Parallel Programming for HPC - Project

Davide Rossi

University of Trieste

July 8, 2024

Table of contents

Distributed matrix-matrix multiplication

Code versions

- Basic version with the naive algorithm (triple loop)

Code versions

- Basic version with the naive algorithm (triple loop)
- Improved CPU version using BLAS library

Code versions

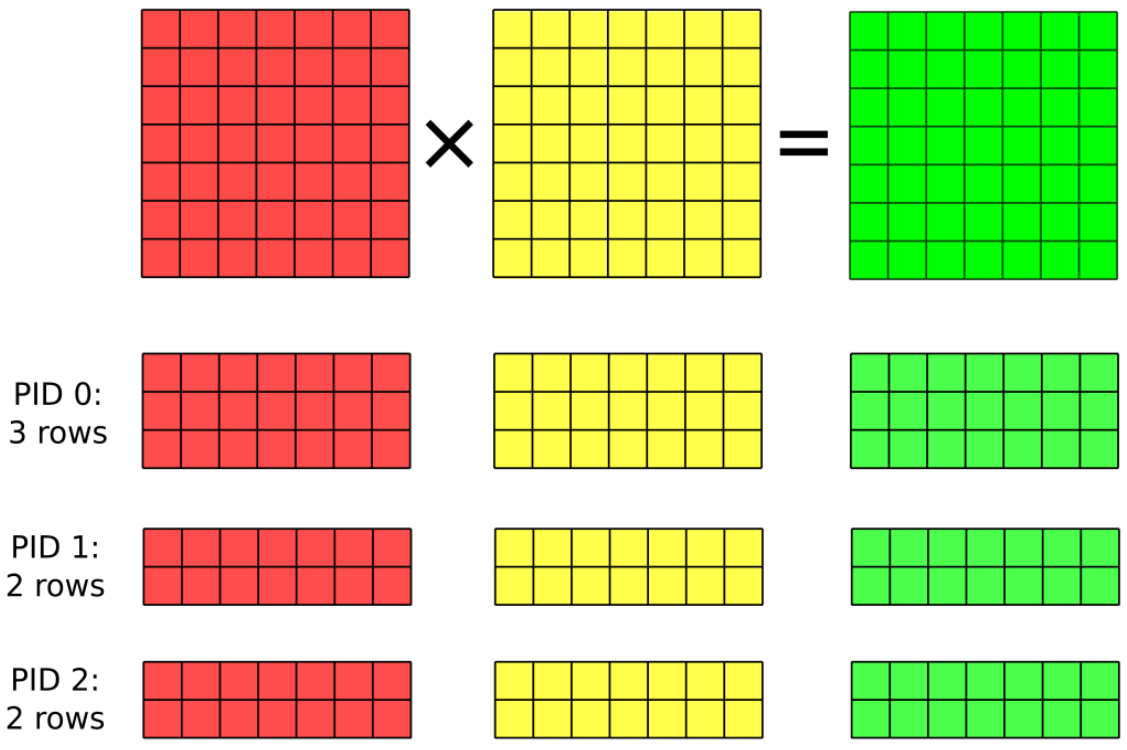
- Basic version with the naive algorithm (triple loop)
- Improved CPU version using BLAS library
- GPU version using CUDA and CUBLAS library

Domain distribution

```
const uint workSize = N / NPEs;
const uint workSizeRem = N % NPEs;
const uint myNRows = workSize + ((uint)myRank < workSizeRem ? 1 : 0);
```

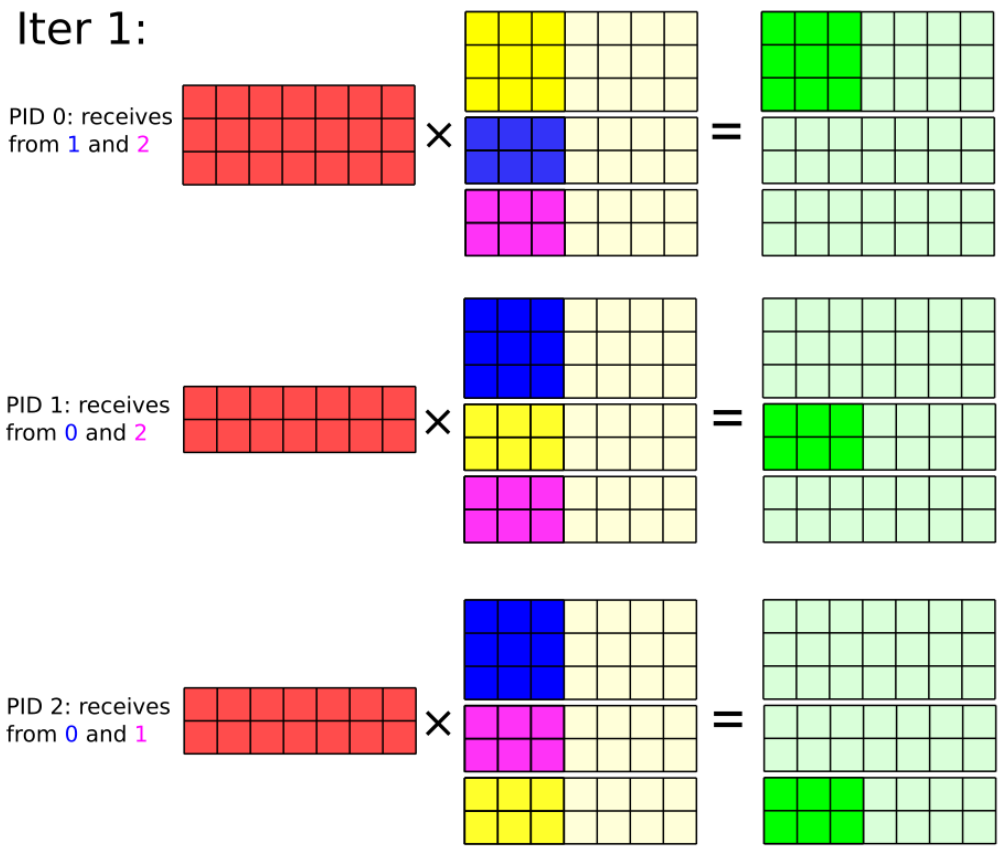
Domain distribution

```
const uint workSize = N / NPEs;
const uint workSizeRem = N % NPEs;
const uint myNRows = workSize + ((uint)myRank < workSizeRem ? 1 : 0);
```

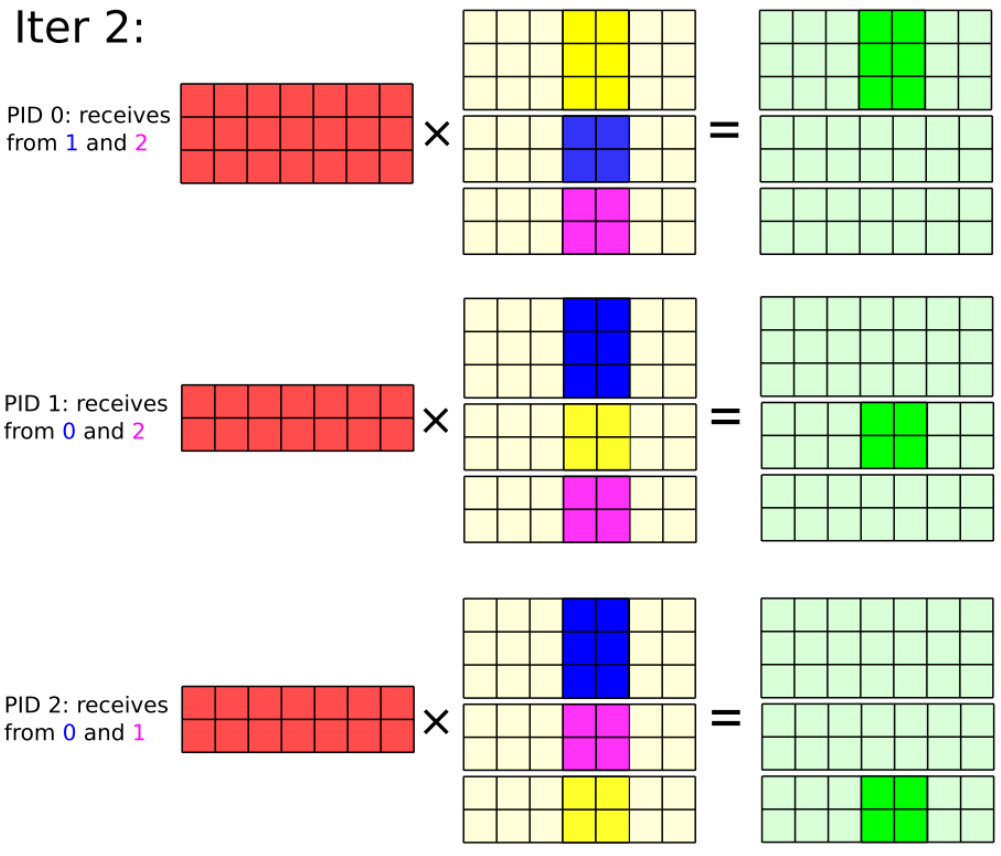


Example: $N = 7$, $NPEs = 3$

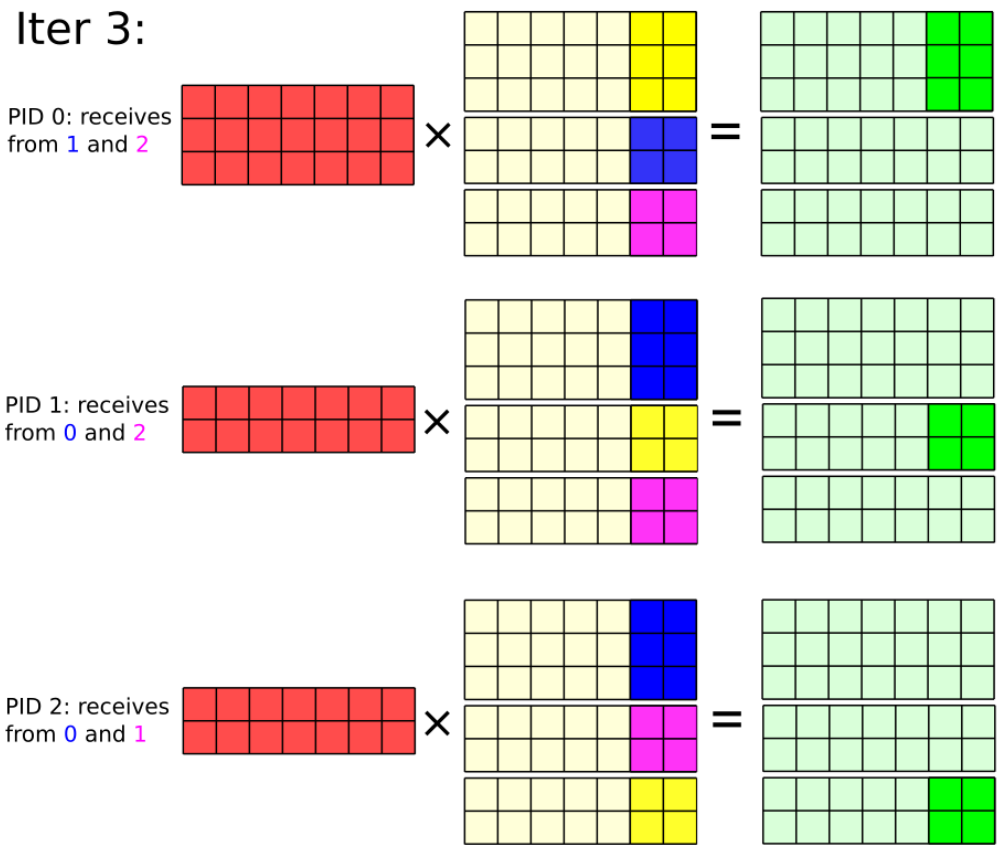
Example: first iteration



Example: second iteration



Example: third iteration



Main code

```
for(uint i = 0; i < (uint)NPEs; i++)
{
    nColumnsBblock = workSize + (i < workSizeRem ? 1 : 0);
    startPoint = i*workSize + (i < workSizeRem ? i : workSizeRem);
    readBlockFromMatrix(myBblock, myB, myNRows, nColumnsBblock, N, startPoint);
    buildRecvCountsAndDispls(recvcounts, displs, NPEs, N, i);
    MPI_Allgatherv(myBblock, myNRows*nColumnsBblock, MPI_DOUBLE, columnB, recvcounts, displs, MPI_DOUBLE, MPI_COMM_WORLD);

    <--  matMul(...)  -->
}
```

CPU baseline: naive algorithm

```
for (uint i = 0; i < myNRows; i++)
    for (uint j = 0; j < nColumnsBblock; j++)
        for (uint k = 0; k < N; k++)
            myC[i*N + j + startPoint] += myA[i*N + k] * columnB[k*N + j];
```

