EPFL

HPC for numerical methods and data analysis

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QR Factorization

Exercise I Splitting communicators

In the previous exercise we splat the matrix in either columns or rows. But we can split such matrix into blocks as well using the `comm.Split` function on MPI. It splits the communicator by color and key.

Every process gets a `color` (a parameter) depending on which communicator they will be. Same color process will end up on the same communicator. In other words, `color` controls the subset assignment, processes with the same color belong to the same new communicator.

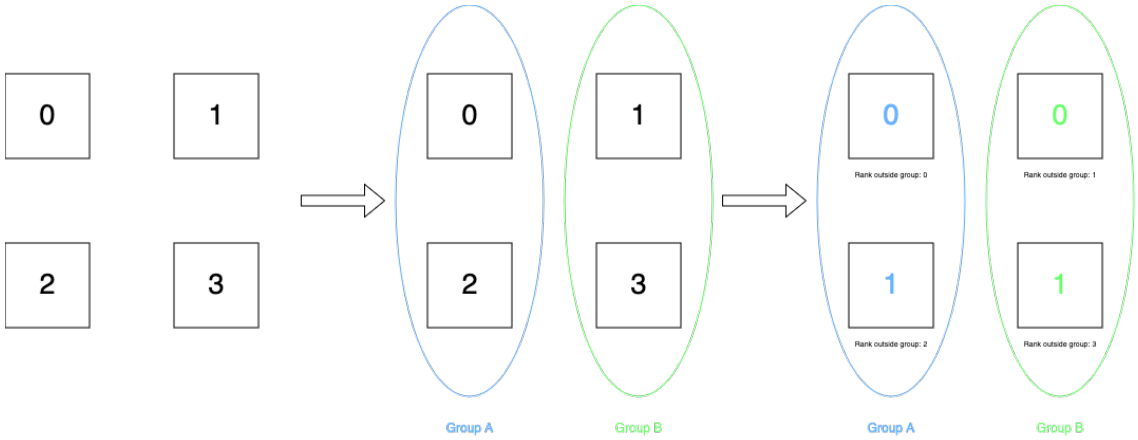
The `key` parameter is an indication of the rank each process will get on the new communicator. The process with the lowest key value will get rank 0, the process with the second lowest will get rank 1, and so on. By default, if you don't care about the order of the processes, you can simply pass their rank in the original communicator as key, this way, the processes will retain the same order. In other words, `key` controls the rank assignment.

Run the following script on 4 processors, how is the communicator being split? What is the difference between `new_comm0`, `new_comm1` and `new_comm2`? In this case, what is `key` doing?

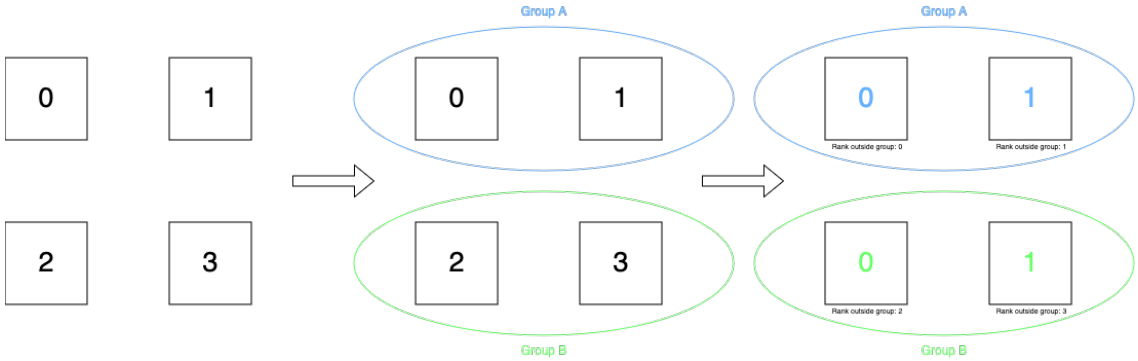
```
from mpi4py import MPI
import numpy as np

# Testing what comm.Split() does

# Initialize MPI (world)
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Defining the subset assignment
if rank == 0:
    color0 = 0
else:
```

```
    color0 = 1
if rank%2 == 0:
    color1 = 0
else:
    color1 = 1
if int(rank/2) == 0:
    color2 = 0
else:
    color2 = 1

new_comm0 = comm.Split(color = color0)
new_rank0 = new_comm0.Get_rank()
new_size0 = new_comm0.Get_size()

new_comm1 = comm.Split(color = color1, key = rank)
new_rank1 = new_comm1.Get_rank()
new_size1 = new_comm1.Get_size()

new_comm2 = comm.Split(color = color2, key = rank)
new_rank2 = new_comm2.Get_rank()
new_size2 = new_comm2.Get_size()

print("Original rank: ", rank,
      " color0: ", color0,
      " new rank0: ", new_rank0,
      " color1: ", color1,
      " new rank1: ", new_rank1,
      " color2: ", color2,
      " new rank2: ", new_rank2)
```

