aware for GPUs) | |

# Dataset and number of processors

- Small number of processors ($P < r$, practical regime)
  - For $\mathrm{B} = \mathrm{A}\Omega$ computation, communication cost $= 0$
  - For $\mathrm{B} = \mathrm{A}\Omega$ and $\mathrm{C} = \Omega^{\mathsf{T}}\mathrm{B}$ computations, communication cost $= nr/P$ (for *Redist*ribution) and $r^2 - r^2/P$ (for *No-Redist*ribution)

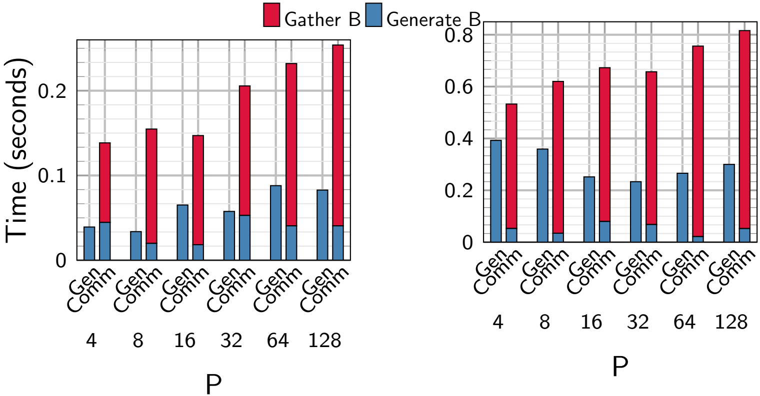
- $n$ and $r$ are selected based on CIFAR-10 dataset
  - $n = 50,000$ and $r = 500$ and $5000$

# C++ vs Python: 3D-distributed memory matrix multiplication




- Comparison to multiply two $50k \times 50k$ double precision matrices
- Use a processor grid as cubical as possible
- Python (mpi4py version 3.1.5) performance is hard to explain
- We focus on C++ implementation

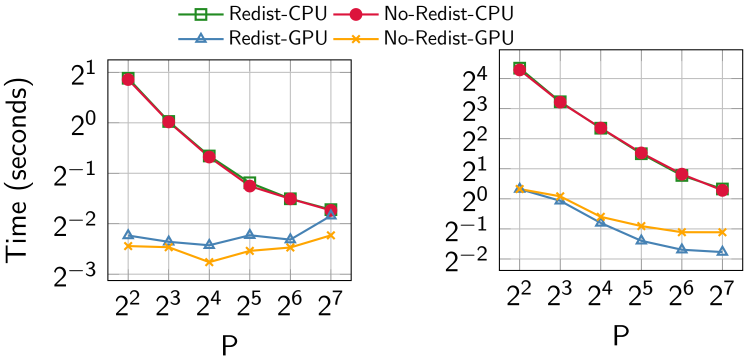
# Communicating vs redundantly generating $\Omega$ in $B = A\Omega$




$r = 500$ $r = 5000$

- Generating $\Omega$ is cheaper than communicating it

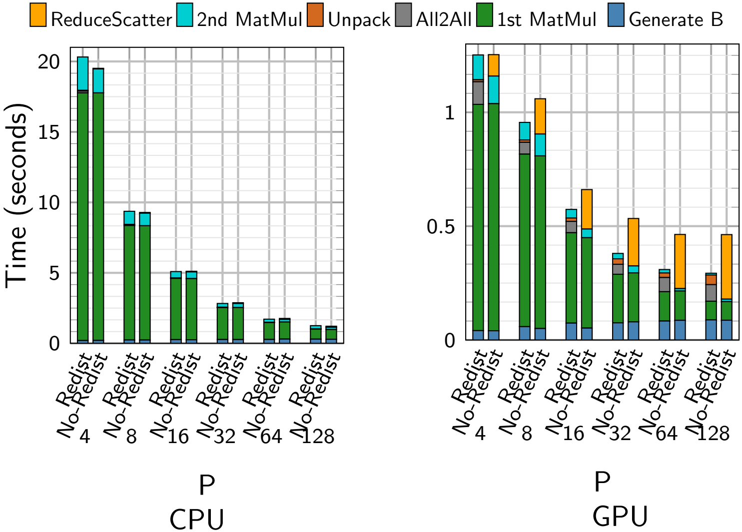
# $B = A\Omega$ and $C = \Omega^T B$ computations




$r = 500$ $r = 5000$

- CPU-only implementations scale better
- *Redist* approach scales better on GPU

# Runtime breakdown for both approaches with $r = 5000$




- CPU-only implementation is dominated by the local matrix multiplication

# Table of Contents

# Conclusion and future work

## Conclusion

- Communication lower bounds and optimal algorithms for $B = A\Omega$ and $C = \Omega^T B$
- Parallel scalability of our algorithms on both CPUs and GPUs
- *Redist* approach scales better on GPUs

## Future Work

- Exploit symmetry to further reduce computation and communication costs
- Study how to perform all computations of generalized Nyström approximations for nonsymmetric matrices efficiently
- Extend our approaches to other sketching methods that use structured matrices, such as CountSketch and Subsampled Randomized Hadamard Transform methods

# Thank You!