CPU improvement: BLAS

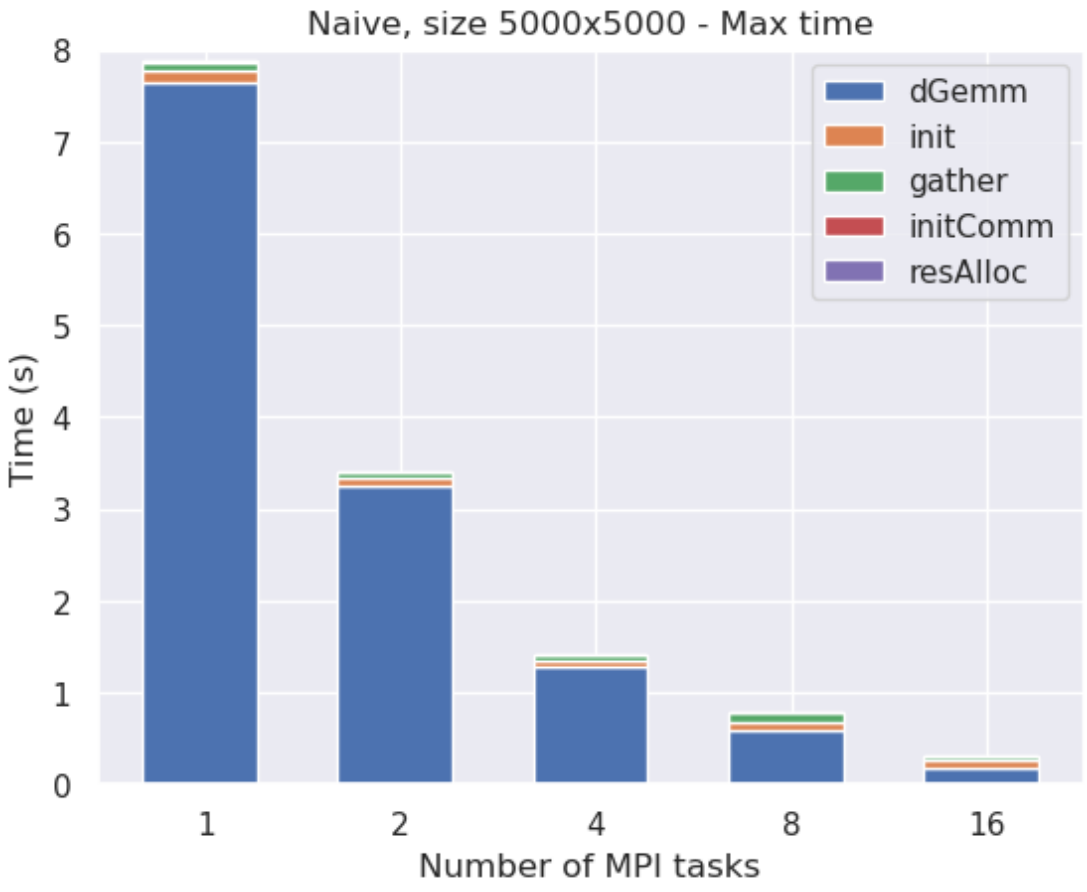
```
cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans, myNRows, nColumnsBblock,
    N, 1.0, myA, N, columnB, nColumnsBblock, 0.0, myCBlock, nColumnsBblock);
placeBlockInMatrix(myCBlock, myC, myNRows, nColumnsBblock, N, startPoint);
```

GPU: CUBLAS

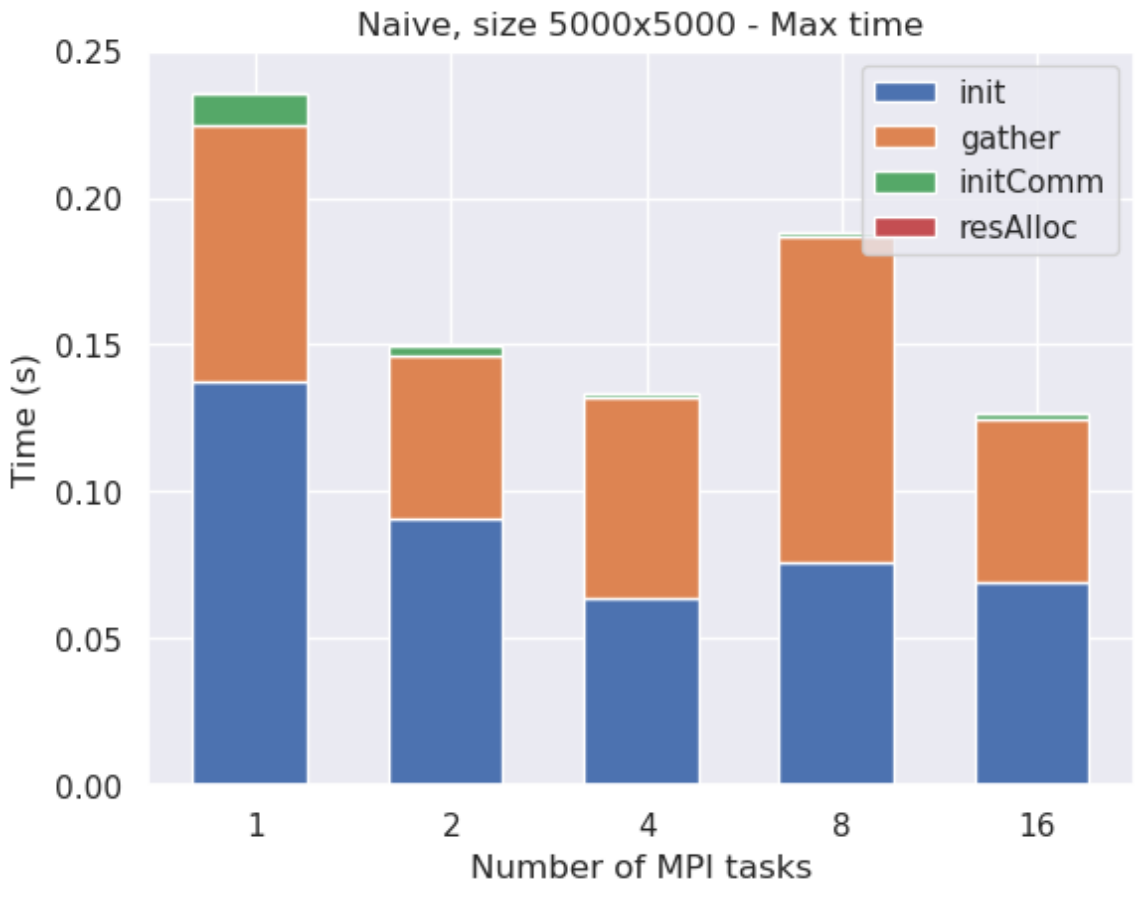
```
cudaMemcpy(columnB_dev, columnB, nColumnsBblock*N*sizeof(double), cudaMemcpyHostToDevice);
cublasDgemm(handle, CUBLAS_OP_N, CUBLAS_OP_N, nColumnsBblock, myNRows,
        N, &alpha, columnB_dev, nColumnsBblock, A_dev, N, &beta, myCBlock_dev, nColumnsBblock);
placeBlockInMatrixKernel<<<numBlocks, threadsPerBlock>>>(myCBlock_dev, C_dev, myNRows, nColumnsBblock, N, startPoint);
```

