SUPERCOMPUTING @ GEORGIA TECH

Attendance

Club Linktree

WORKSHOP 2:

Matrix Multiplication Optimization

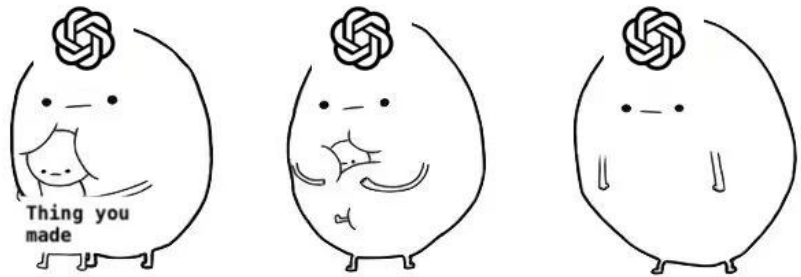
Slides by: Panya B., Min L., Saatvik A.

Agenda

1. Introduction on Matrix Multiplication
2. Tools Overview
3. More on HPC
4. The Message-Passing Paradigm (MPI)
5. **The Matrix Multiplication Algorithm**
6. Solution 1: Brute Force
7. Optimization 0: Divide-and-conquer
8. Time/Space Complexity Analysis
9. Caching
10. Optimization 1: Tiling
11. Optimization 2: Cannon's Algorithm
12. Optimization 3: Sparse Matrix Multiplication
13. **Implementation Time!**
14. Applications
15. Key Takeaways

Why matrix multiplication?

- Mathematical concept that most of you guys already know.
- Most classic and straightforward problem to emphasise the importance of HPC.
- Well-studied and foundational algorithms
- Able to be implemented using a variety of HPC paradigms relatively straightforwardly.
- Broad applications in many areas.



Tools Overview

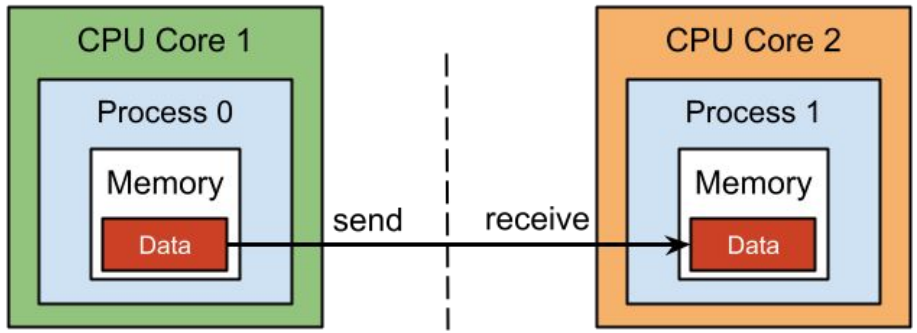
- Python 3.11
- mpi4py
- PACE Instructional Cluster (ICE)
- Your brains!

A little more on HPC...

- Despite what NVIDIA may want you to think, CUDA is not the only software stack that exists in the HPC world!
- There are many programming paradigms in the HPC world, with pros and cons for each.
  - Data-Parallel,
  - Shared-Memory,
  - Message-Passing,
  - …
- In this workshop we will be focused on message-passing using the MPI protocol!
- MPI allows communication between different machines with their own distributed memory.

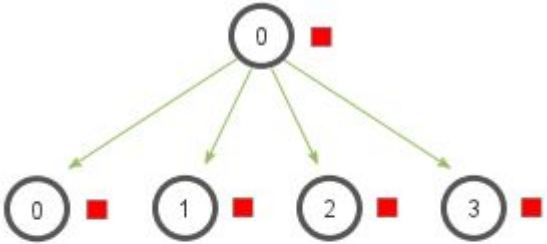
The Message-Passing Paradigm

- Group of nodes = “world”
- Each node has a “rank”
- Send and receive messages between different ranks
- Common functions:
  - Broadcast
  - Scatter
  - Reduce / AllReduce
  - Gather / AllGather
  - All-to-all / Many-to-many