Solution: The following diagrams might be helpful to understand how the splitting is done.



(a) Splitting done in new comm1



(b) Splitting done in new comm2

Exercise II Getting submatrices

Suppose that you are given a matrix $A \in \mathbb{R}^{2n \times 2n}$, for $n \in \mathbb{N}$:

$$A = \begin{bmatrix} A_0 & A_1 \\ A_2 & A_3 \end{bmatrix},$$

where $A_k \in \mathbb{R}^{n \times n}$. Write a Python script using MPI such that:

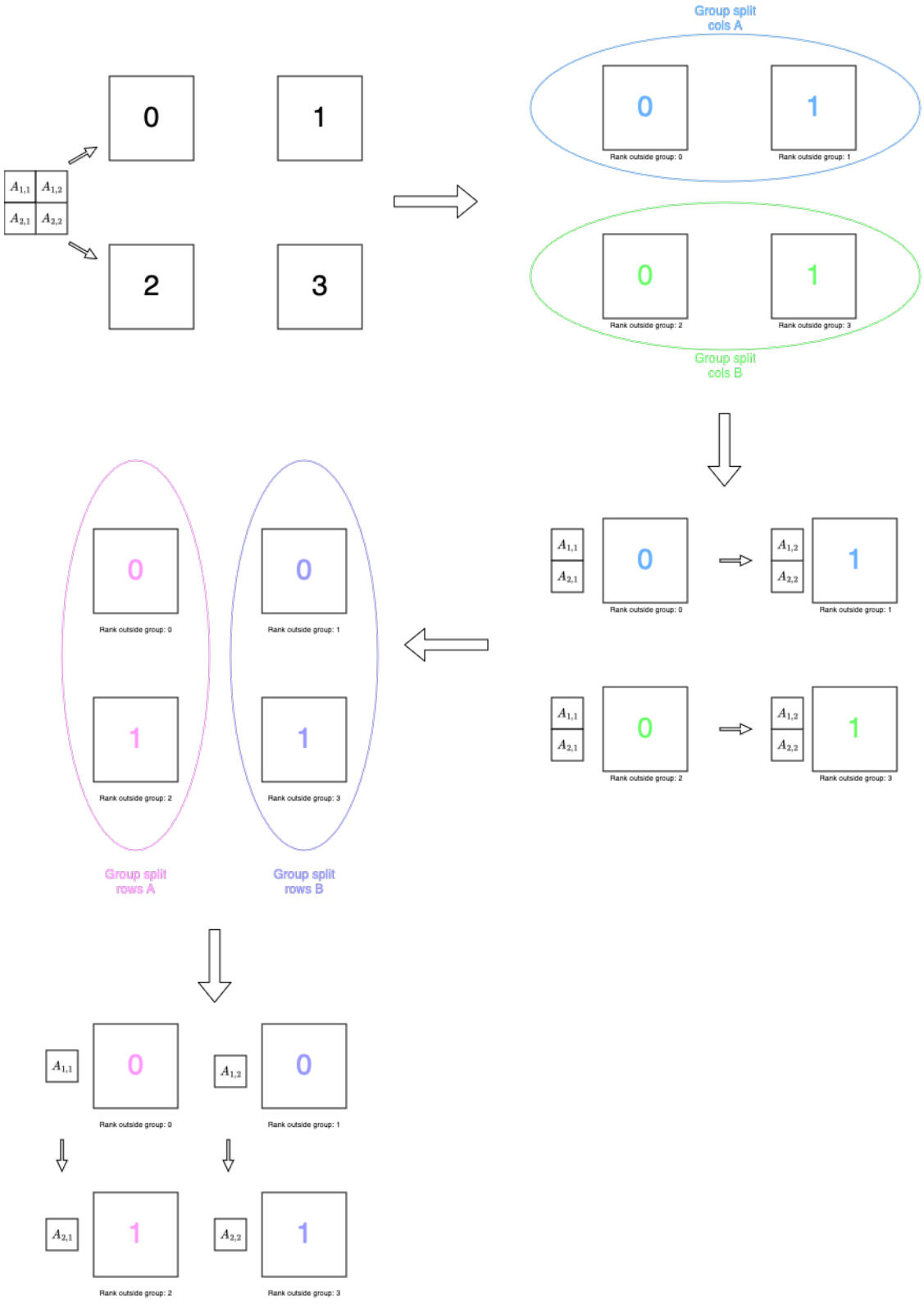
- In the root process it defines a matrix $A \in \mathbb{R}^{2n \times 2n}$, with n the number of processors.
- Using `comm.Split` and `comm.Scatter` distributes the matrix into 4 square sub-blocks by first splitting the matrix into columns and then splitting those columns into rows.
- Prints the sub-blocks in the correct sub-communicator.