Results

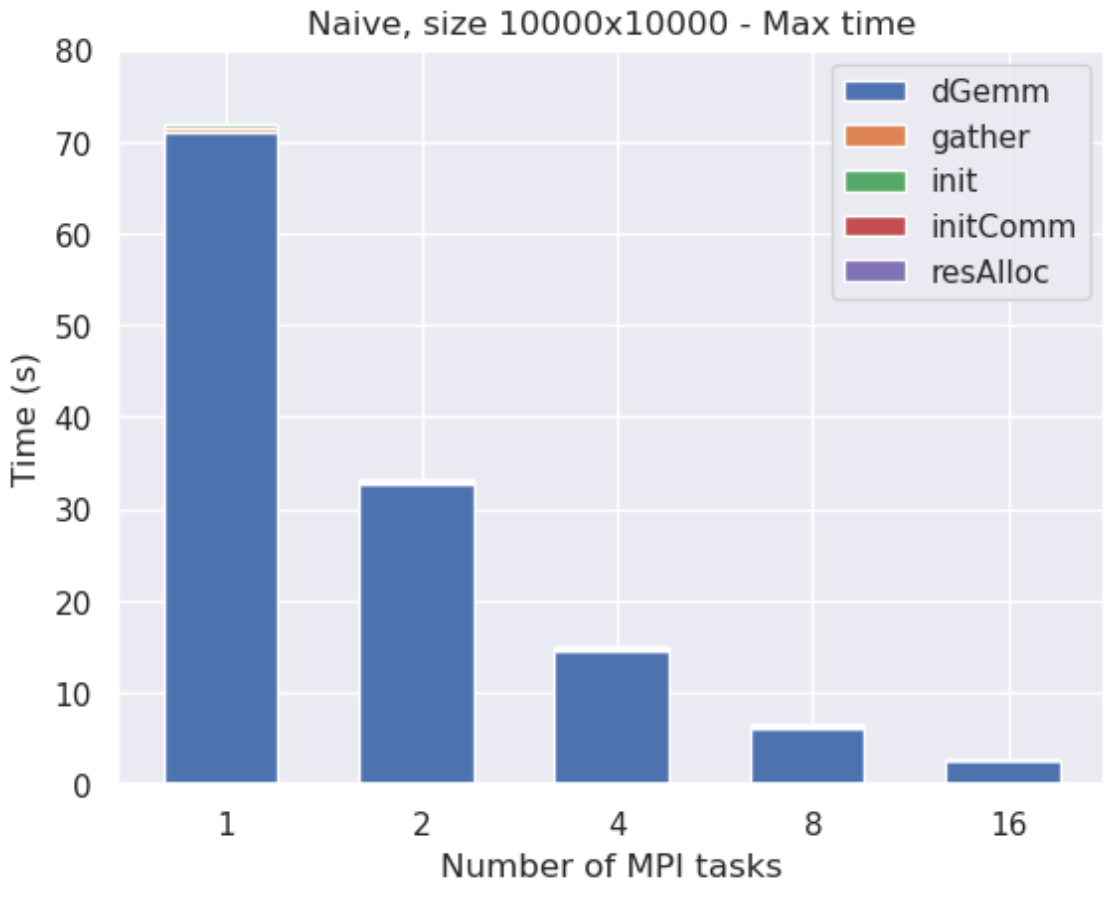
Naive algorithm: size 5000



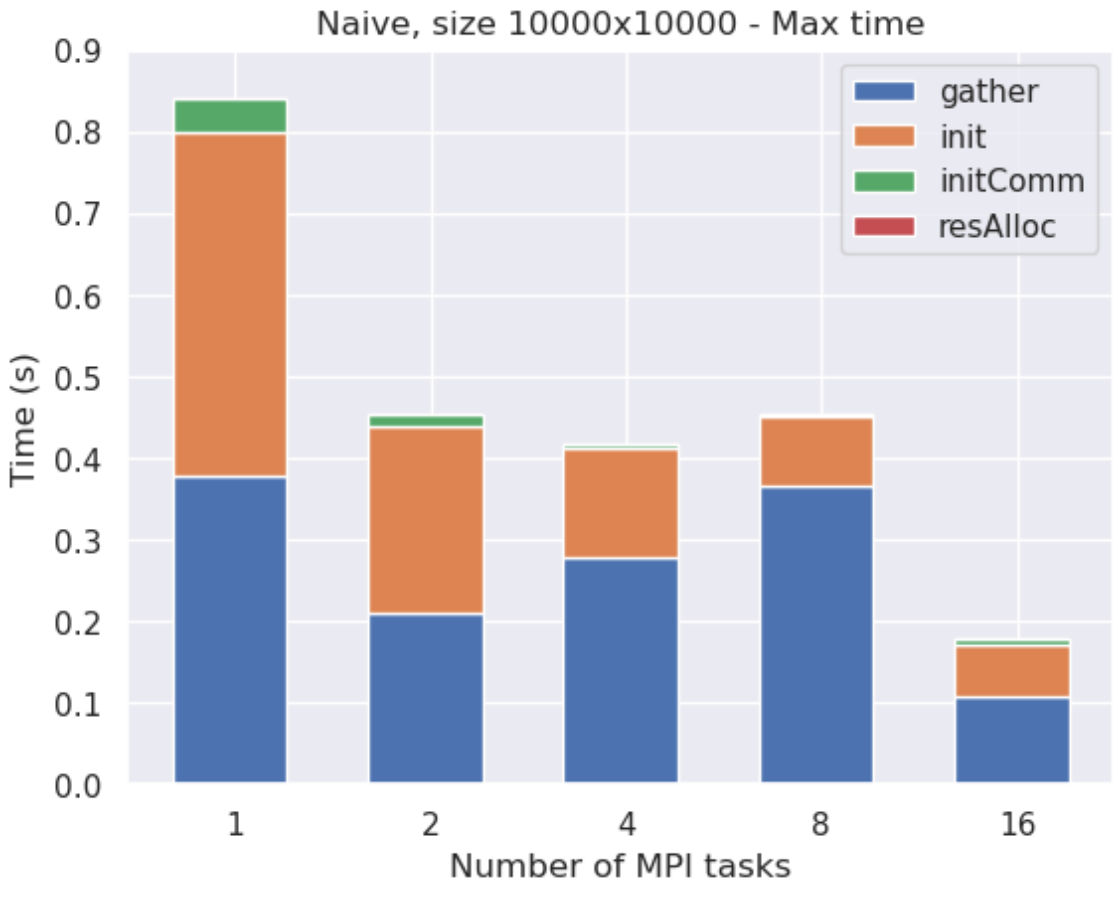
Naive algorithm: size 5000



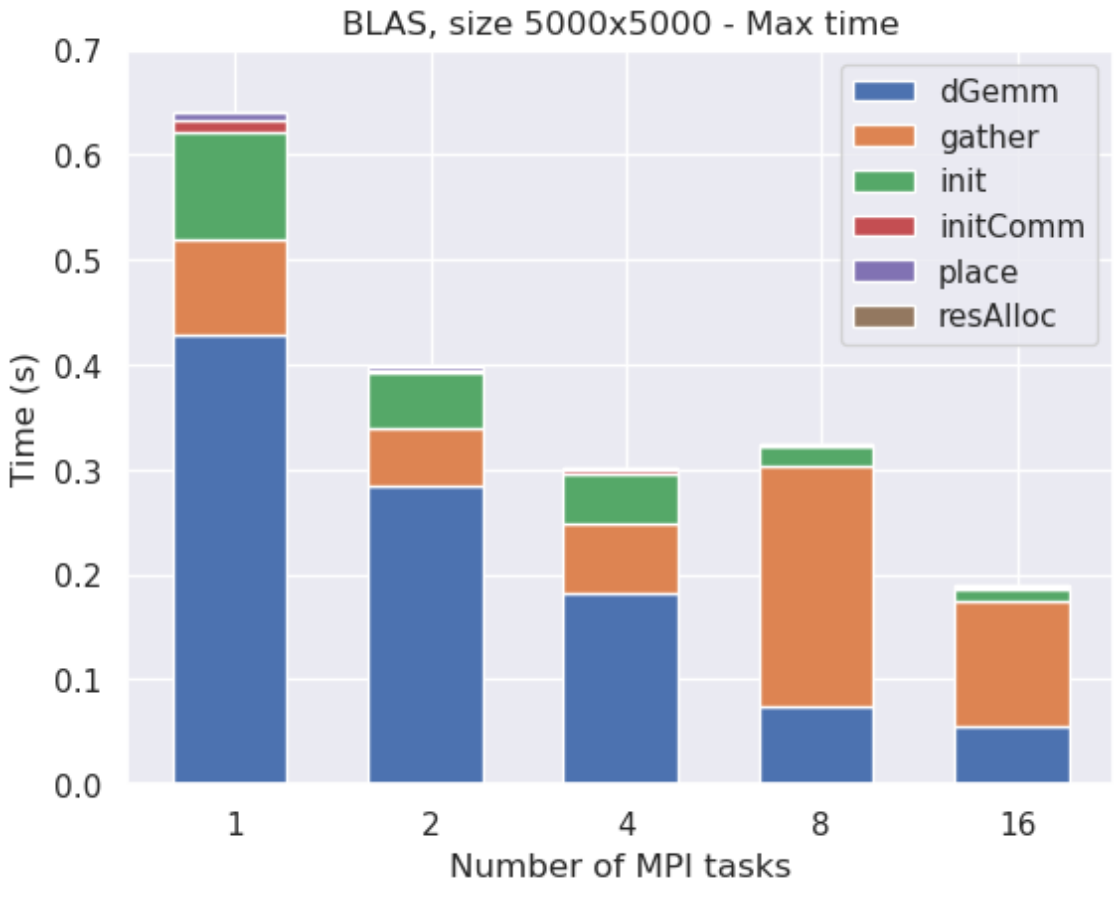
Naive algorithm: size 10000



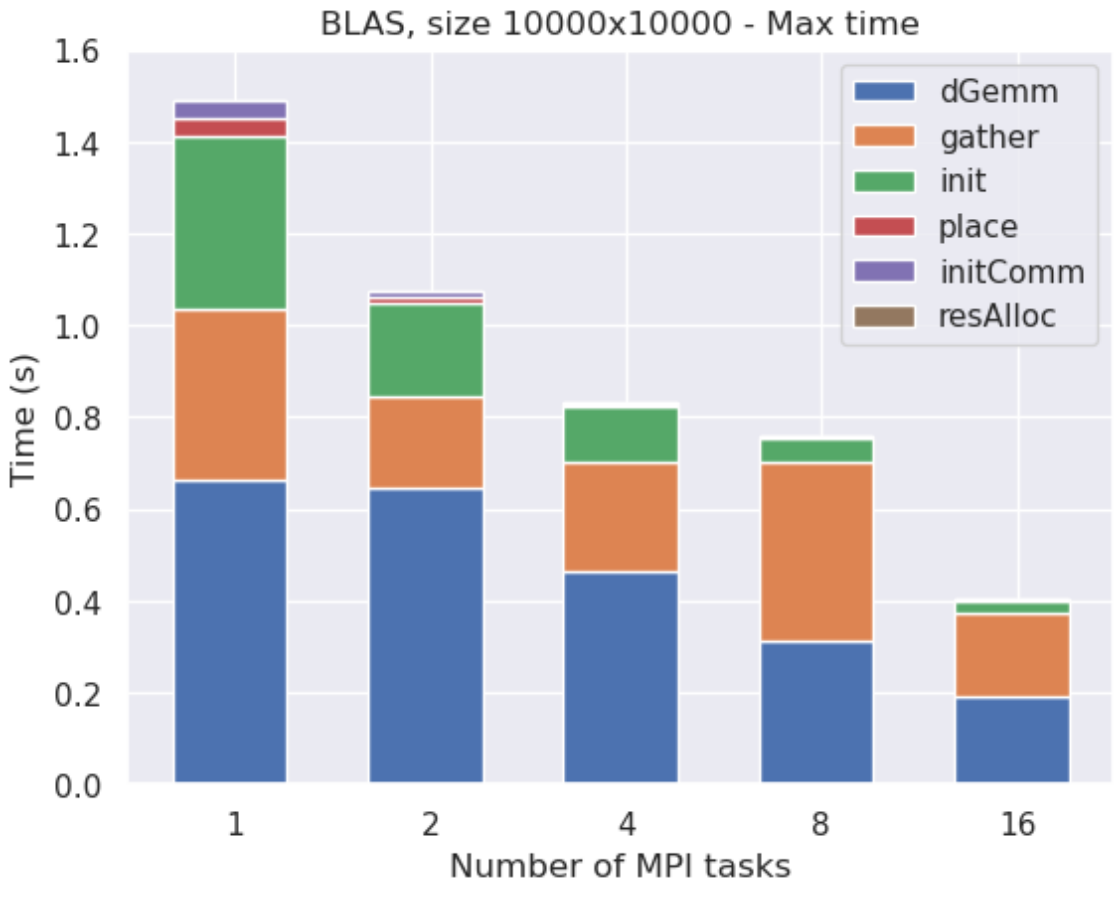
Naive algorithm: size 10000



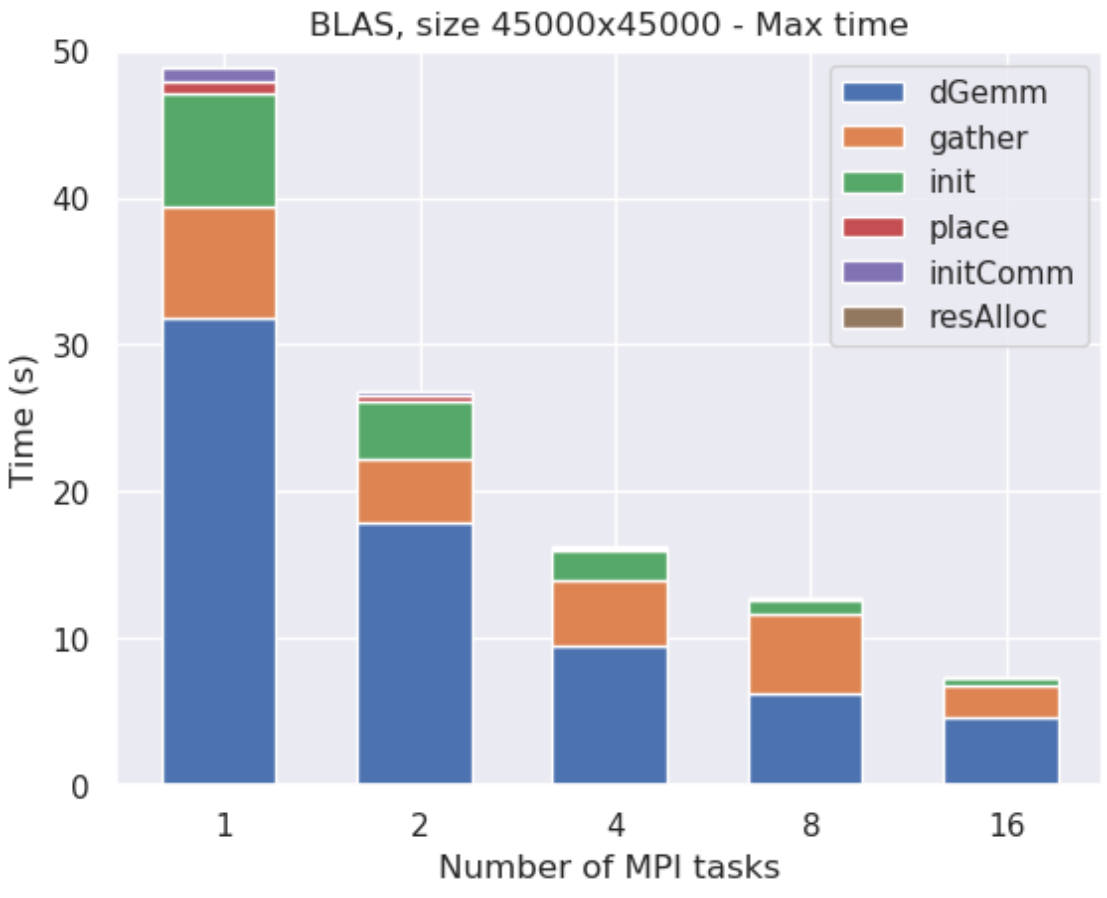
BLAS: size 5000



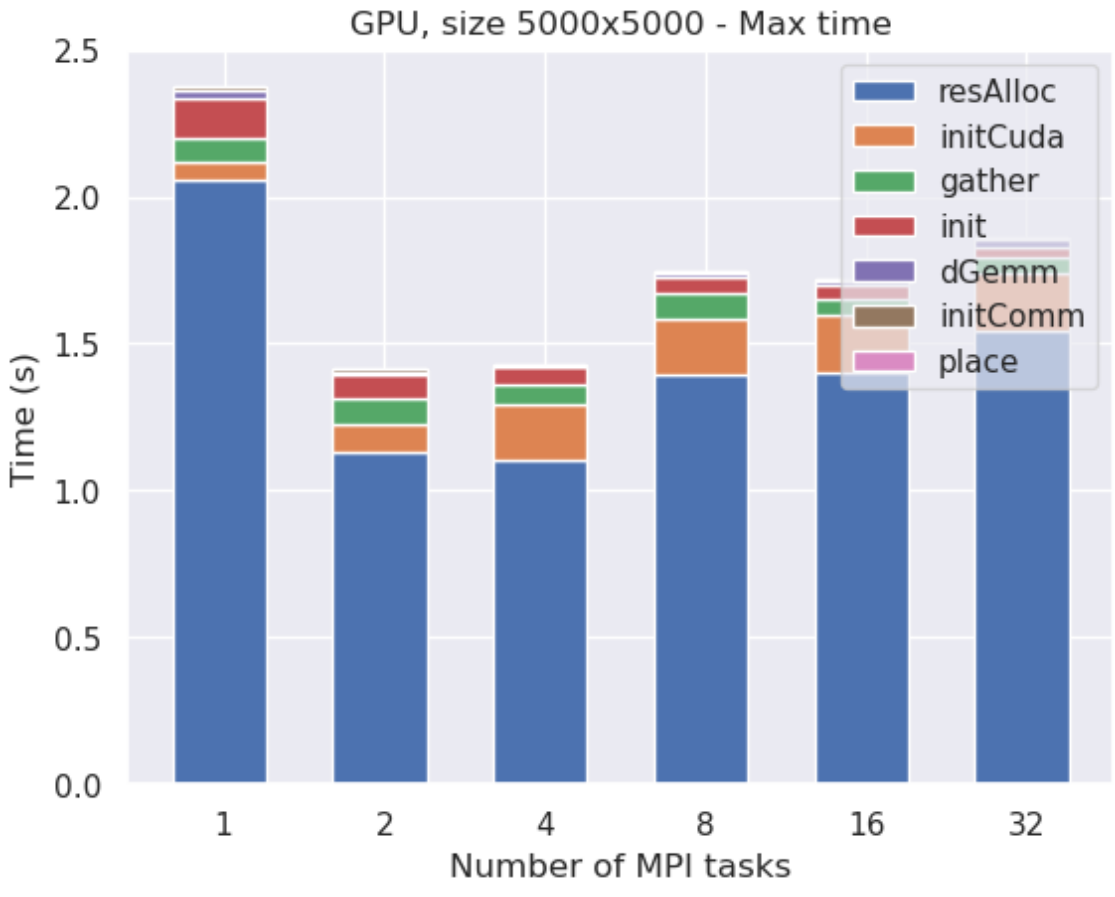
BLAS: size 10000



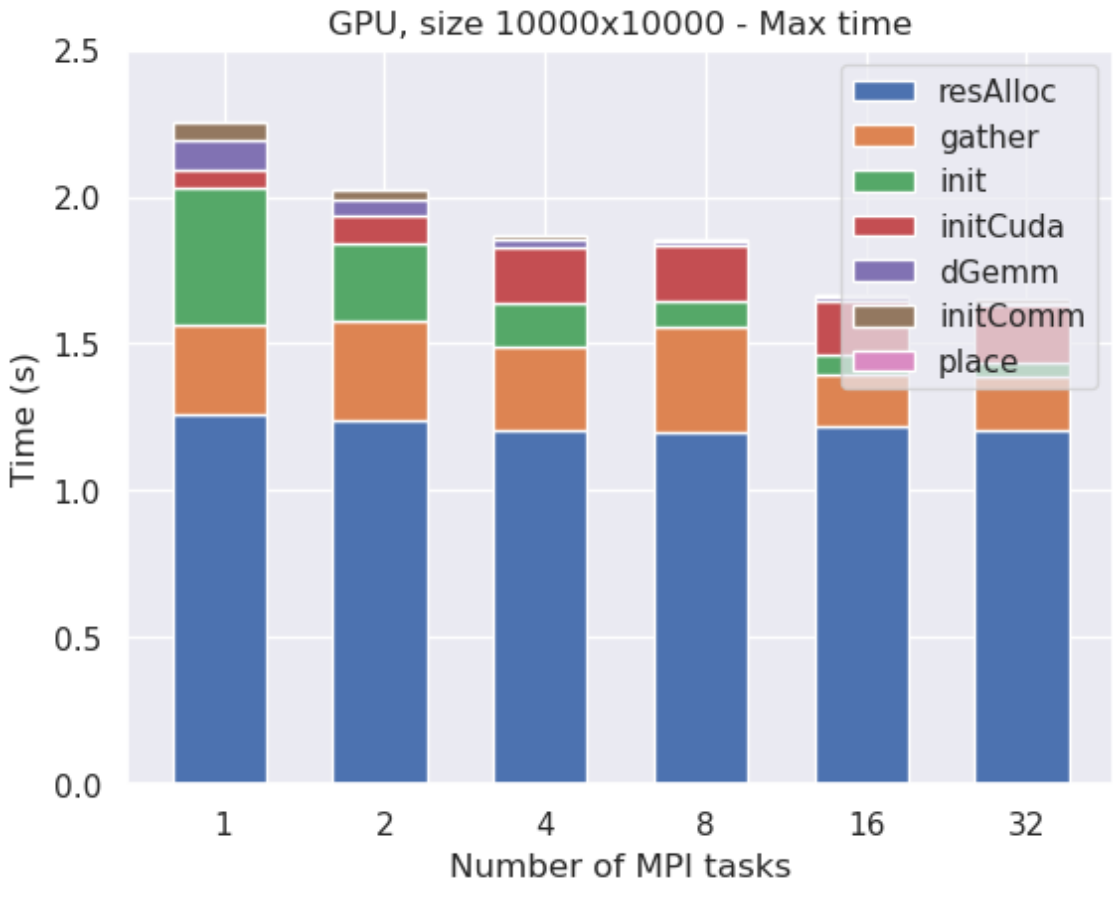
