Supplemental: MPI Matrix Multiplication

High-Performance Computing

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Matrix-Matrix multiplication

Multiplying two square matrices:
$C \leftarrow A \times B, \qquad A, B, C \in \Re^{n \times n}$
can be achieved by calculating each element of the result matrix as

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

where a_{ij}, b_{ij} and c_{ij} are the element on i^{th} row and j^{th} column of A, B and C respectively.

Pseudocode:

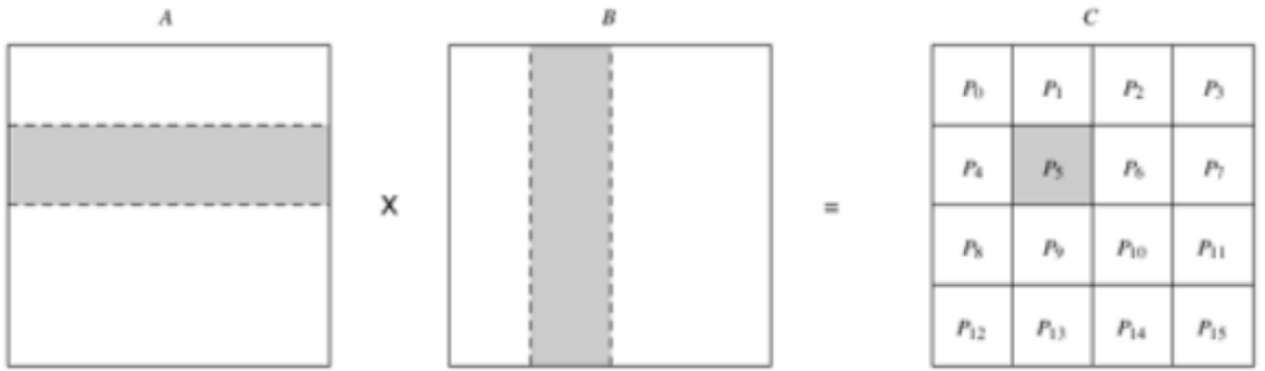
```
1:  Procedure MAT-MULT (A, B, C)
2:  begin
3:      for i ← 0 to n − 1 do
4:          for j ← 0 to n − 1 do
5:              begin
6:                  c_ij = 0
6:                  for k ← 0 to n − 1 do
7:                      c_ij += a_ik · b_kj
8:              endfor
9:  end MAT-MULT
```

Since we assume that floating point multiplications take one time unit, and that floating point additions are very fast (they take zero time units), the time needed for the serial algorithm to complete is expressed as $\Theta(n^3)$.

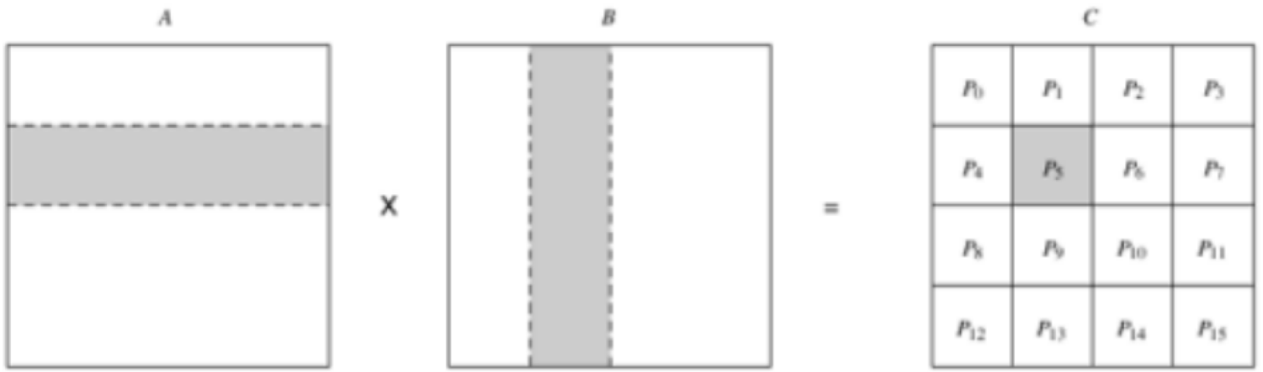
A Simple Parallel Matrix-Matrix Multiplication