Hint: if we want to distribute a matrix $A \in \mathbb{R}^{m \times n}$ first by columns and then by rows, we would need to split the communicator twice. Is there another way of doing this?

Solution: the code that does what was described is the following. Notice that there might be a lot of different ways to obtain the same result.

```
from mpi4py import MPI
import numpy as np

# Testing what comm.Split() does

# Initialize MPI (world)
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Define the matrix
n_blocks = 2
n = size
npr = 2

matrix = None
matrix_transpose = None

if rank%npr == 0:
  matrix = np.arange(1, n*n + 1, 1, dtype=int)
  matrix = np.reshape(matrix, (n,n))
  arrs = np.split(matrix, n, axis=1)
  raveled = [np.ravel(arr) for arr in arrs]
  matrix_transpose = np.concatenate(raveled)
  print(matrix)

comm_cols = comm.Split(color = rank/npr, key = rank%npr)
comm_rows = comm.Split(color = rank%npr, key = rank/npr)

# Get ranks of subcommunicator
rank_cols = comm_cols.Get_rank()
rank_rows = comm_rows.Get_rank()

# Select columns
submatrix = np.empty((n_blocks, n), dtype = 'int')

# Then we scatter the columns and put them in the right order
receiveMat = np.empty((n_blocks*n), dtype = 'int')
comm_cols.Scatterv(matrix_transpose, receiveMat, root = 0)
subArrs = np.split(receiveMat, n_blocks)
raveled = [np.ravel(arr, order='F') for arr in subArrs]
submatrix = np.ravel(raveled, order = 'F')

# Then we scatter the rows
blockMatrix = np.empty((n_blocks, n_blocks), dtype = 'int')
comm_rows.Scatterv(submatrix, blockMatrix, root = 0)


print("Original rank: ", rank,
      " rank in splitrows: ", rank_rows, " rank in splitcols: ", rank_cols,
      "submatrix after scattering columns: ", submatrix,
      "block matrix: ", blockMatrix, "\n\n")
```

The following diagram explains what the code is doing.