BLAS: size 45000



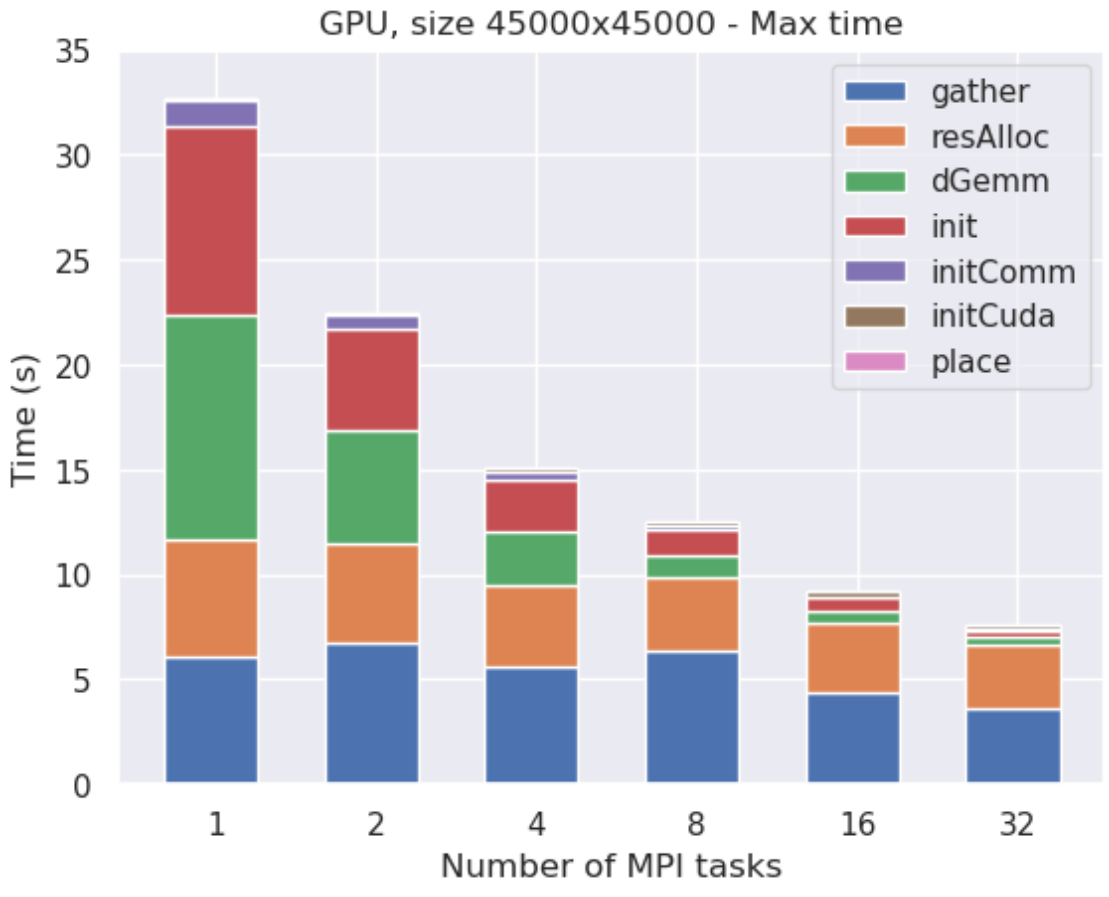
GPU: size 5000



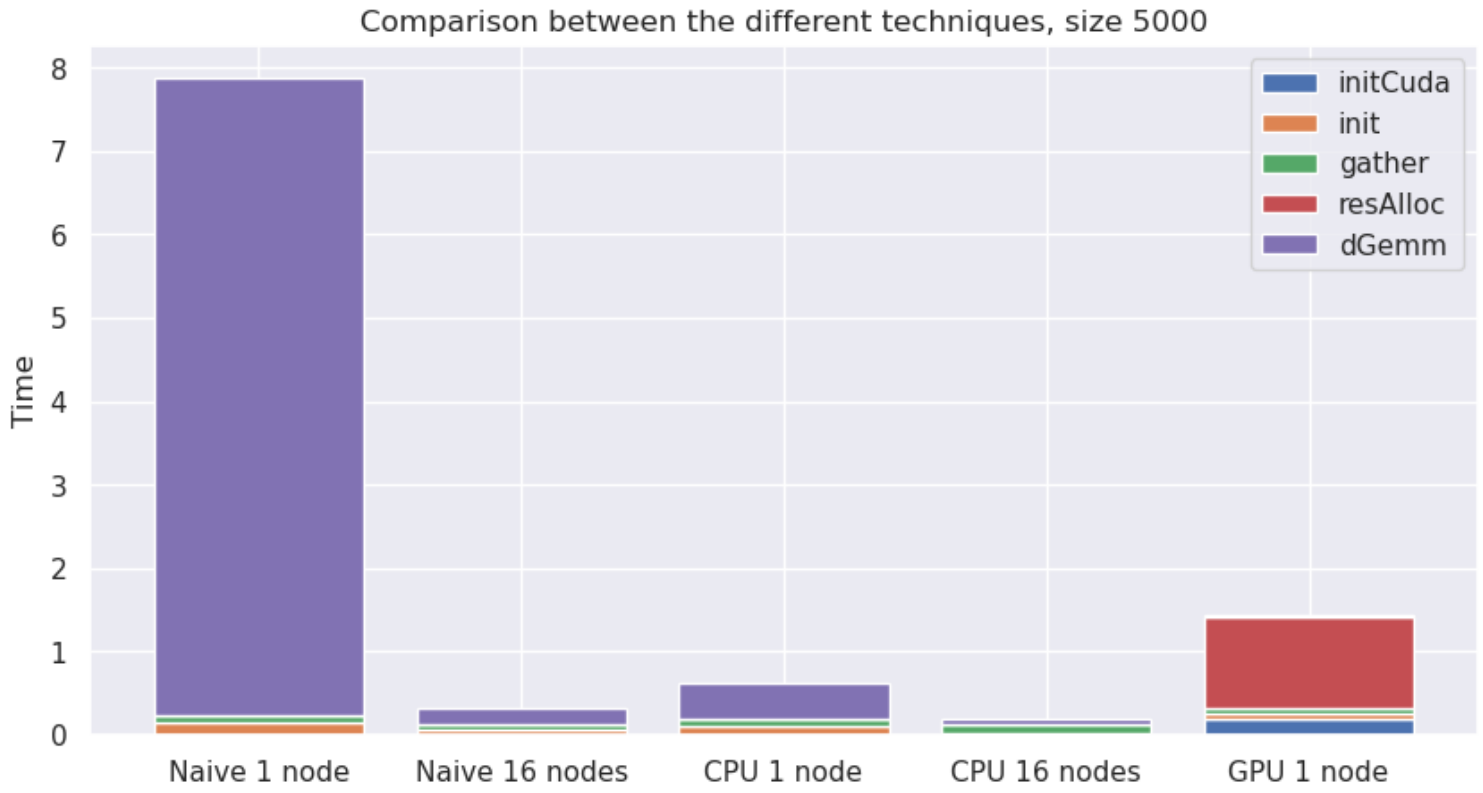
GPU: size 10000



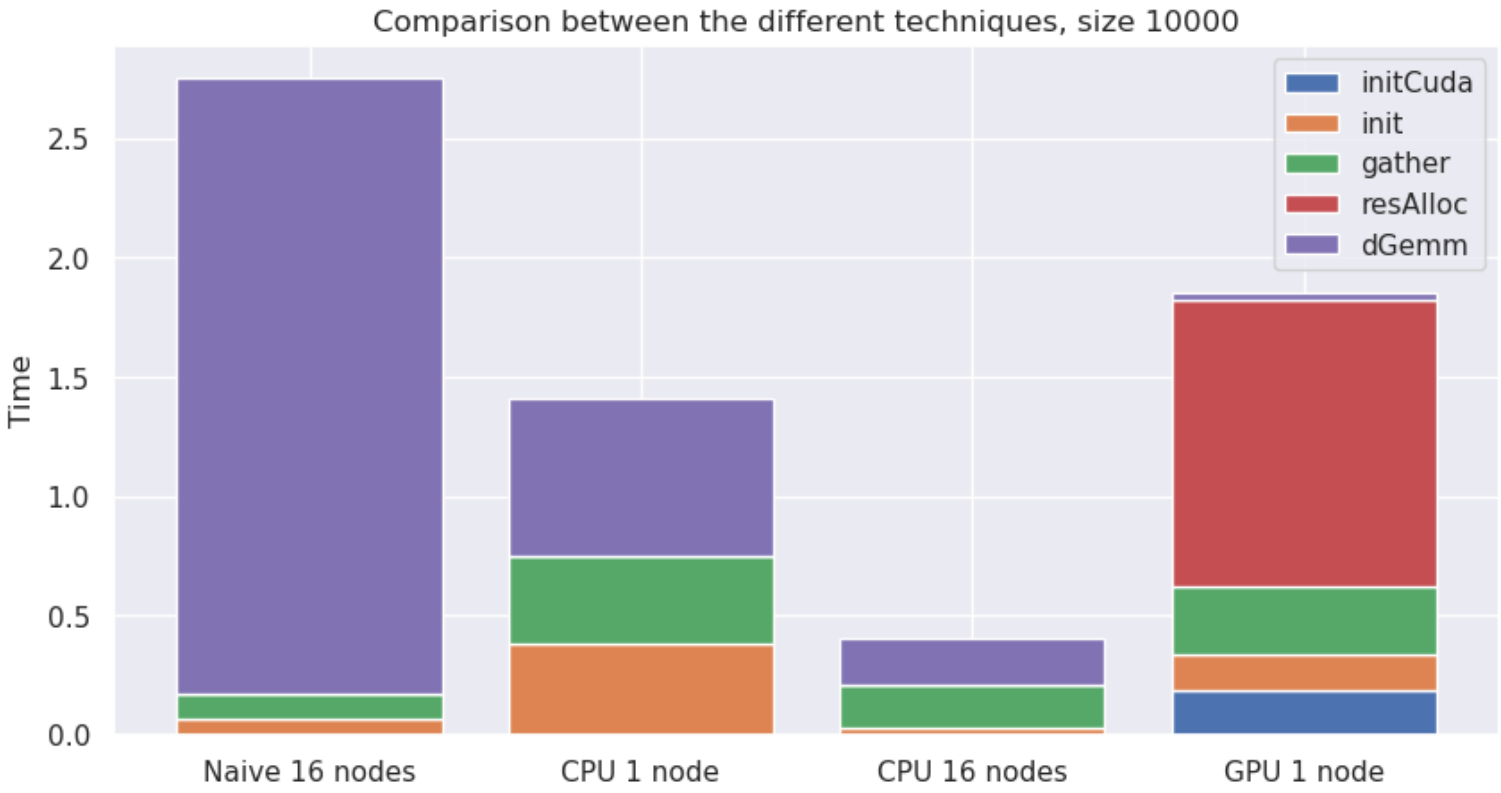
GPU: size 45000



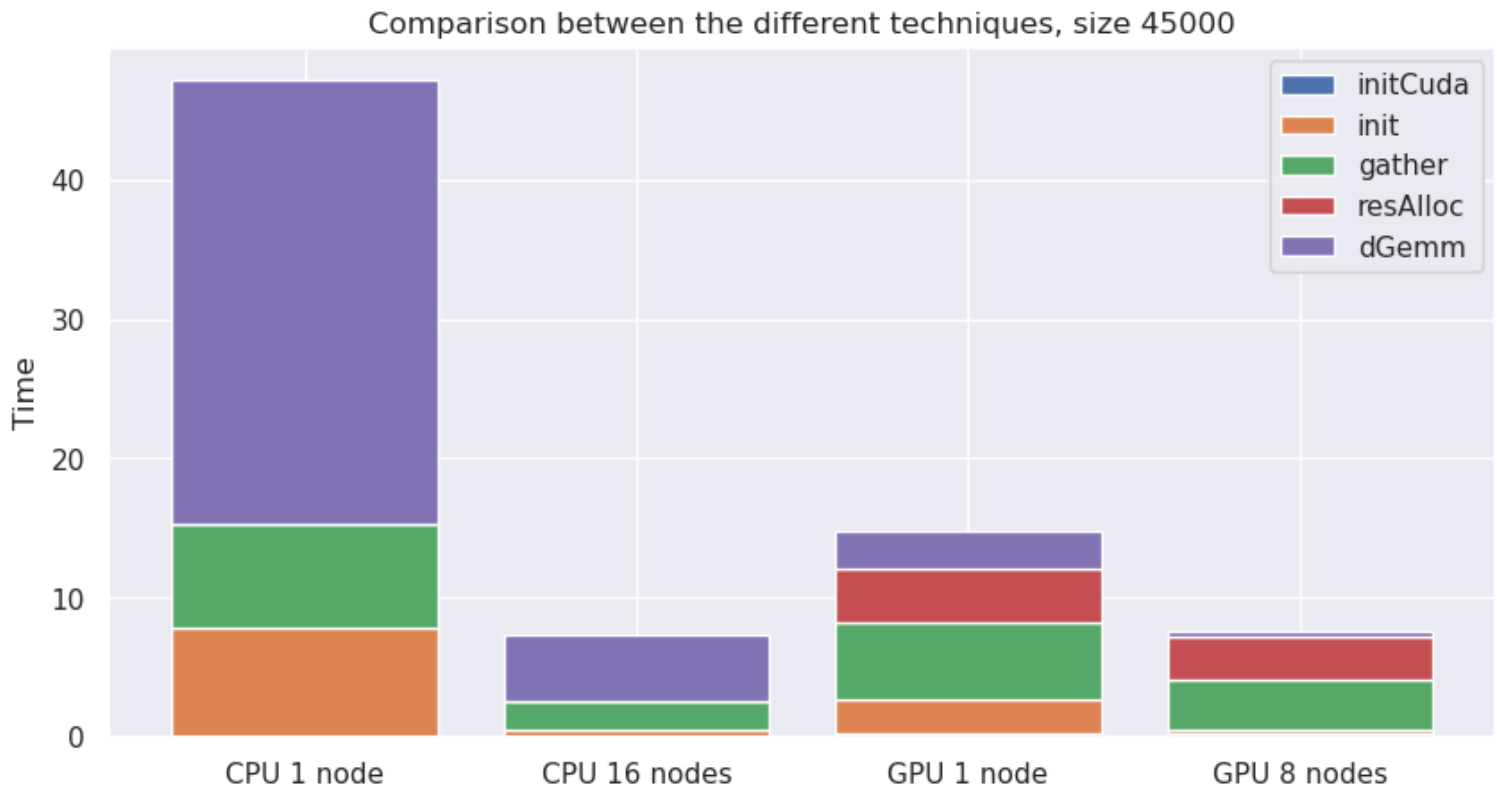
Comparison: size 5000



Comparison: size 10000



Comparison: size 45000



Jacobi's algorithm with Send-Recv communication

Laplace's equation

$$\nabla^2 V = 0$$

Laplace's equation

$$\nabla^2 V = 0$$

In $\mathbb{R}^2$:

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0$$

The algorithm

1. Initialize two matrices as:

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
40.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
50.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
70.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
80.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
100.0	90.0	80.0	70.0	60.0	50.0	40.0	30.0	20.0	10.0	0.0

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
20.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
30.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
40.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
50.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
60.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
70.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
80.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
90.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.0
100.0	90.0	80.0	70.0	60.0	50.0	40.0	30.0	20.0	10.0	0.0

2. Perform the update as:

$$V_{i,j}^{k+1} = \frac{1}{4}\left(V_{i-1,j}^{k} + V_{i+1,j}^{k} + V_{i,j-1}^{k} + V_{i,j+1}^{k}\right)$$

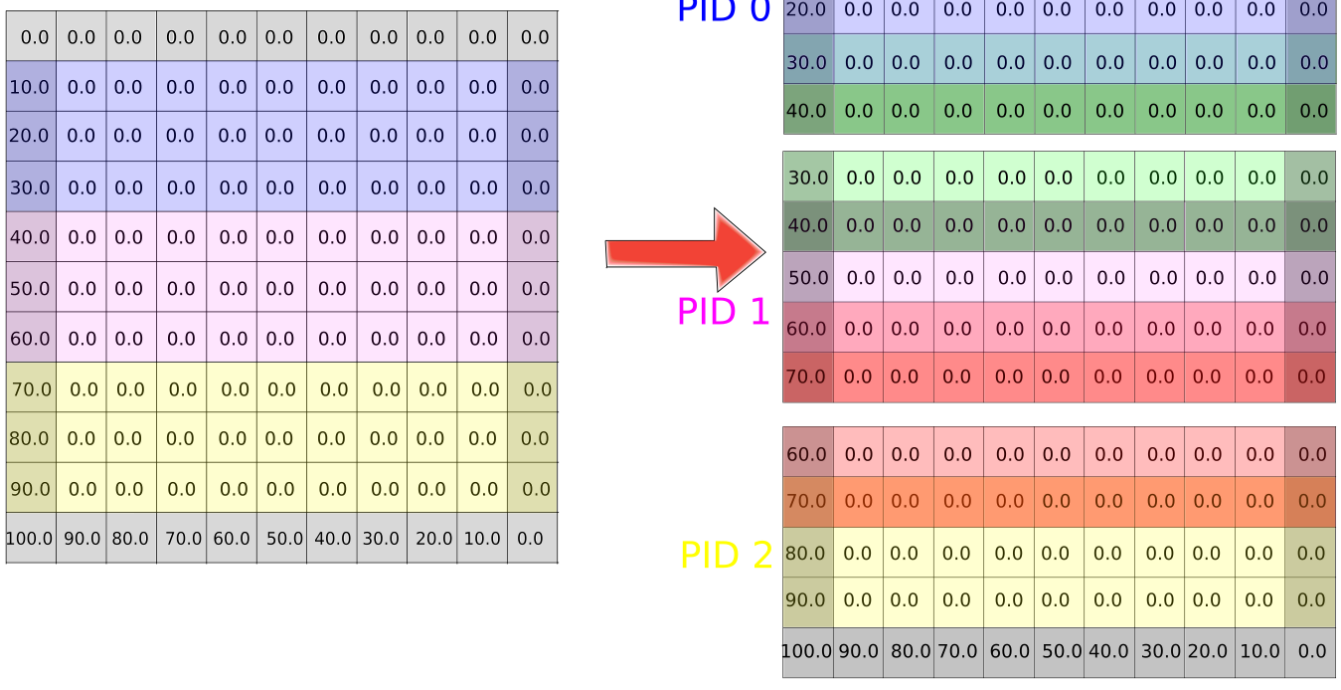
3. swap the pointers of the two matrices and repeat 2 and 3

Domain distribution

```
size_t dim = atoi(nptr: argv[1]);
size_t iterations = atoi(nptr: argv[2]);
size_t dimWithEdge = dim + 2;
const uint workSize = dim/NPEs;
const uint workSizeRemainder = dim % NPEs;
const uint myWorkSize = workSize + ((uint)myRank < workSizeRemainder ? 1 : 0) + 2;  // 2 rows added for the borders
```

Domain distribution

```
size_t dim = atoi(nptr: argv[1]);
size_t iterations = atoi(nptr: argv[2]);
size_t dimWithEdge = dim + 2;
const uint workSize = dim/NPEs;
const uint workSizeRemainder = dim % NPEs;
const uint myWorkSize = workSize + ((uint)myRank < workSizeRemainder ? 1 : 0) + 2;  // 2 rows added for the borders
```



Example: $dim = 9$, $NPEs = 3$

Code

- Update:

```
for(size_t i = 1; i < nRows-1; ++i )
  for(size_t j = 1; j < nCols-1; ++j ) {
    size_t currentEl = i*nCols + j;
    matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                   matrix[currentEl+nCols] + matrix[currentEl-1] );
  }
```

Code

- Update:

```
for(size_t i = 1; i < nRows-1; ++i )
  for(size_t j = 1; j < nCols-1; ++j ) {
    size_t currentEl = i*nCols + j;
    matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                   matrix[currentEl+nCols] + matrix[currentEl-1] );
  }
```

- Communication:

```
MPI_Isend(&matrix_new[nCols], nCols, MPI_DOUBLE, prev, 1, MPI_COMM_WORLD, &send_request[0]);
MPI_Irecv(&matrix_new[0], nCols, MPI_DOUBLE, prev, 0, MPI_COMM_WORLD, &recv_request[0]);

MPI_Isend(&matrix_new[(nRows - 2) * nCols], nCols, MPI_DOUBLE, next, 0, MPI_COMM_WORLD, &send_request[1]);
MPI_Irecv(&matrix_new[(nRows - 1) * nCols], nCols, MPI_DOUBLE, next, 1, MPI_COMM_WORLD, &recv_request[1]);
```

Move to GPU: OpenACC

```
#pragma acc data create(matrix[:myWorkSize*dimWithEdge], matrix_new[:myWorkSize*dimWithEdge]) copyout(matrix[:myWorkSize*dimWithEdge])
{
  init( matrix, matrix_new, myWorkSize, dimWithEdge, prev, next, shift, &t);
  for(size_t it = 0; it < iterations; ++it )
  {
    evolve( matrix, matrix_new, myWorkSize, dimWithEdge, prev, next, &t);
    tmp_matrix = matrix;
    matrix = matrix_new;
    matrix_new = tmp_matrix;
  }
}
```

Move to GPU: OpenACC

```
#ifdef _OPENACC
#pragma acc parallel loop collapse(2) present(matrix[:nRows*nCols], matrix_new[:nRows*nCols])
#else
#pragma omp parallel for collapse(2)
#endif
  for(size_t i = 0; i < nRows; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      matrix[ i*nCols + j ] = 0.5;
      matrix_new[ i*nCols + j ] = 0.0;
    }
```

Move to GPU: OpenACC

```
#ifdef _OPENACC
#pragma acc parallel loop collapse(2) present(matrix[:nRows*nCols], matrix_new[:nRows*nCols])
#else
#pragma omp parallel for collapse(2)
#endif
  for(size_t i = 0; i < nRows; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      matrix[ i*nCols + j ] = 0.5;
      matrix_new[ i*nCols + j ] = 0.0;
    }
```

```
#ifdef _OPENACC
#pragma acc parallel loop collapse(2) present(matrix[:nRows*nCols], matrix_new[:nRows*nCols])
#else
#pragma omp parallel for collapse(2)
#endif
  for(size_t i = 1; i < nRows-1; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      size_t currentEl = i*nCols + j;
      matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                     matrix[currentEl+nCols] + matrix[currentEl-1] );
    }
```

Move to GPU: OpenACC

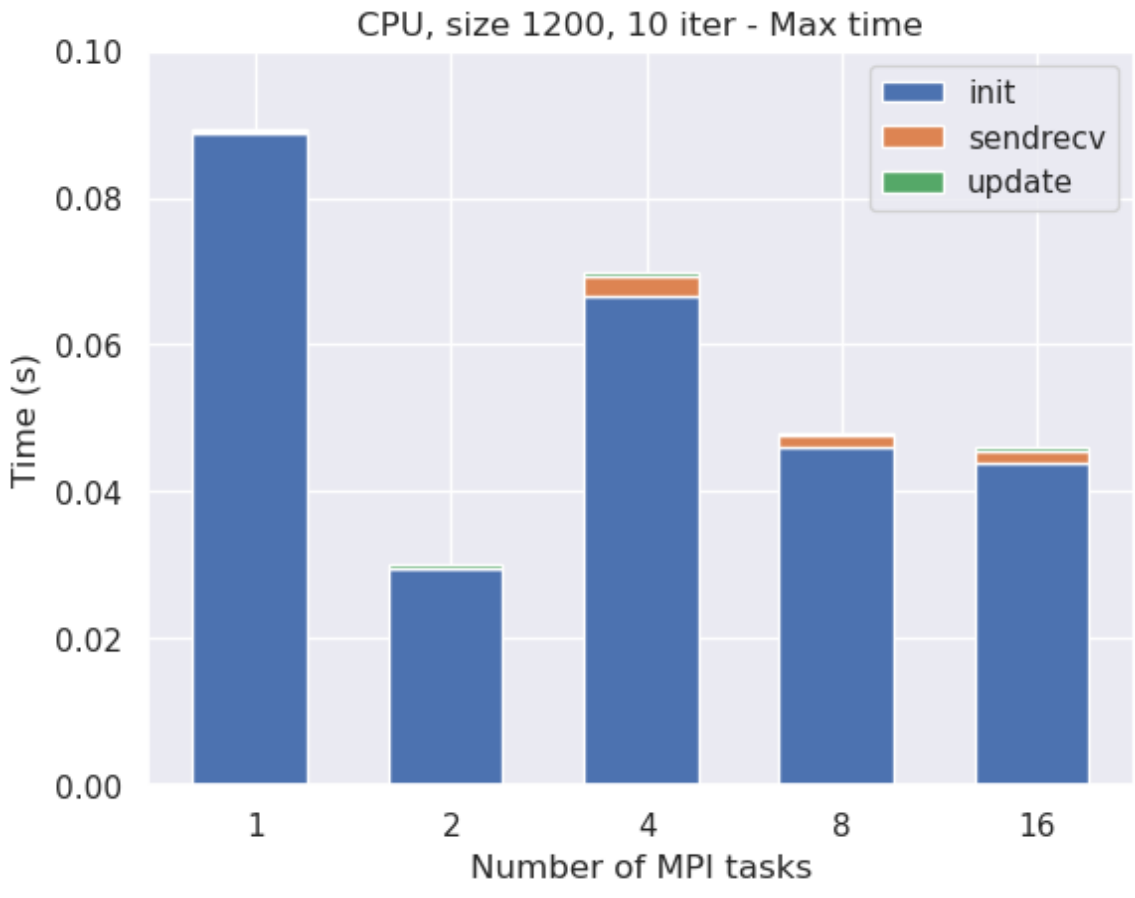
```
#ifdef _OPENACC
#pragma acc parallel loop collapse(2) present(matrix[:nRows*nCols], matrix_new[:nRows*nCols])
#else
#pragma omp parallel for collapse(2)
#endif
  for(size_t i = 0; i < nRows; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      matrix[ i*nCols + j ] = 0.5;
      matrix_new[ i*nCols + j ] = 0.0;
    }
```

```
#ifdef _OPENACC
#pragma acc parallel loop collapse(2) present(matrix[:nRows*nCols], matrix_new[:nRows*nCols])
#else
#pragma omp parallel for collapse(2)
#endif
  for(size_t i = 1; i < nRows-1; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      size_t currentEl = i*nCols + j;
      matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                     matrix[currentEl+nCols] + matrix[currentEl-1] );
    }
```