Let $A = [a_{ij}]_{n\times n}$ and $B = [b_{ij}]_{n\times n}$ be n × n matrices. Compute $C = AB$

- Computational complexity of sequential algorithm: $O(n^3)$
- Partition A and B into p square blocks $A_{i,j}$ and $B_{i,j}$ $(0 \le i, j < \sqrt{p})$ of size $(n/\sqrt{p}) \times (n/\sqrt{p})$ each.
- Use Cartesian topology to set up process grid. Process $P_{i,j}$ initially stores $A_{i,j}$ and $B_{i,j}$ and computes block $C_{i,j}$ of the result matrix.
- Remark: Computing submatrix $C_{i,j}$ requires all submatrices $A_{i,k}$ and $B_{k,j}$ for $0 \le k < \sqrt{p}$.



Algorithm

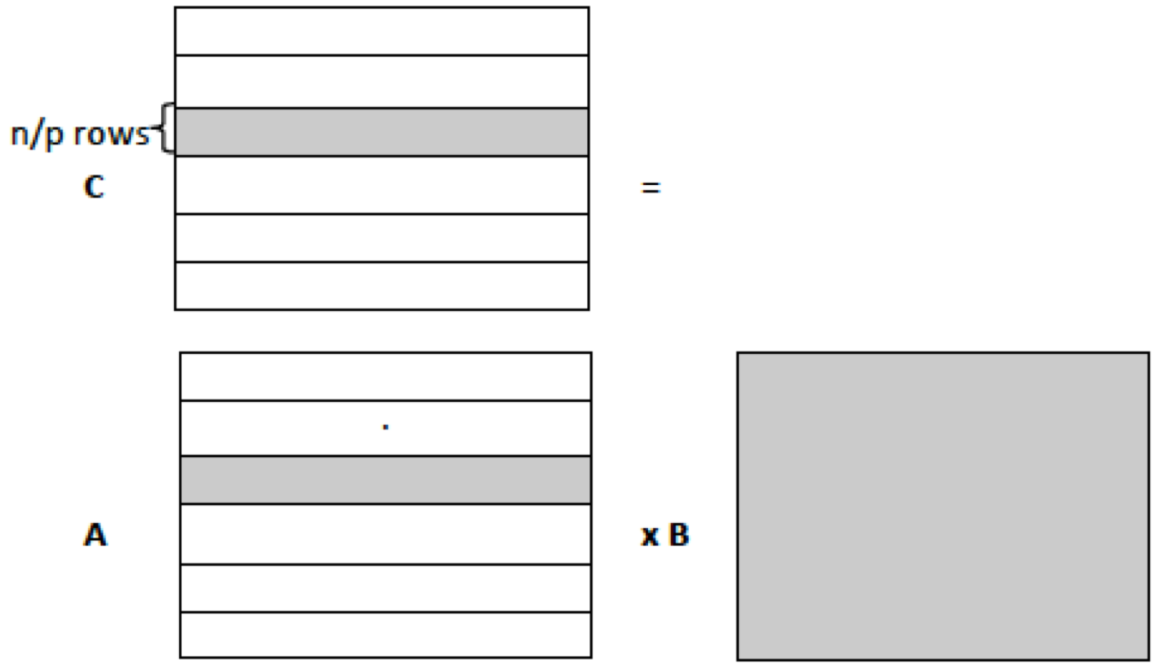


- Perform all-to-all broadcast of blocks of A in each row of processes
- Perform all-to-all broadcast of blocks of B in each column of processes
- Each process $P_{i,j}$ perform $C_{i,j} = \sum_{k=0}^{\sqrt{p}-1} A_{i,k} B_{k,j}$