Exercise III 2D distribution for matrix vector multiplication

Consider a matrix $A \in \mathbb{R}^{n \times n}$. We can write this matrix as blocks:

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,p} \\ A_{2,1} & A_{2,2} & \dots & A_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ A_{p,1} & A_{p,2} & \dots & A_{p,p} \end{bmatrix},$$

where $p \leq n$. With this notation, not all blocks necessarily have the same dimensions. Then we can write the block version of the matrix-vector multiplication:

$$y = Ax = \begin{bmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,p} \\ A_{2,1} & A_{2,2} & \dots & A_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ A_{p,1} & A_{p,2} & \dots & A_{p,p} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix} = \begin{bmatrix} \sum_{k=1}^{p} A_{1,k} x_k \\ \sum_{k=1}^{p} A_{2,k} x_k \\ \vdots \\ \sum_{k=1}^{p} A_{p,k} x_k \end{bmatrix}.$$

First let $p = 2n$ where n is the number of processors being used. With your answer from the previous exercise, write a Python script such that:

- In the root process defines the matrix A and the vector x
- Using `comm.Split` distributes the blocks of both the matrix and the vector accordingly, the matrix should be split first by columns and then into rows (like on the previous exercise)
- Computes the matrix-vector multiplication using `broadcast`, `scatter`, and/or `reduction`, both on a subset of processors (this is a 2D blocked layout for matrix-vector multiplication)

Solution: the following code solves the problem (even though there are different ways of achieving this). Notice that we also compare our result to the one given by numpy.

```
from mpi4py import MPI
import numpy as np

# 2D distribution for matrix-vector multiplication

# Initialize MPI (world)
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Define the matrix
n_blocks = 4
n = size*2
npr = 2
matrix = None
matrix_transpose = None
x = None
y = None
sol = None

if rank%npr == 0:
  matrix = np.arange(1, n*n + 1, 1, dtype=int)
  matrix = np.reshape(matrix, (n,n))
  arrs = np.split(matrix, n, axis=1)
  raveled = [np.ravel(arr) for arr in arrs]
```

```
  matrix_transpose = np.concatenate(raveled)
  x = np.arange(1, n+1, 1, dtype = int)
  x = np.reshape(x, (n,1) )
  sol = np.empty((n,1), dtype = int)

comm_cols = comm.Split(color = rank/npr, key = rank%npr)
comm_rows = comm.Split(color = rank%npr, key = rank/npr)

# Get ranks of subcommunicator
rank_cols = comm_cols.Get_rank()
rank_rows = comm_rows.Get_rank()

### DISTRIBUTE THE MATRIX
# Select columns
submatrix = np.empty((n_blocks, n), dtype = 'int')

# Then we scatter the columns and put them in the right order
receiveMat = np.empty((n_blocks*n), dtype = 'int')
comm_cols.Scatterv(matrix_transpose, receiveMat, root = 0)
subArrs = np.split(receiveMat, n_blocks)
raveled = [np.ravel(arr, order='F') for arr in subArrs]
submatrix = np.ravel(raveled, order = 'F')

# Then we scatter the rows
blockMatrix = np.empty((n_blocks, n_blocks), dtype = 'int')
comm_rows.Scatterv(submatrix, blockMatrix, root = 0)

### DISTRIBUTE X USING COLUMNS
x_block = np.empty((n_blocks, 1), dtype = 'int')
comm_cols.Scatterv(x, x_block, root = 0)

# Multiply in place each block matrix with each x_block
local_mult = blockMatrix@x_block

# Now sum those local multiplications along rows
rowmult = np.empty((n_blocks, 1), dtype = 'int')
comm_cols.Reduce(local_mult, rowmult, op = MPI.SUM, root = 0)

# # Now we gather all of this on the root process of the original comm
if rank_cols == 0:
    comm_rows.Gather(rowmult, sol, root = 0)

# Print in the root process
if(rank == 0):
    print("Solution with MPI: ", np.transpose(sol),
          "Solution with Python: ", np.transpose(matrix@x))
```