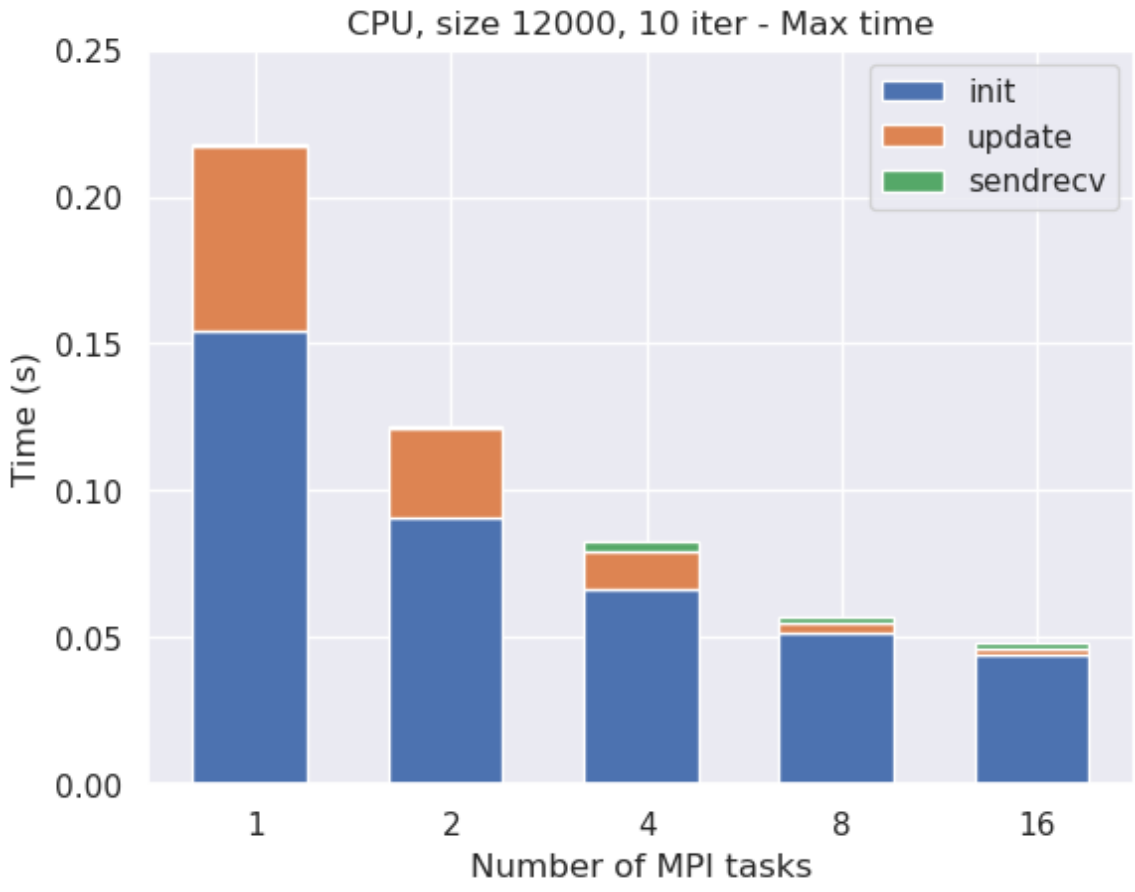
```
  MPI_Request send_request[2], recv_request[2];
#pragma acc host_data use_device(matrix, matrix_new)
  {
    MPI_Isend(&matrix_new[nCols], nCols, MPI_DOUBLE, prev, 1, MPI_COMM_WORLD, &send_request[0]);
    MPI_Irecv(&matrix_new[0], nCols, MPI_DOUBLE, prev, 0, MPI_COMM_WORLD, &recv_request[0]);

    MPI_Isend(&matrix_new[(nRows - 2) * nCols], nCols, MPI_DOUBLE, next, 0, MPI_COMM_WORLD, &send_request[1]);
    MPI_Irecv(&matrix_new[(nRows - 1) * nCols], nCols, MPI_DOUBLE, next, 1, MPI_COMM_WORLD, &recv_request[1]);
  }
  MPI_Waitall(2, send_request, MPI_STATUSES_IGNORE);
  MPI_Waitall(2, recv_request, MPI_STATUSES_IGNORE);
```