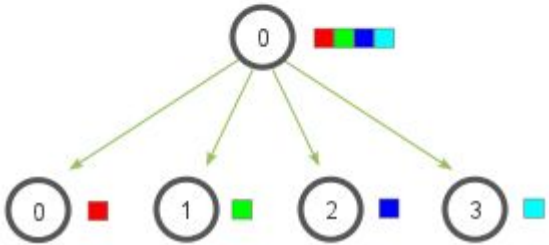


MPI Functions

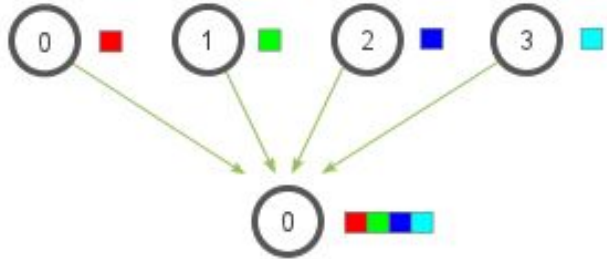
MPI_Bcast



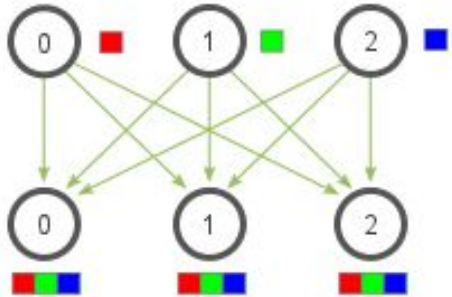
MPI_Scatter



MPI_Gather

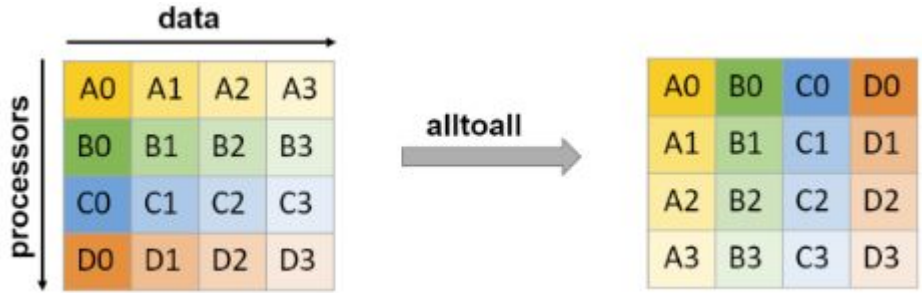


MPI_Allgather



MPI Functions

- All-to-All:



- Many-to-many is similar, but with variable data lengths

mpi4py

Rank, Size, COMM: comm.Get_rank(), comm.Get_size(), MPI.COMM_WORLD

Send: comm.send(sendbuf, dest, tag)

Receive: comm.recv(source, tag)

Broadcast: comm.bcast(sendbuf, root)

Reduce: comm.reduce(int, root, operation)

AllReduce: comm.allreduce(int, operation)

Scatter: comm.scatter(sendbuf, recvbuf, root=root)

Gather: comm.gather(sendbuf, recvbuf, root=root)

AllGather: comm.allgather(sendbuf, recvbuf)

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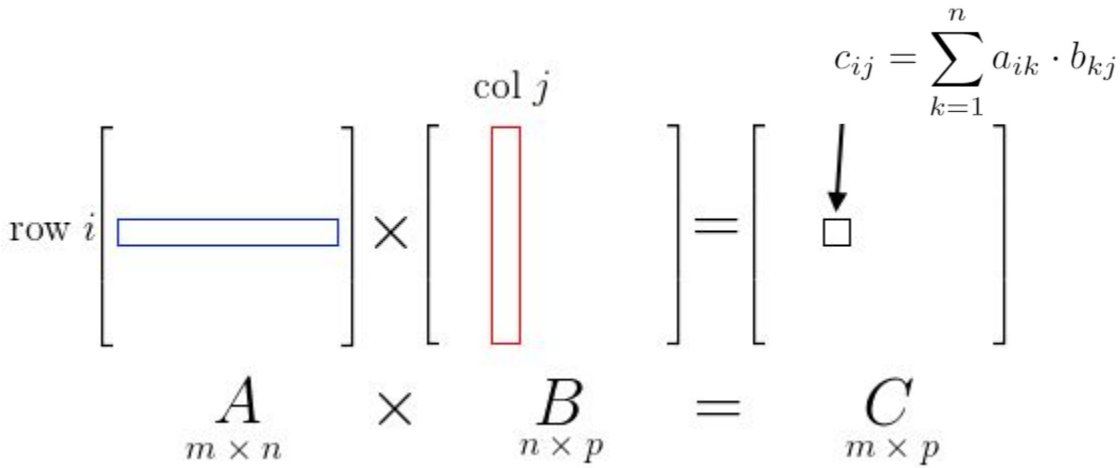
Inner Matrix Multiplication Algorithm

Problem Statement: Given matrices A and B of size (m x n) and (n x p) respectively, where, $m \neq n \neq p$ and $m, n, p > 0$, calculate their inner product AB.