Exercise IV: Reminder of QR

If we recall what a QR factorization is, given a matrix $W \in \mathbb{R}^{m\times n}$, with $m \geq n$, its QR factorization is

$$W = QR = \begin{bmatrix}\tilde{Q} & \bar{Q}\end{bmatrix}\begin{bmatrix}\tilde{R}\\ 0\end{bmatrix} = \tilde{Q}\tilde{R},$$

where $Q \in \mathbb{R}^{m\times n}$ orthogonal and $R \in \mathbb{R}^{m\times n}$ upper triangular. Note that W can be seen as a map $W : \mathbb{R}^n \to \mathbb{R}^m$.

a) Using this factorization, state an orthonormal basis for the span of W and one for the nullspace of W. *Solution:* an orthonormal basis is given by the columns of $\tilde{Q}$ while an orthonormal basis is given by the columns of $\bar{Q}$.

b) Consider the code below, it computes $\tilde{Q}$ without using MPI. Try running the code with the two matrices defined. Do you notice any problems with CGS here? What could be improved when building the projector P? Compute $\|I - \tilde{Q}^\top \tilde{Q}\|$, $\kappa(W)$, and $\kappa(\tilde{Q})$. State the time it takes for this code to run. Compare this implementation with `numpy`'s QR function. What would happen if we just use Python's built in matrix-matrix/vector multiply `@` instead of the user-defined `matrixVectorMultiply` and `matrixMatrixMultiply`?

```
import numpy as np
from numpy.linalg import norm
import time
import matplotlib.pyplot as plt

# Non paralell implementation of QR algorithm (just get Q)

def matrixVectorMultiply(A, x):
    '''
    Serial implementation of matrix vector multiply
    '''
    m = A.shape[0]
    y = np.zeros((m,), dtype = 'd')
    for i in range(m):
        y[i] = A[i, :]@x
    return y

def matrixMatrixMultiply(A, B):
    '''
    Computes the product C = A@B with outer
    product summation
    '''
    m = A.shape[0]
    n = A.shape[1]
    p = B.shape[1]
    C = np.zeros((m, p), dtype = 'd')
    for i in range(n):
        C += A[:, i]@B[i, :]
    return C

wt = time.time() # We are going to time this

# Define the matrix
## TEST1: MATRIX1
size = 4
m = 50*size
n = 20*size
W = np.arange(1, m*n + 1, 1, dtype = 'd')
W = np.reshape(W, (m, n))
W = W + np.eye(m, n) # Make this full rank
# ## TEST2: MATRIX2
# m = 4
# n = 3
# ep = 1e-12
```

```
# W = np.array([[1, 1, 1], [ep, 0, 0], [0, ep, 0], [0, 0, ep]])
I = np.eye(m, m, dtype = 'd')
Q = np.zeros((m,n), dtype = 'd')

# First column
qk = W[:, 0]
qk = qk/norm(qk)
Q[:, 0] = qk

# Start itarating through the columns of W
for k in range(1, n):
    ## Build the projector
    # Is there a better way of defining this projector?
    P = I - Q@Q.T
    qk = matrixVectorMultiply(P, W[:, k]) # project
    qk = qk/norm(qk) # Normalize
    Q[:, k] = qk

wt = time.time() - wt
#print(Q)
print("Time taken: ", wt)

wt = time.time()
Q_true, R_true = np.linalg.qr(W)
wt = time.time() - wt
print("Time with numpy's QR: ", wt)


# We see the loss in orthogonality
loss_orth = np.empty((n, ))
for k in range(1,n+1):
    loss_orth[k-1] = norm( np.eye(k) - Q[:, 0:k].T@Q[:, 0:k], 'fro' )

plt.figure()
plt.loglog(range(1,n+1), loss_orth)
plt.title("Loss in orthogonality, Frobenius norm")
plt.xlabel("k")
plt.ylabel("$\| I - Q_{k}^{T}Q_{k} \|_{F}$")

plt.show()
```

Solution: What could be improved when building the projector P is not using the whole Q matrix on each iteration. Notice that before reaching the last iteration, the last columns of this matrix are just zeros. We could just use the non zero columns when computing the projector. Python's built-in matrix-matrix/vector multiply will make our code faster since it uses optimized run times.