Results

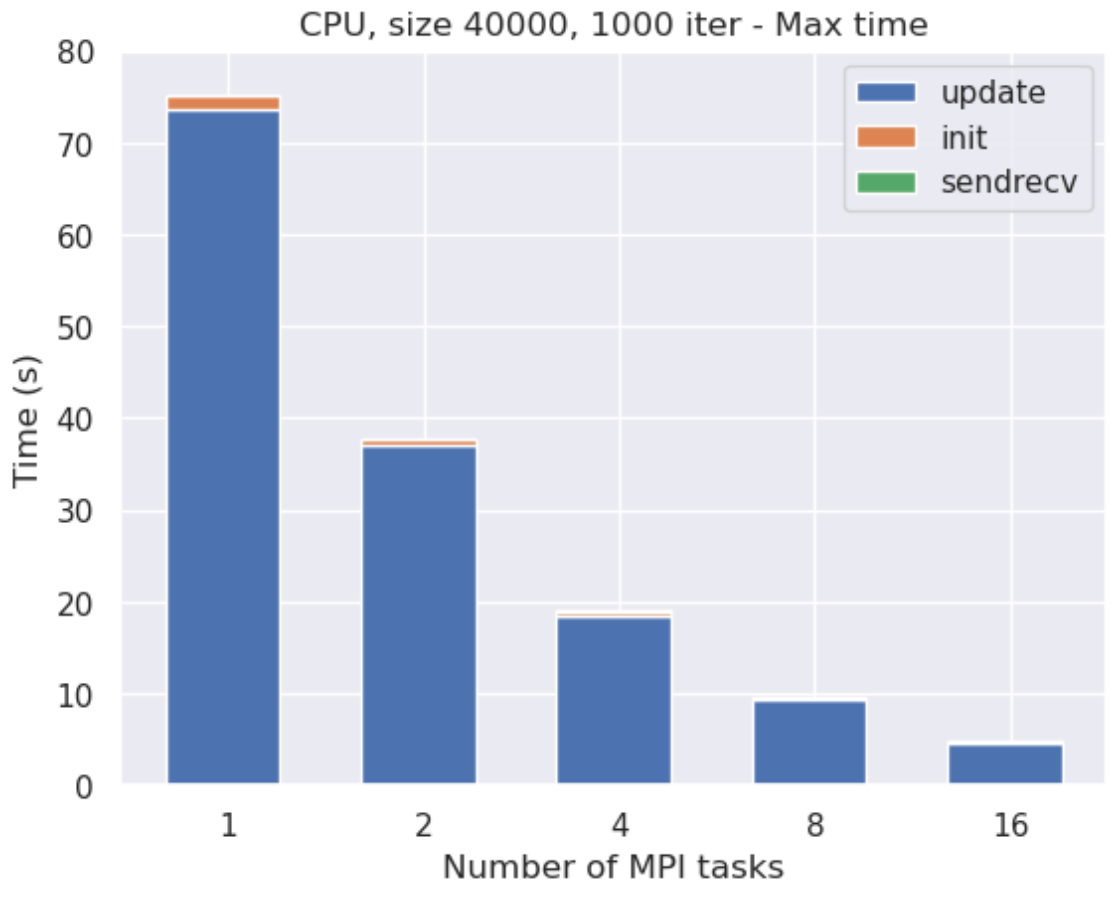
CPU, size 1200, 10 iterations



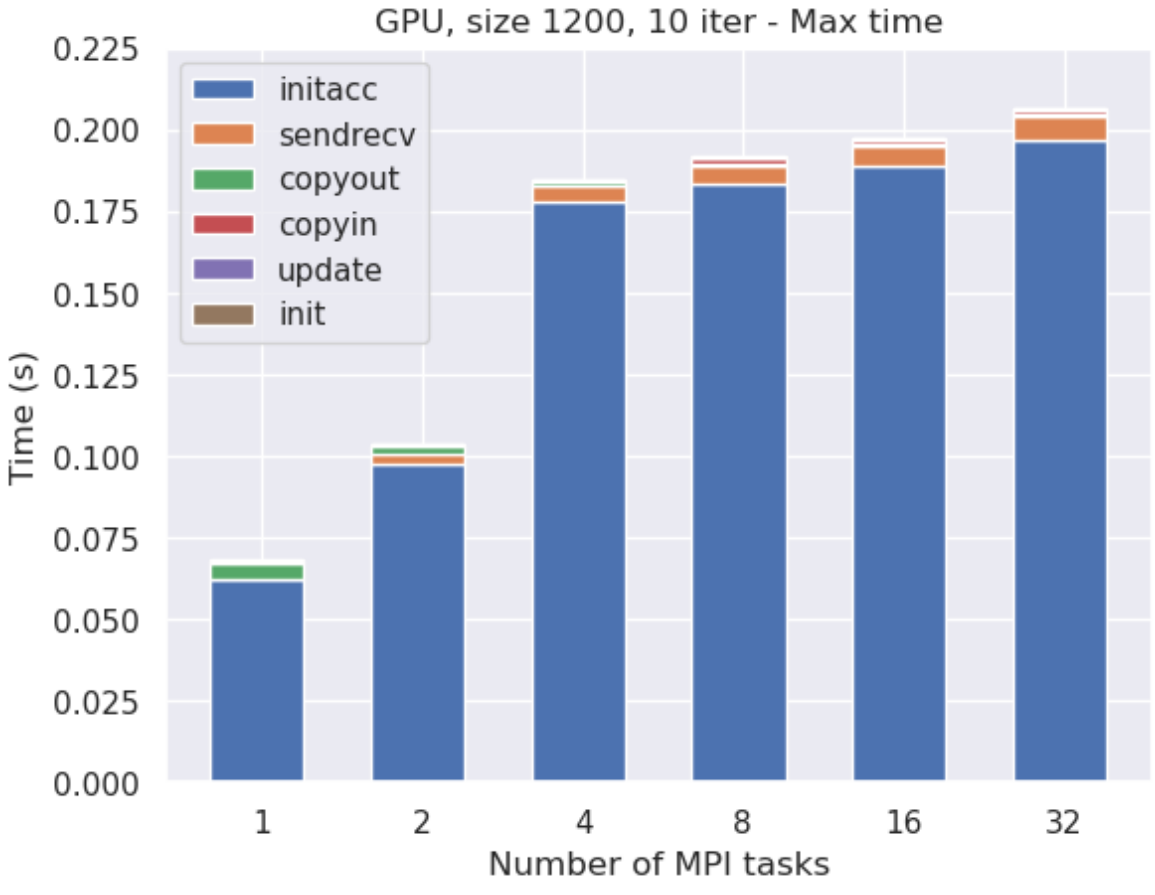
CPU, size 12000, 10 iterations



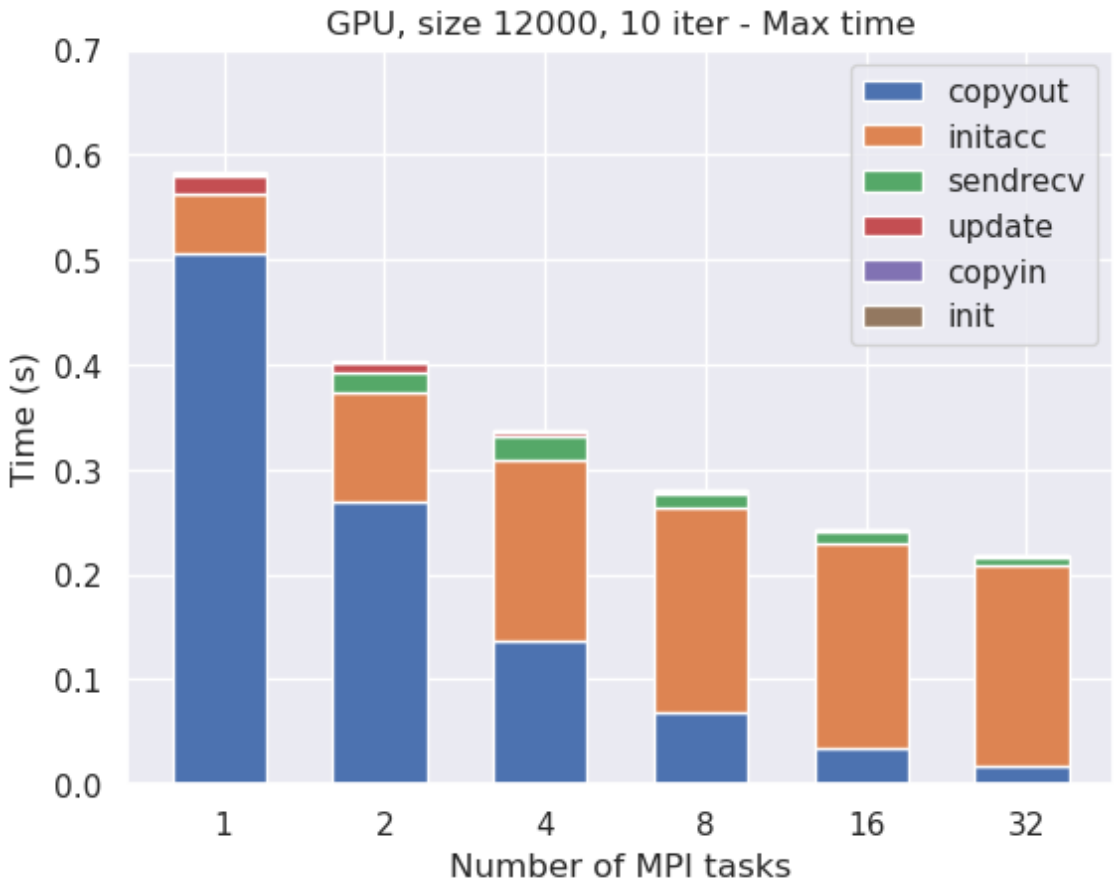
CPU, size 40000, 1000 iterations



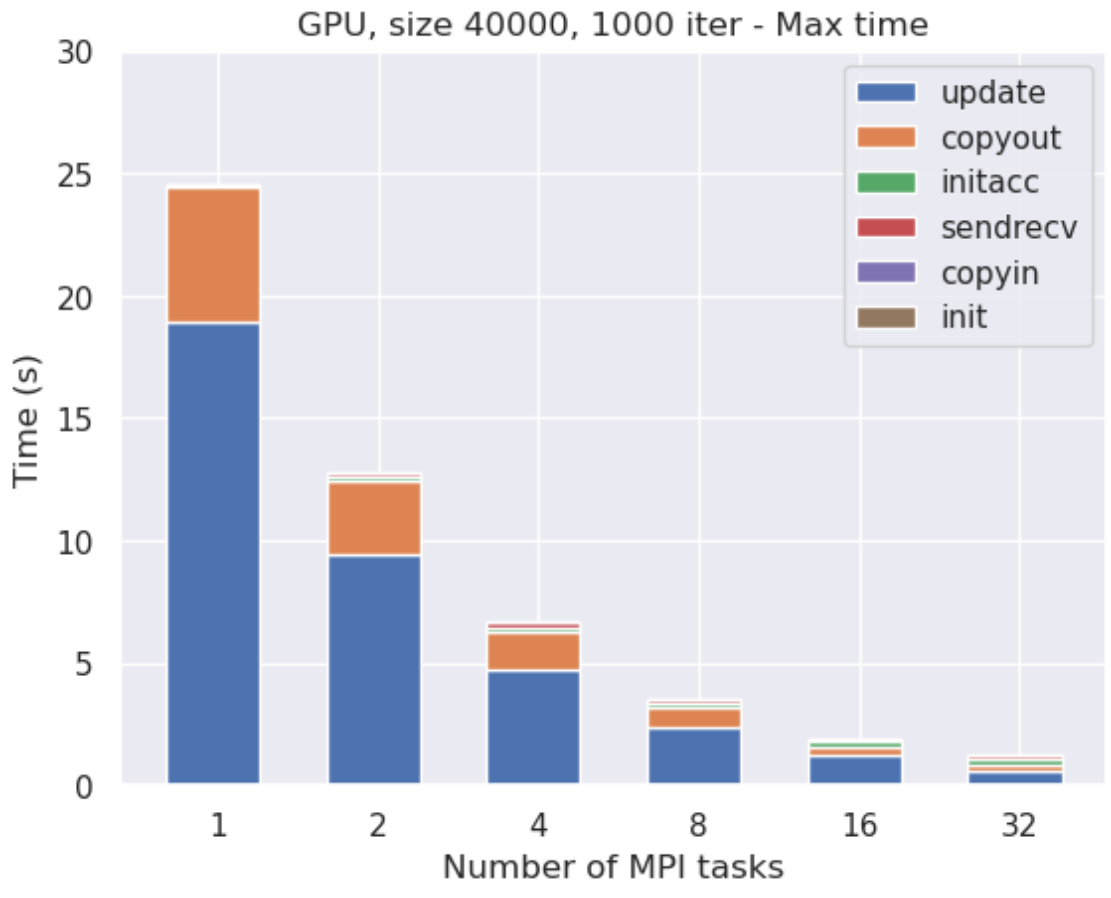
GPU, size 1200, 10 iterations



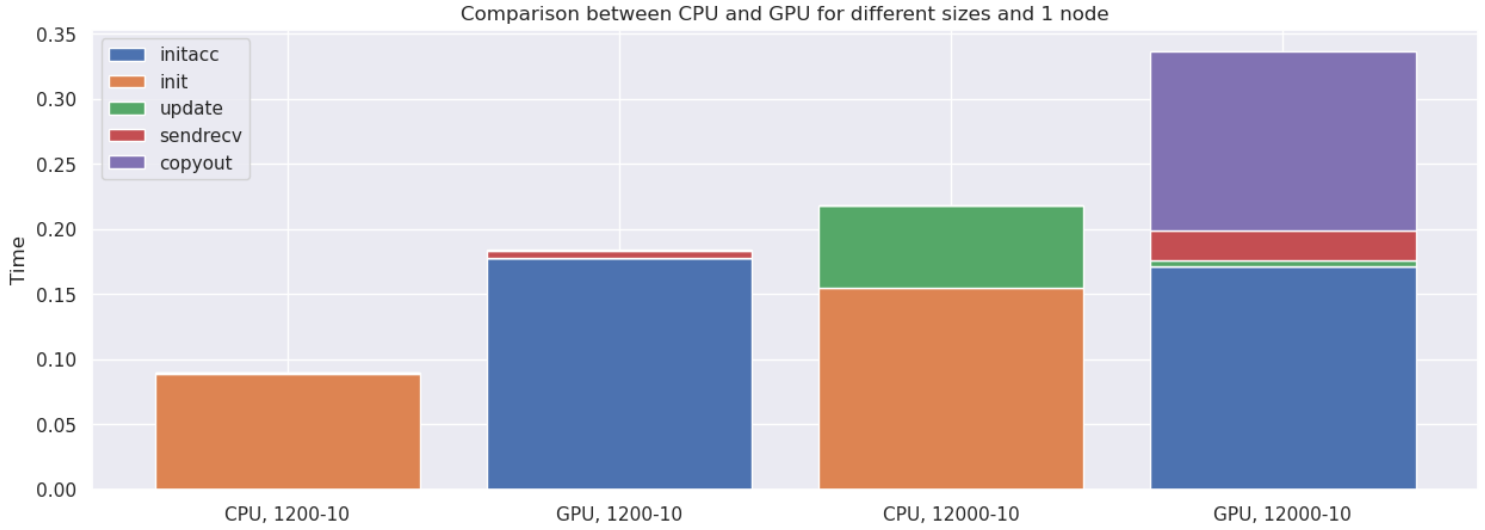
GPU, size 12000, 10 iterations

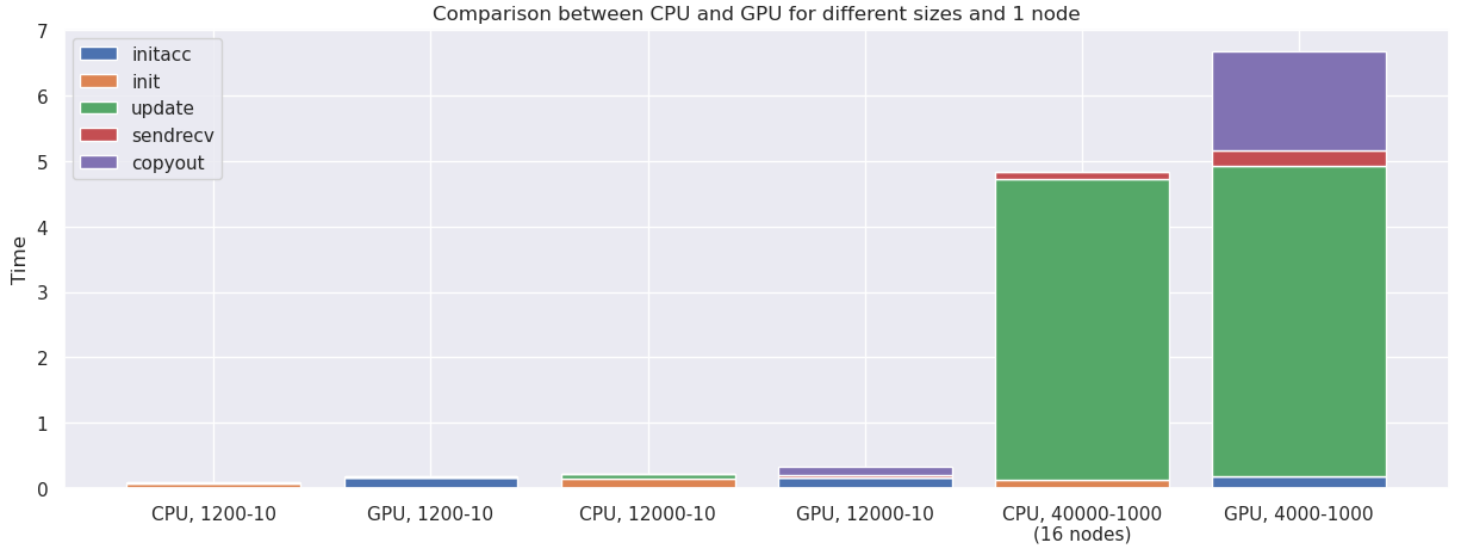


GPU, size 40000, 1000 iterations

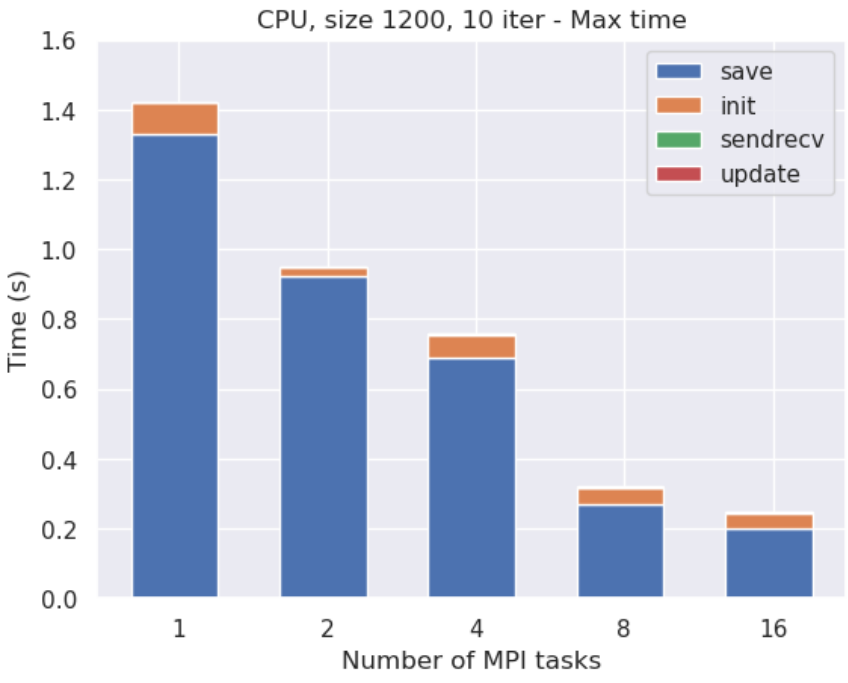


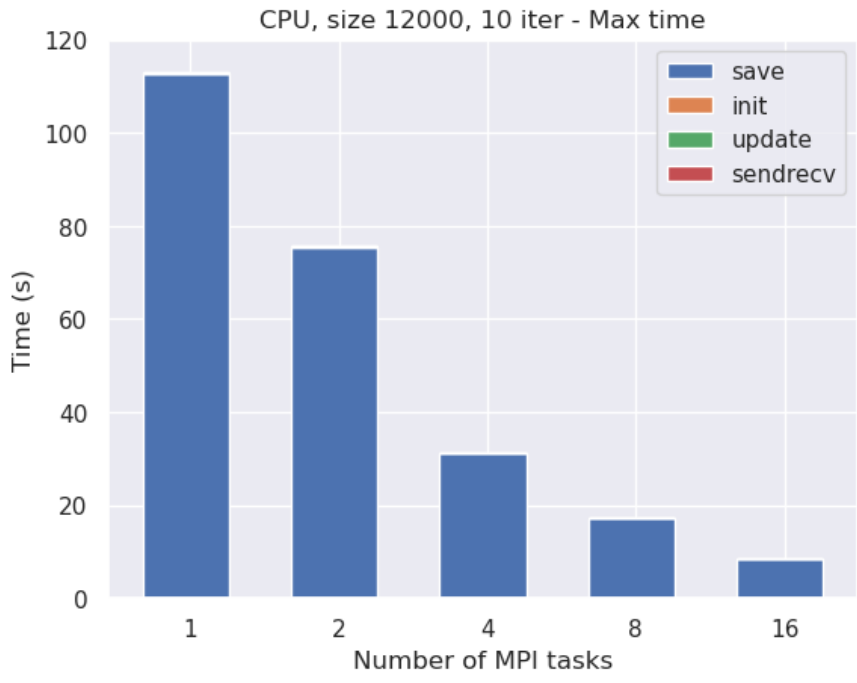
Comparison


Comparison between CPU and GPU for different sizes and 1 node
initacc
init
update
sendrecv
copyout
Time
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
CPU, 1200-10
GPU, 1200-10
CPU, 12000-10
GPU, 12000-10


Comparison between CPU and GPU for different sizes and 1 node
initacc
init
update
sendrecv
copyout
Time
7
6
5
4
3
2
1
0
CPU, 1200-10
GPU, 1200-10
CPU, 12000-10
GPU, 12000-10
CPU, 40000-1000
(16 nodes)
GPU, 4000-1000

Save time


CPU, size 1200, 10 iter - Max time
Time (s)
Number of MPI tasks
save
init
sendrecv
update
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1
2
4
8
16


CPU, size 12000, 10 iter - Max time
Time (s)
Number of MPI tasks
save
init
update
sendrecv
0
20
40
60
80
100
120
1
2
4
8
16

Jacobi's algorithm with One-Sided communication

Domain distribution

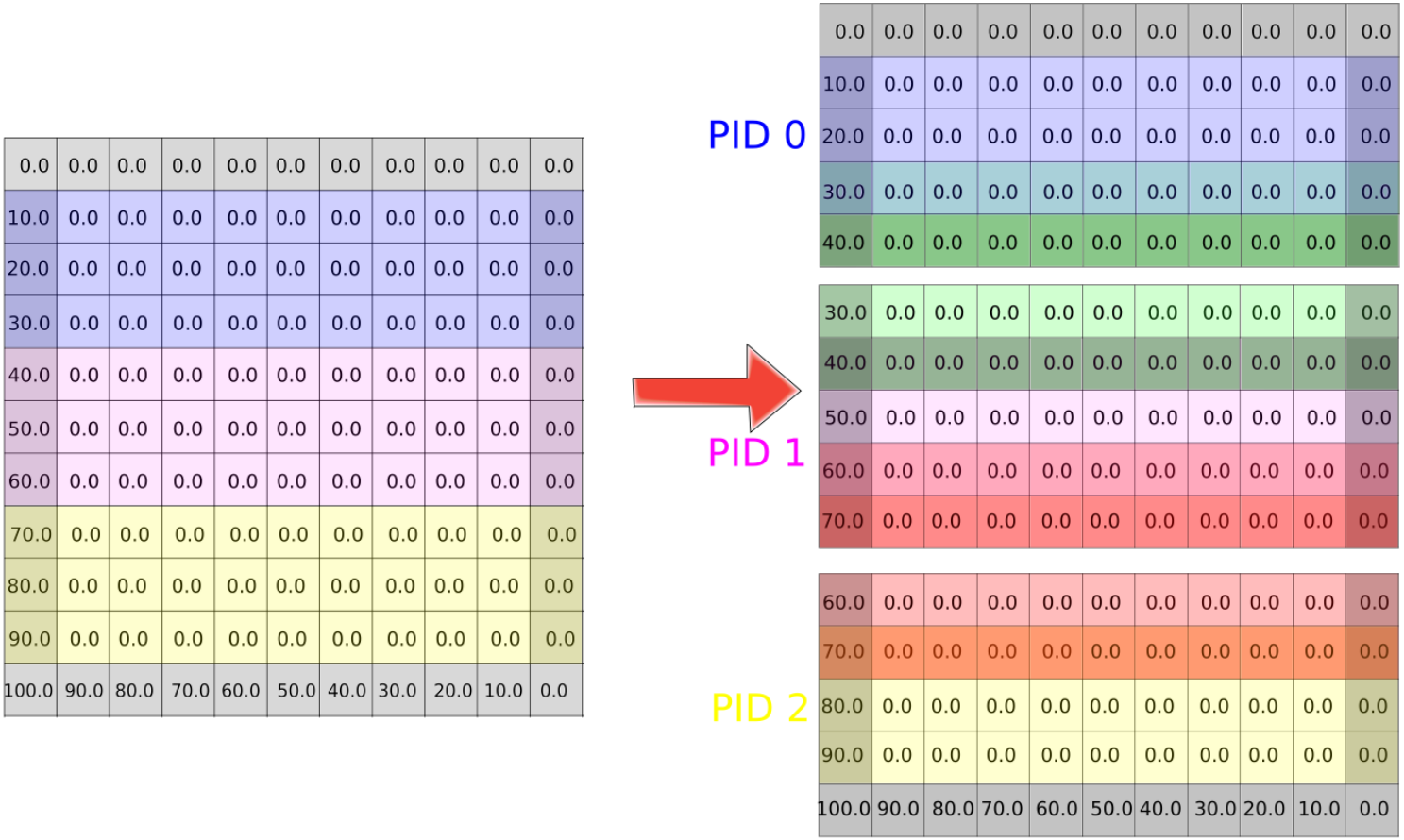
```
size_t dim = atoi(nptr: argv[1]);
size_t dimWithEdges = dim + 2;
size_t iterations = atoi(nptr: argv[2]);
const uint workSize = dim/NPEs;
const uint workSizeRemainder = dim % NPEs;
const uint myWorkSize = workSize + ((uint)myRank < workSizeRemainder ? 1 : 0);
const size_t my_byte_dim = sizeof(double) * myWorkSize * dimWithEdges;
double *matrix     = ( double* )malloc( size: my_byte_dim );
double *matrix_new = ( double* )malloc( size: my_byte_dim );
double *firstRow = (double *)malloc(size: dimWithEdges * sizeof(double));
double *lastRow = (double *)malloc(size: dimWithEdges * sizeof(double));
```