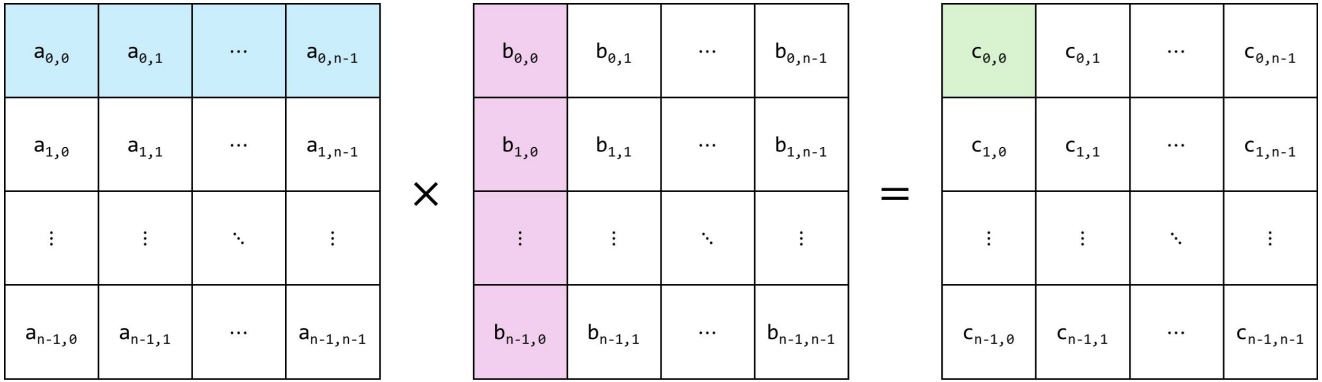
Solution 1: Brute Force Approach

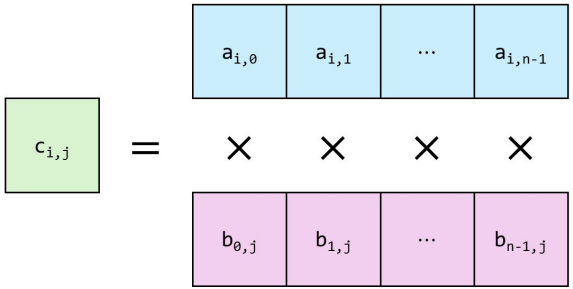
Naive Approach: Using Nested Loops – $O(n^3)$ Time and $O(n^2)$ Space

RECTANGULAR-MATRIX-MULTIPLY(A, B, C, p, q, r)

```
1  for i = 1 to p
2      for j = 1 to r
3          for k = 1 to q
4              c_ij = c_ij + a_ik · b_kj
```

Solution 1: Brute Force Approach





RECTANGULAR-MATRIX-MULTIPLY(A, B, C, p, q, r)

```
1  for i = 1 to p
2      for j = 1 to r
3          for k = 1 to q
4              c_ij = c_ij + a_ik · b_kj
```

Why do we need parallelization?

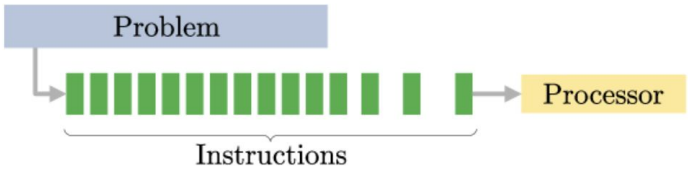
- Suppose matrices are of size (3×3) ⇒ total number of instructions = 27
- Suppose matrices are of size (10^6x10^6) ⇒ total number of instructions = 10^{18}

How do we make this faster?

Time Complexity Analysis of Parallel Programs

Serial Programs

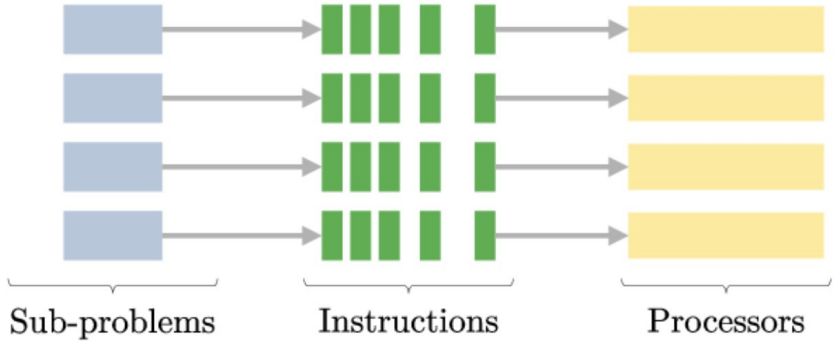
amount of work done by the program = time it takes for the program to finish.



VS

Parallel Programs

amount of work done by the program ≠ time it takes for the program to finish!