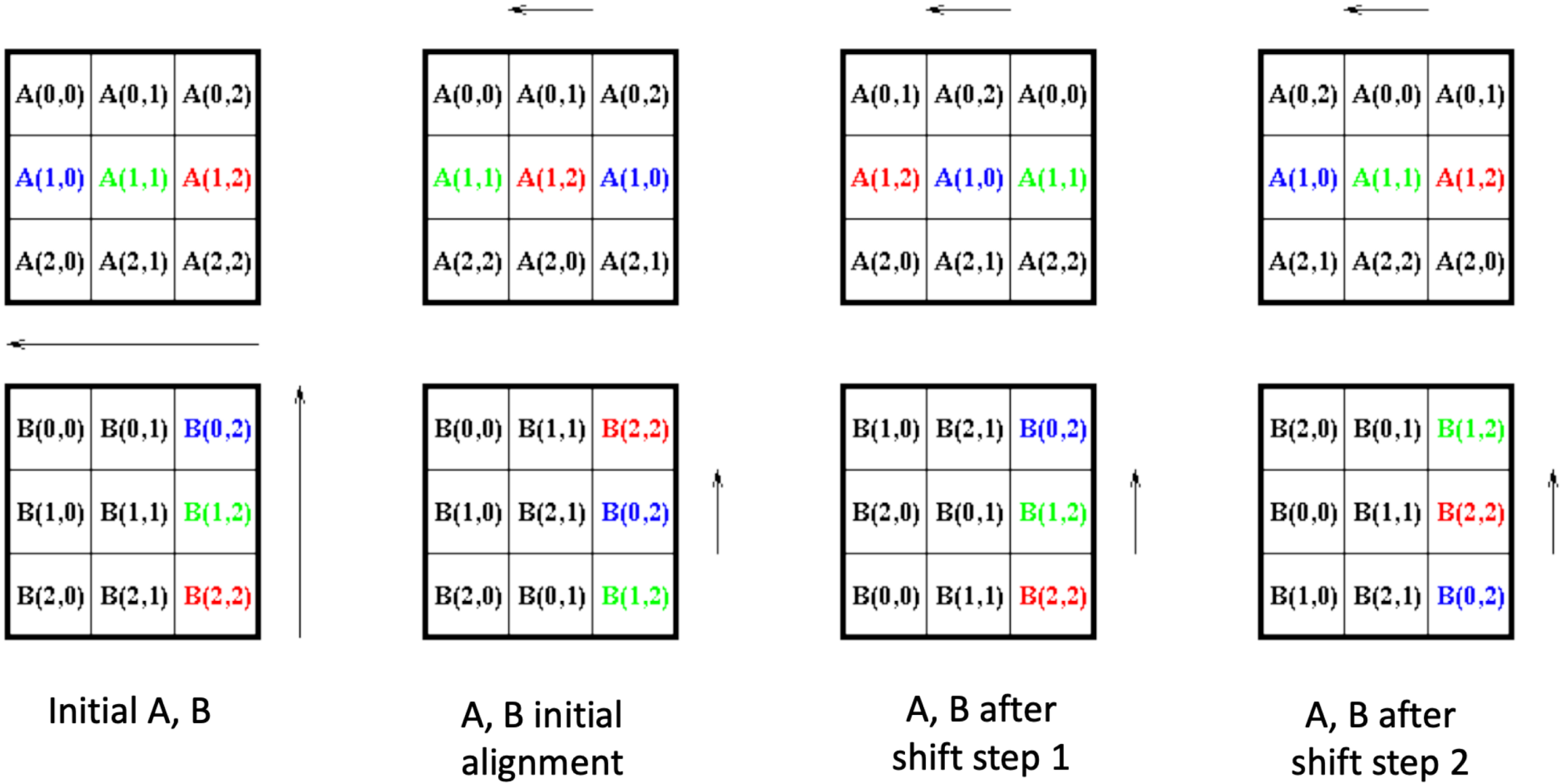
Parallel Matrix Multiplication

Write the parallel matrix multiplication using 1-D partitioning.

- Consider a homogeneous parallel machine with the number of processors p a perfect (i.e., $\sqrt{p}$ is an integer). $P_{i,j}$ is the processor row i and column j where $0 \le i,j \le \sqrt{p}-1$.
- We consider only the simple case where the matrix dimension n is a multiple of $\sqrt{p}$ (i.e., $n/\sqrt{p}$ is an integer).
- Implement the program using collective communications such as MPI_Scatter, MPI_Bcast, and MPI_Gather. For example, scatter A matrix and broadcast B matrix to the processes. Compute partial multiplication and gather partial C into C.