Exercise V: CGS and MPI

Consider the script given above. Which parts could benefit from using MPI? Which information do you need to scatter/broadcast? In this section we are going to implement CGS, this means that for every q_k we need to define the following projector:

$$P_{j-1} = I - \tilde{Q}_{j-1}\tilde{Q}_{j-1}^{\top}.$$

Notice that because of this, every time we want to project a column of W, W_k we need one synchronization. Take this into consideration for your code. There are different ways of implementing this, below is a rough sketch you could use to guide yourself. Using different values for `m` and `n`, compute $\|I - \tilde{Q}^\top \tilde{Q}\|$, $\kappa(W)$, and $\kappa(\tilde{Q})$. State the time it takes for this code to run. Compute the speedup and compare the computation time with `numpy`'s QR function.

Solution: the script would be the following. Notice that it is still slower than numpy's QR decomposition. What could be improved?

```
from mpi4py import MPI
import numpy as np
from numpy.linalg import norm

# CSG

# Initialize MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

wt = MPI.Wtime() # We are going to time this

m = 50*size
n = 10*size
local_size = int(m/size)

# Define
W = None
Q = None
R = None
Qkreceived = None
QT = None
P = None
if rank == 0:
    W = np.arange(1, m*n + 1, 1, dtype = 'd')
    W = np.reshape(W, (m, n))
    W = W + np.eye(m, n) # Make this full rank
    Q = np.zeros((m,n), dtype = 'd')
    QT = np.zeros((n,m), dtype = 'd')
    Qkreceived = np.zeros((m, 1), dtype = 'd')
    R = np.zeros((n,n), dtype = 'd')
    P = np.eye( m, m, dtype = 'd')

# In here: we first build Q and then we build R
W_local = np.zeros((local_size, n), dtype = 'd')
q_local = np.zeros((local_size, 1), dtype = 'd')
QT_local = np.zeros((local_size, m), dtype = 'd')
P_local = np.zeros((local_size, m), dtype = 'd')
W_local = comm.bcast(W, root = 0)
comm.Scatterv(P, P_local, root = 0)

# For the first column
q_local = P_local@W_local[:, 0]

# Normalize
comm.Gather(q_local, Qkreceived, root = 0)
```

```
if( rank == 0):
    col = Qkreceived[:, 0]/norm(Qkreceived)
    Q[:, 0] = col
    QT[0, :] = col
comm.Barrier()
comm.Scatterv(QT, QT_local, root = 0) # We have COLUMNS of Q (or rows of Qt)
# Start interating in the columns

for k in range(1, n):
    # We've already built column 0 so we move to column 1
    # First: we must build the projector P, using SUMMA
    localMult = 1/size*np.eye(m,m) - np.transpose(QT_local)@QT_local
    comm.Reduce(localMult, P, op = MPI.SUM, root = 0) # Projector
    comm.Scatterv(P, P_local, root = 0) # scatter rows of projector
    q_local = P_local@W_local[:, k]
    # Normalize
    comm.Gather(q_local, Qkreceived, root = 0)
    if(rank == 0):
        col = Qkreceived[:, 0]/norm(Qkreceived)
        Q[:, k] = col
        QT[k, :] = col
    comm.Barrier()
    comm.Scatterv(QT, QT_local, root = 0)

# Compute R as R = QtA
W_rows = np.zeros((local_size, n), dtype = 'd')
Q_local = np.zeros((local_size, n), dtype = 'd')
comm.Scatterv(W, W_rows, root = 0)
comm.Scatterv(Q, Q_local, root = 0)
localMult_R = np.transpose(Q_local)@W_rows
comm.Reduce(localMult_R, R, op = MPI.SUM, root = 0)


# Print in rank = 0
if( rank == 0):
    wt = MPI.Wtime() - wt
    print("Size of W: ", W.shape)
    print("Orthogonality of Q: ", norm(np.eye(n) - np.transpose(Q)@Q))
    print("Q: \n", Q.shape)
    print("R: \n", R.shape)
    print("Time taken: ", wt)
```