Optimization 0: Divide and Conquer

- Theorem:

Suppose that we partition each of A, B, and C into four $n/2 \times n/2$ matrices

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}, \quad C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}, \tag{4.9}$$

so that we rewrite the equation $C = A \cdot B$ as

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \cdot \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}. \tag{4.10}$$

Equation (4.10) corresponds to the four equations

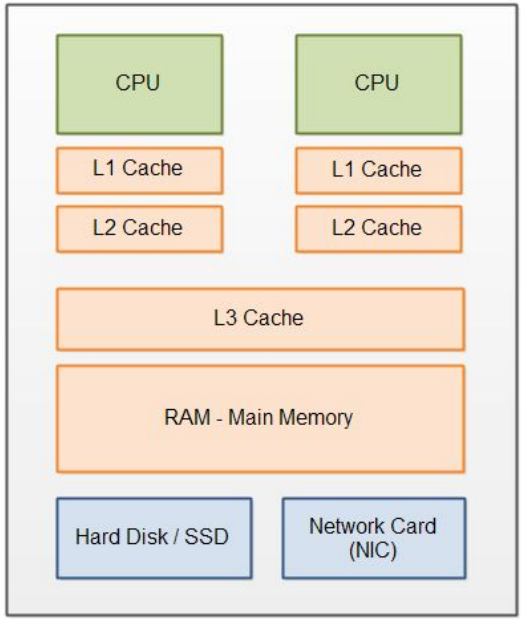
$$C_{11} = A_{11} \cdot B_{11} + A_{12} \cdot B_{21}, \tag{4.11}$$
$$C_{12} = A_{11} \cdot B_{12} + A_{12} \cdot B_{22}, \tag{4.12}$$
$$C_{21} = A_{21} \cdot B_{11} + A_{22} \cdot B_{21}, \tag{4.13}$$
$$C_{22} = A_{21} \cdot B_{12} + A_{22} \cdot B_{22}. \tag{4.14}$$

Cormen et al.

- This can be done on a single processor using the divide-and-conquer paradigm, or alternatively, we can split the workload across multiple processors!

Caching

- Memory access is expensive
- **Caches** are fast, smaller memory near the CPU that stores recently or frequently accessed data
- **Spatial locality:** processor likely to access memory locations near each other
- **Temporal locality:** memory accessed at a specific time is likely to be accessed again
- **Problem with naive matmul:** poor spatial and temporal locality → lots of cache misses



What if we broke the matrices into smaller blocks stored in the cache …

Optimization 1: Blocked Multiplication

Goal: Increase parallelism

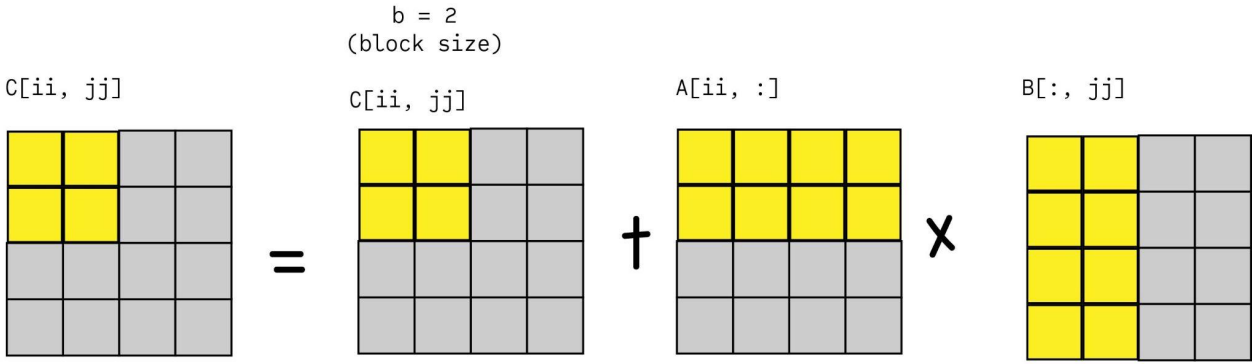
How?

- Divide the matrix into evenly sized blocks, 1 per processor (2D partitioning of both matrices).
- Send all the blocks in a row to all processors in a row, and send all the blocks in a column to all processors in a column.
- Each processor performs matrix multiplication for its block.
- The root collects all of the results.

Pros and Cons?

- Computation is divided among the processors.
- However, total cache usage is still suboptimal as blocks are present multiple times.

Optimization 1: Blocked Multiplication



ii, jj, kk denote block indices while i, j, k denote element indices

```
// C = C + A * B
// b = n / N (where b is the block size)
for ii = 1 to N:
  for jj = 1 to N:
    for kk = 1 to N:
      C[ii, jj] += A[ii, kk] * B[kk, jj]
```