Cannon's Algorithm: Memory Efficient Algorithm



Initial A, B

A, B initial alignment

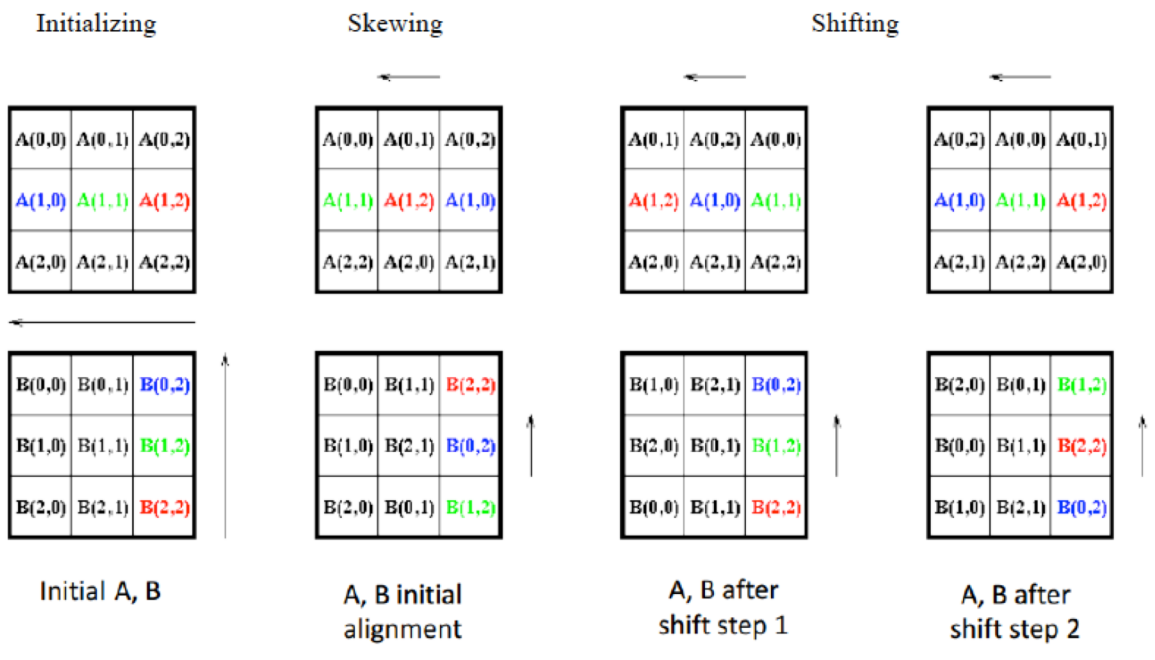
A, B after shift step 1

A, B after shift step 2

Cannon's Algorithm: Memory Efficient Algorithm

```
1:  Set c_ij = 0, for ∀ i and j
2:  Skew A: for i = 0 : (√p − 1)
3:              left circular shift i^th sub-block row of A by i
4:  Skew B: for j = 0 : (√p − 1)
5:              up circular shift j^th sub-block column of B by j
6:  for i = 0 : (√p − 1)
7:      Each processor multuplies the current sub-block of A by the current sub-block of B
8:      and adds the result to the sub-block of C of the processor
9:      Roll A: left circular shift sub-blocks of A by 1
10:     Roll B: up circular shift sub-blocks of B by 1
11: end
```

Example:



Cannon's Algorithm: Memory Efficient Algorithm

Goal: to improve the memory efficiency.

Let $A = [a_{ij}]_{n\times n}$ and $B = [b_{ij}]_{n\times n}$ be n × n matrices. Compute $C = AB$

- Partition A and B into p square blocks $A_{i,j}$ and $B_{i,j}$ $(0 \le i, j < \sqrt{p})$ of size $(n/\sqrt{p}) \times (n/\sqrt{p})$ each.
- Use Cartesian topology to set up process grid. Process $P_{i,j}$ initially stores $A_{i,j}$ and $B_{i,j}$ and computes block $C_{i,j}$ of the result matrix.
- Remark: Computing submatrix $C_{i,j}$ requires all submatrices $A_{i,k}$ and $B_{k,j}$ for $0 \le k < \sqrt{p}$.
- **The contention-free formula**:

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

Cannon's Algorithm

```
// inialize matrices
if (rank == root && isValid == true) {

// set up cartesian topology
int ndims, dims[2], sqrt_np;
bool periods[2], reorder;
ndims = 2;                                  // 2D matrix/grid
dims[0] = dims[1] = sqrt_np = sqrt(np);     // dimensions
periods[0] = periods[1] = true;             // wraparound both column and row
reorder = true;                             // allows processes reordered for efficiency

// MPI new Cartcomm (grid_comm) by Create_cart
MPI::Cartcomm grid_comm = MPI::COMM_WORLD.Create_cart(ndims, dims, periods, reorder);

// get the rank and coordinates with respect to the new topology
int grid_rank, grid_coords[2];
grid_rank = grid_comm.Get_rank();
grid_comm.Get_coords(grid_rank, ndims, grid_coords);

// compute ranks of the up and left shifts
int leftrank, rightrank, uprank, downrank;
//grid_comm.Shift(0, 1, uprank, downrank);
//grid_comm.Shift(1, 1, leftrank, rightrank);
//cout << "Process:" << rank << "> leftrank: " << leftrank << ", rightrank:" << rightrank <<
endl;
//cout << "Process:" << rank << "> uprank: " << uprank << ", downrank:" << downrank << endl;
grid_comm.Shift(0, -1, downrank, uprank);
grid_comm.Shift(1, -1, rightrank, leftrank);

// determine the dimension of the local matrix block
int block_n, block_count;
block_n = n / sqrt_np;
block_count = block_n * block_n;
```

Cannon's Algorithm

```
  // determine the dimension of the local matrix block
  int block_n, block_count;
  block_n = n / sqrt_np;
  block_count = block_n * block_n;

  // define MPI block datatype and vector
  MPI::Datatype block = MPI::FLOAT.Create_vector(block_n, block_n, n).Create_resized(0,
sizeof(float));
  block.Commit();        // commit the defined datatype

  // prepare sendcounts and displs for MPI Scatterv
  int sendcounts[np], displs[np];
  for (int i = 0; i < sqrt_np; i++) {
    for (int j = 0; j < sqrt_np; j++) {
      displs[i*sqrt_np + j] = (i * sqrt_np * block_n + j) * block_n;
      sendcounts[i*sqrt_np + j] = 1;
    }
  }

  // send block using scatterv
  float block_A[block_n][block_n], block_B[block_n][block_n], block_C[block_n][block_n];
  for (int i = 0; i < block_n; i++) {
    for (int j = 0; j < block_n; j++) {
      block_A[i][j] = block_B[i][j] = block_C[i][j] = 0;
    }
  }
  //MPI::COMM_WORLD.Scatterv(A, sendcounts, displs, block, block_A, block_count, MPI::FLOAT, 0);
  grid_comm.Scatterv(A, sendcounts, displs, block, block_A, block_count, MPI::FLOAT, 0);
```

Cannon's Algorithm

```
  // Cannon Step1: skewing
  int src, dst;

  // shift all blocks in A to the left by i steps
  grid_comm.Shift(1, -grid_coords[0], src, dst);
  grid_comm.Sendrecv_replace(block_A, block_count, MPI::FLOAT, dst, 1, src, 1);
  //cout << "Process:" << rank << ", grid_coords = (" << grid_coords[0] << "," << grid_coords[1]
<< ")" << ", A[1][2]=" << A[1][2] << endl;

  // shift all blocks in B up by j steps


// Cannon Step2: calculate and shifting
for (int i = 0; i < sqrt_np; i++) {
  for (int row = 0; row < block_n; row++) {
    for (int col = 0; col< block_n; col++) {
      for (int k = 0; k < block_n; k++) {
        block_C[row][col] += block_A[row][k] * block_B[k][col];
      }
    }
  }
  grid_comm.Shift(1, -1, src, dst);    // left 1
  grid_comm.Sendrecv_replace(block_A, block_count, MPI::FLOAT, dst, 0, src, 0);
  grid_comm.Shift(0, -1, src, dst);    // up 1
  grid_comm.Sendrecv_replace(block_B, block_count, MPI::FLOAT, dst, 0, src, 0);
}

// gather the partial results
```