Optimization 2: Cannon's Algorithm

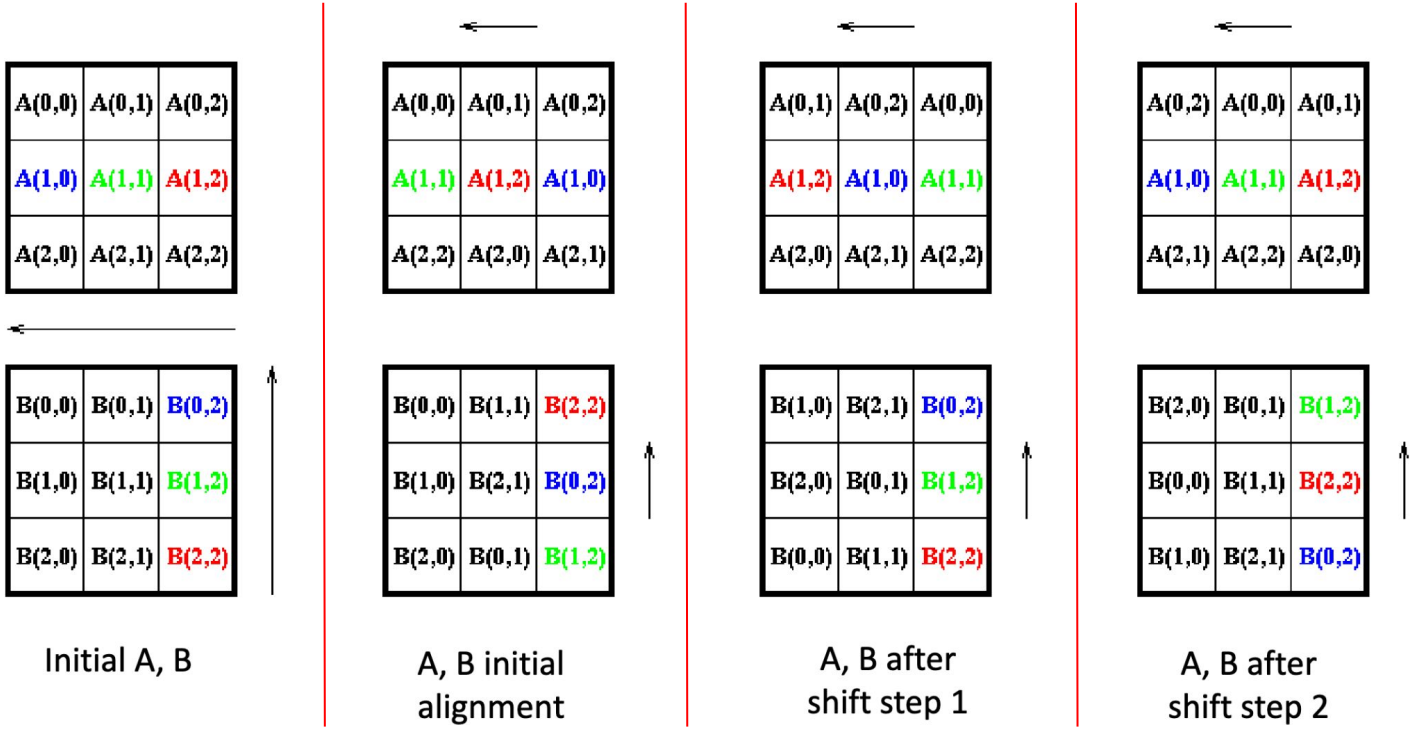
$$c_{ij} = \sum_{k=1}^{n} a_{ik} \cdot b_{kj}$$

Key Observation:

- Partition A and B in p square blocks, denoted A_{ij} and B_{ij}.
- Computing C_{ij} just needs all submatrices A_{ik} and B_{kj} for $0 \leq k \leq \sqrt{p}$.

$$C_{i,j} = \sum_{k=0}^{\sqrt{p}-1} A_{i,(i+j+k)\%\sqrt{p}} B_{(i+j+k)\%\sqrt{p},j}$$

Optimization 2: Cannon's Algorithm



Optimization 2: Cannon's Algorithm

Goal: Improve memory efficiency

How?

- Multiplies 2 square matrices using processors in a 2D grid.
- Distributes submatrices (blocks) of A and B to each processor.
- Minimizes communication by reusing data blocks over multiple computation steps.

Key Steps

- **Align data:** Shift matrix A's blocks left by row index i. Shift matrix B's blocks up by column index j.
- **Main Loop** (repeat $\sqrt{p}$ times): Each processor multiplies local A_{ij} X B_{ij} and accumulates the result in C_{ij} Then:
  - Shift all blocks of A left by 1 (wraparound)
  - Shift all blocks of B up by 1 (wraparound)

Optimization 2: Cannon's Algorithm

What improvements does this have?

- Avoids global all-to-all broadcast (reduces computation time)
- Computation dominates for larger matrices
- Memory needed does not increase as processors increase

Optimization 3: Sparse Matrix Mult.

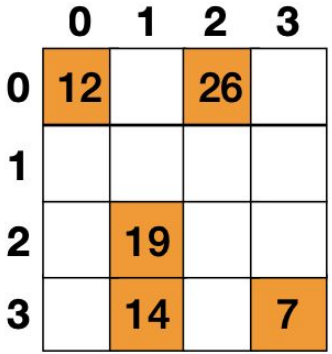
- **Sparse Matrix:** Matrix with primarily zeros.
- Much of matrix multiplication done in HPC is SpMM.
- Sometimes using dense matrix multiplication algorithms is not necessary and wastes time and memory.
- Notice that (nonzero x nonzero) calculations will occur much lesser in frequency than multiplications that involve 0s.
- ⇒ Optimize matmul by making sure we only do (nonzero x nonzero) multiplications!
- Use a better data structure to ensure this!

$$c_i \sum_{a_{iv} \neq 0} a_{iv} b_v. \quad \text{for } 1 \leq i \leq p.$$

"The ith row of resulting matrix C is the linear combination of the v rows of B for which $a_{iv} \neq 0$."
– **Gustavson (September, 1978)**

Designing A SpMM Algorithm

Step 1. Designing a better data structure:
→ One Solution: The **Coordinate Representation (COO)**



(0, 0, 12)
(0, 2, 26)
(2, 1, 19)
(3, 1, 14)
(3, 3, 7)

row + column index + weight per nonzero (easy to build / modify)

Designing A SpMM Algorithm

Step 2. Minimize the number of multiplications we are doing with 0 elements by using the dot product formula.

$$c_i \sum_{a_{iv} \neq 0} a_{iv} b_v. \quad \text{for } 1 \leq i \leq p.$$

"The ith row of resulting matrix C is the linear combination of the v rows of B for which $a_{iv} \neq 0$."
– **Gustavson (September, 1978)**

RowWise_SpGEMM(C, A, B)

```
1  // set matrix C to ∅
2  for a_{i*} in matrix A in parallel
3    do for a_{ik} in row a_{i*}
4         do for b_{kj} in row b_{k*}
5              do value ← a_{ik} b_{kj}
6                 if c_{ij} ∉ c_{i*}
7                    then insert (c_{ij} ← value)
8                    else  c_{ij} ← c_{ij} + value
```

Pseudocode Credit: Gustavson's Formula (1978) described in a workshop proceeding by Nagasaka, et al. (August, 2018)

But wait... Limitations of COO

- Revisit step 1: Notice that the only way to implement COO data structure results in **low cache locality!**
- Solution: A new data structure called **Compressed Sparse Row (CSR) representation.**

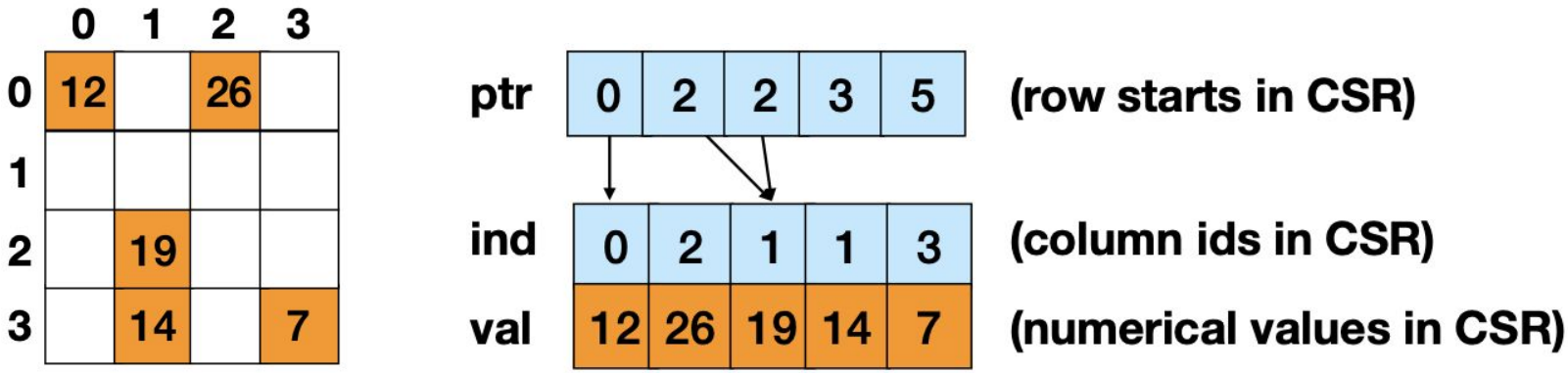


Photo Credit: UC Berkeley CS267

Implementation Time!

Set Up

Getting Started with PACE

SSH Instructions

- **IMPORTANT: Make sure that you are connected to the GT VPN!**
- Connect to Host: For everyone, the host name is <gt-username>@login-ice.pace.gatech.edu
- Type in your GT password upon seeing the prompt. DO NOT BE ALARMED IF NOTHING SHOWS UP AS YOU TYPE (its for safety etc.) Just finish typing your password and press <Enter>.

https://gatech.service-now.com/home?id=kb_article_view&sysparm_article=KB0042100

Remote SSH w/ Terminal

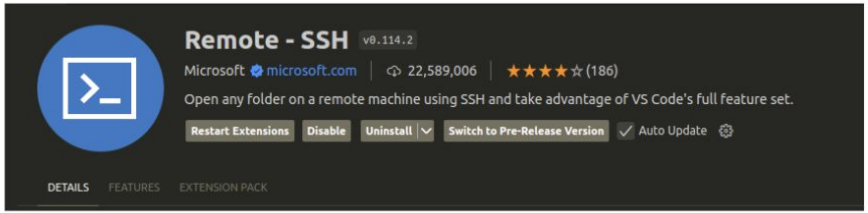
- Please check that you have access to an **SSH-Capable Terminal**!
  - → Windows Powershell
  - → MacOS Terminal
  - → Linux Terminal
- We'll use **SSH** to log onto the cluster you'll be using today.
- Follow the previous instructions to login to the PACE cluster. If you've successfully logged in, you'll see a prompt like the following:

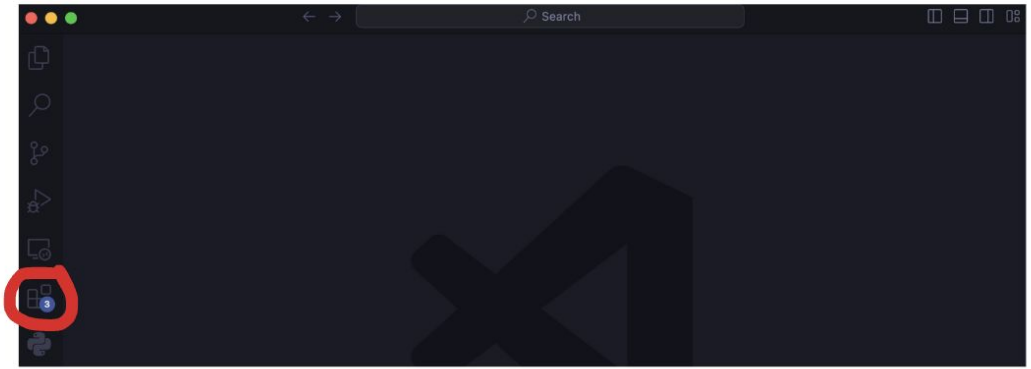
```
[pbhinder3@login-ice-3 ~]$
```

- You are now in a **login node** of the cluster, which you can use to access files, write code, submit jobs, etc.

Remote SSH w/ VSCode

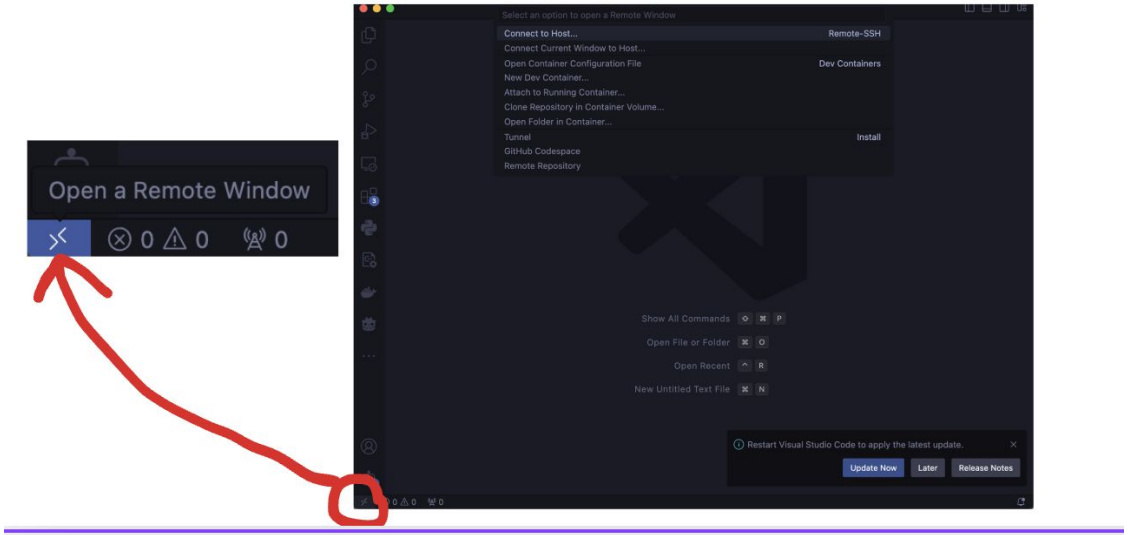
Install the extension from the VSCode extension store.





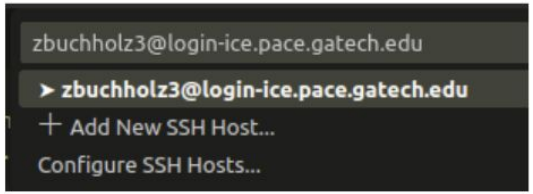
Remote SSH w/ VSCode

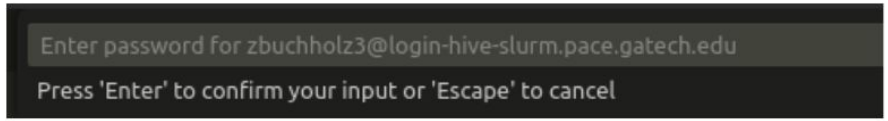
2. Notice that at the bottom left of the application, you will now see a button which appears to show a broken link. Click on it.



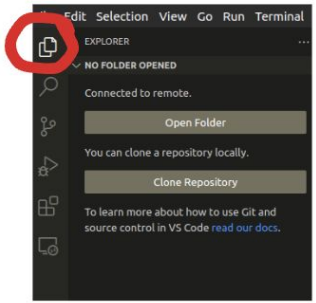
Remote SSH w/ VSCode

3. Select Connect-to-Host (should be the first option) and enter the hostname and password as shown previously.





4. You should now be able to open the folders icon to see the contents of the remote.



Set up repository

In your terminal, clone the workshop repository:

```
git clone https://github.com/suco-gt/Parallel-Optimization-Workshop.git
```

Follow the setup instructions in the README:

- Run `chmod +x *.sh` to give executable permissions to the shell scripts that are going to be used for this workshop.
- Run `./get_nodes.sh [num_nodes]` to allocate nodes on the cluster for 1 hour. Default num_nodes is 4.
- `module load anaconda3`
- Install conda environment: `conda create --name sp25_suco2 -c conda-forge python=3.11 numpy openmpi mpi4py -y`
- `conda activate sp25_suco2`
- Test if mpi4py is working for you successfully by running `./run.sh test`.
- You will run your code with the given bash file “run.sh”:
- For example: To run the intro exercises– “./run.sh intro”

Your Job

Your tasks (choose at least 1):

Complete the introduction to MPI problems in `0-mpi-intro.py`

OR

Race to implement each optimization! (Feel free to work in groups)

1. Implement the brute force matmul implementation in `bruteforce.py`
2. Implement the blocked matrix multiplication optimization in `blocked.py`
3. Implement Cannon's Algorithm in `cannon.py`
4. Implement COO SpGEMM in `spgemm.py`

Let us know if you have any questions!

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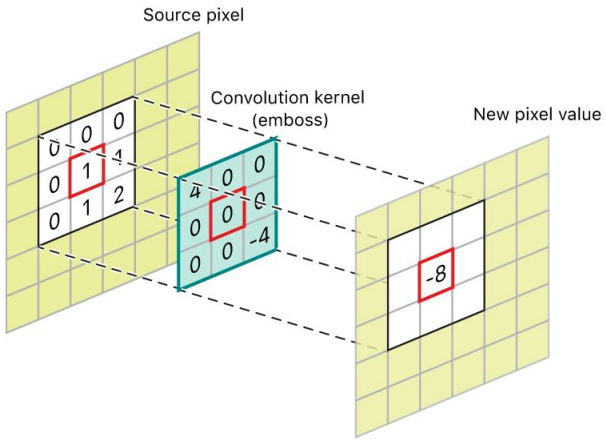
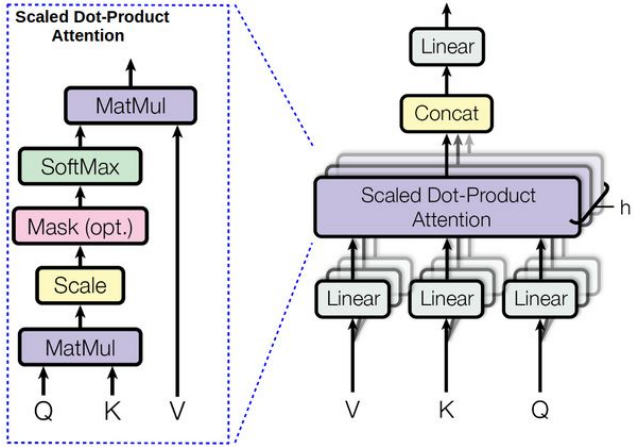
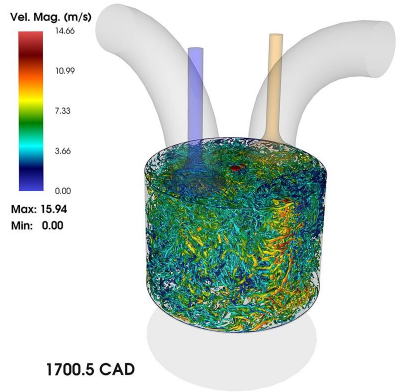
Applications







Key Takeaways

- Parallelism and scaling
  - → Breaking up computation into smaller tasks speed up execution
  - → Difference between shared memory (OpenMP) and distributed memory parallelism (MPI)
- Memory hierarchy and data locality - hardware impacts efficiency
  - → Tiling and blocking improves cache efficiency
  - → Impact of sparsity on performance
- Algorithmic trade-off
  - → Communication vs computation bottlenecks
  - → Choosing right optimization based on problem size and hardware constraints