Domain distribution

```
size_t dim = atoi(nptr: argv[1]);
size_t dimWithEdges = dim + 2;
size_t iterations = atoi(nptr: argv[2]);
const uint workSize = dim/NPEs;
const uint workSizeRemainder = dim % NPEs;
const uint myWorkSize = workSize + ((uint)myRank < workSizeRemainder ? 1 : 0);
const size_t my_byte_dim = sizeof(double) * myWorkSize * dimWithEdges;
double *matrix     = ( double* )malloc( size: my_byte_dim );
double *matrix_new = ( double* )malloc( size: my_byte_dim );
double *firstRow = (double *)malloc(size: dimWithEdges * sizeof(double));
double *lastRow = (double *)malloc(size: dimWithEdges * sizeof(double));
```

```
MPI_Win firstRowWin, lastRowWin;
MPI_Info info;
MPI_Info_create(info: &info);
MPI_Info_set(info, key: "same_size", value: "true");
MPI_Info_set(info, key: "same_disp_unit", value: "true");
MPI_Win_create(base: firstRow, size: dimWithEdges*sizeof(double), disp_unit: sizeof(double),
               info, comm: MPI_COMM_WORLD, win: &firstRowWin);
MPI_Win_create(base: lastRow, size: dimWithEdges*sizeof(double), disp_unit: sizeof(double),
               info, comm: MPI_COMM_WORLD, win: &lastRowWin);
```

Domain distribution



Example: $dim = 9$, $NPEs = 3$

Code

- Update:

```
#pragma omp for collapse(2)
  for(size_t i = 1; i < nRows-1; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      currentEl = i*nCols + j;
      matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                     matrix[currentEl+nCols] + matrix[currentEl-1] );
    }
```

Code

- Update:

```
#pragma omp for collapse(2)
  for(size_t i = 1; i < nRows-1; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      currentEl = i*nCols + j;
      matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                     matrix[currentEl+nCols] + matrix[currentEl-1] );
    }
```

- Update bounds:

```
#pragma omp for
  for(size_t j = 1; j < nCols-1; ++j){
    matrix_new[j] = 0.25*( firstRow[j] + matrix[j+1] + matrix[j+nCols] + matrix[j-1] );
    currentEl = (nRows-1)*nCols + j;
    matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                   lastRow[j] + matrix[currentEl-1] );
  }
```

Code

- Update:

```
#pragma omp for collapse(2)
  for(size_t i = 1; i < nRows-1; ++i )
    for(size_t j = 1; j < nCols-1; ++j ) {
      currentEl = i*nCols + j;
      matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                     matrix[currentEl+nCols] + matrix[currentEl-1] );
    }
```

- Update bounds:

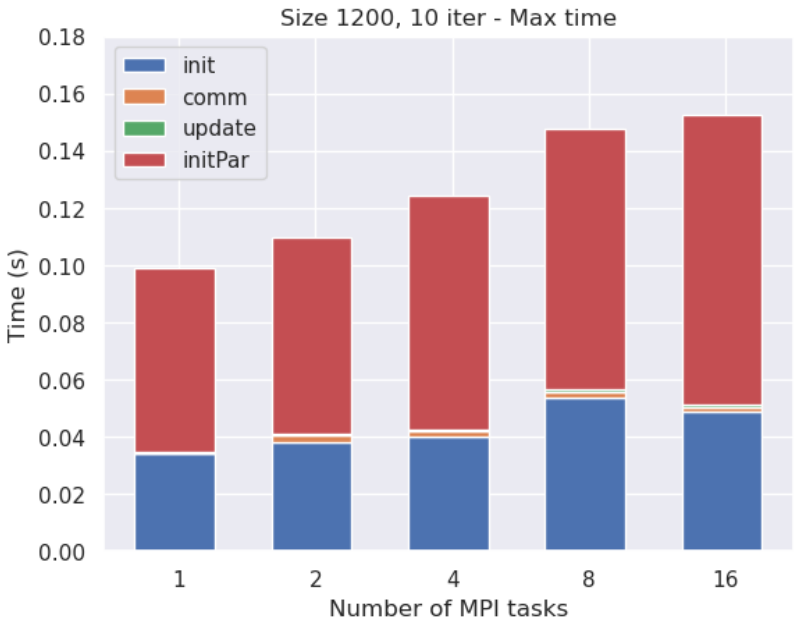
```
#pragma omp for
  for(size_t j = 1; j < nCols-1; ++j){
    matrix_new[j] = 0.25*( firstRow[j] + matrix[j+1] + matrix[j+nCols] + matrix[j-1] );
    currentEl = (nRows-1)*nCols + j;
    matrix_new[currentEl] = 0.25*( matrix[currentEl-nCols] + matrix[currentEl+1] +
                                   lastRow[j] + matrix[currentEl-1] );
  }
```

- Communication:

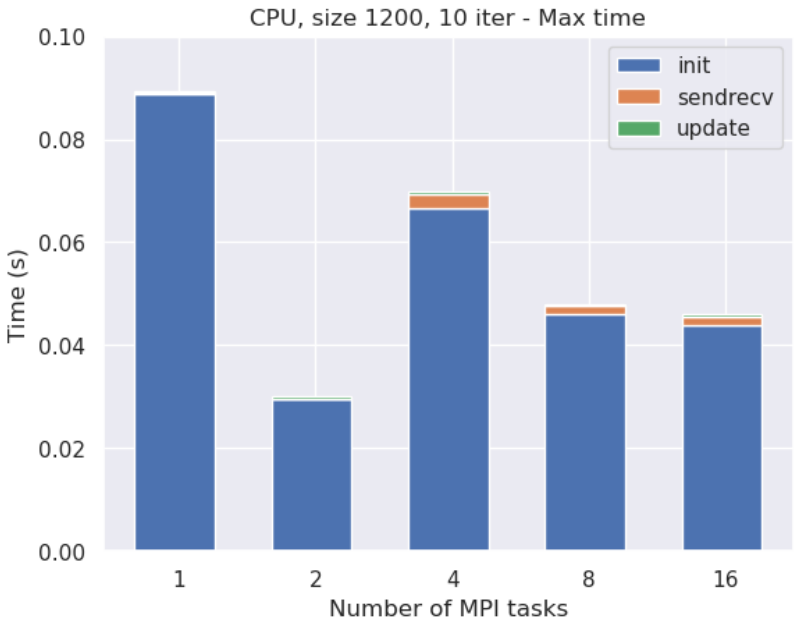
```
if(myRank<NPEs-1){
  MPI_Win_lock(MPI_LOCK_EXCLUSIVE, myRank+1, MPI_MODE_NOCHECK, firstRowWin);
  MPI_Put(&matrix_new[(myWorkSize-1)*dimWithEdges], dimWithEdges, MPI_DOUBLE,
                                   myRank+1, 0, dimWithEdges, MPI_DOUBLE, firstRowWin);
  MPI_Win_unlock(myRank+1, firstRowWin);
}
if(myRank){
  MPI_Win_lock(MPI_LOCK_EXCLUSIVE, myRank-1, MPI_MODE_NOCHECK, lastRowWin);
  MPI_Put(matrix_new, dimWithEdges, MPI_DOUBLE,
      myRank-1, 0, dimWithEdges, MPI_DOUBLE, lastRowWin);
  MPI_Win_unlock(myRank-1, lastRowWin);
}
```

Results

CPU, size 1200, 10 iterations

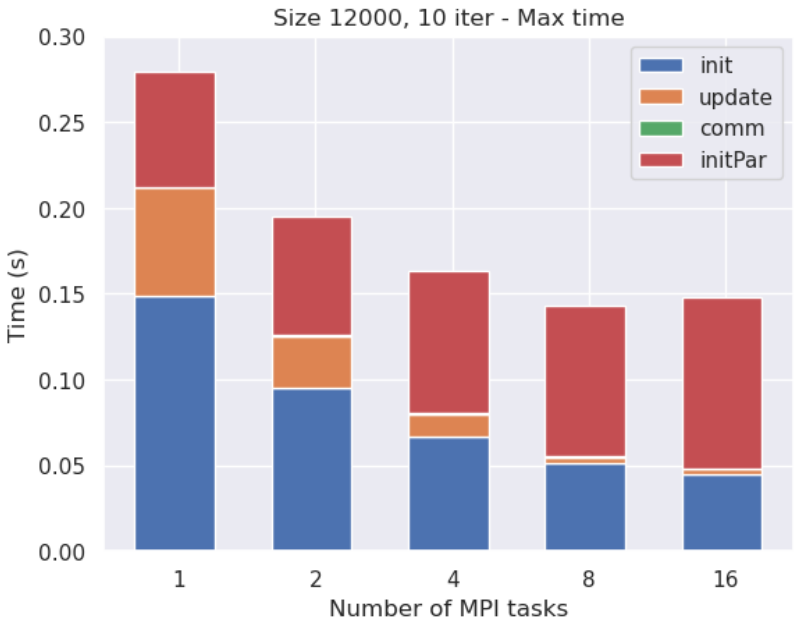


One-Sided comm

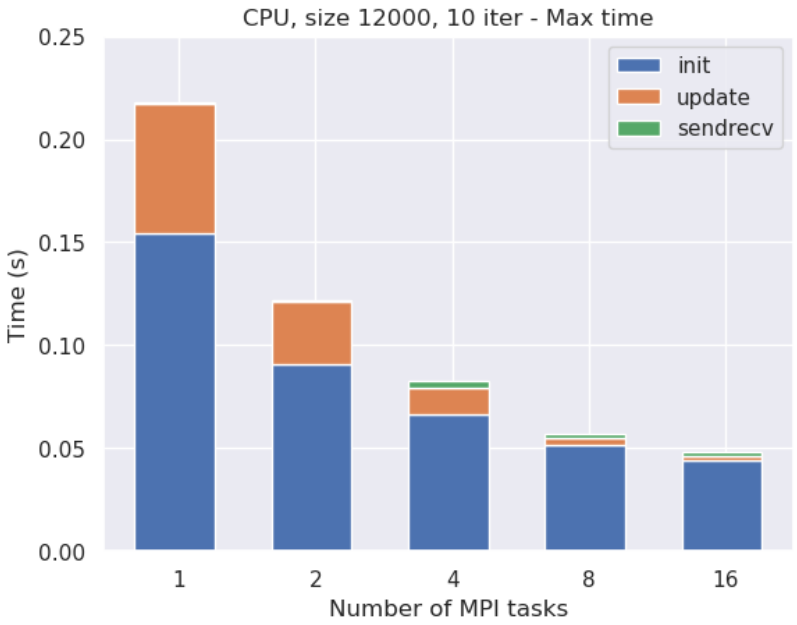


Send-Recv comm

CPU, size 12000, 10 iterations

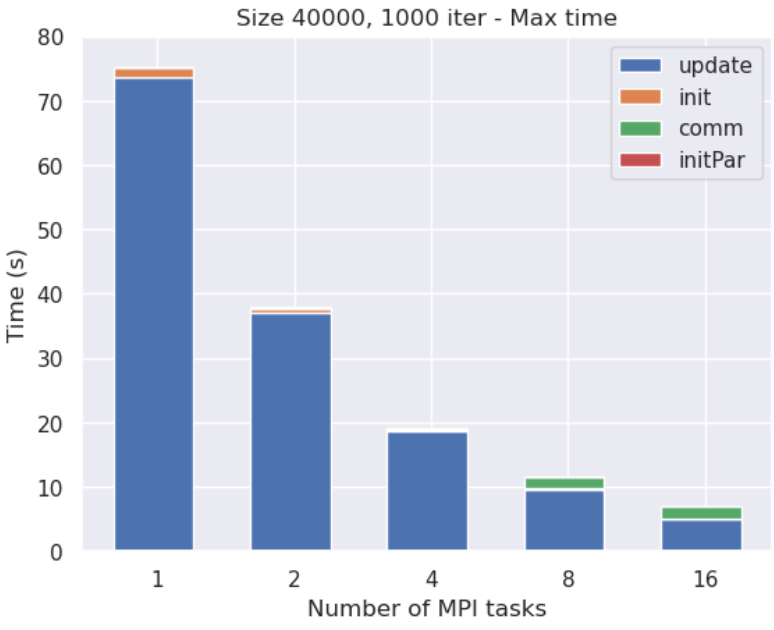


One-Sided comm



Send-Recv comm

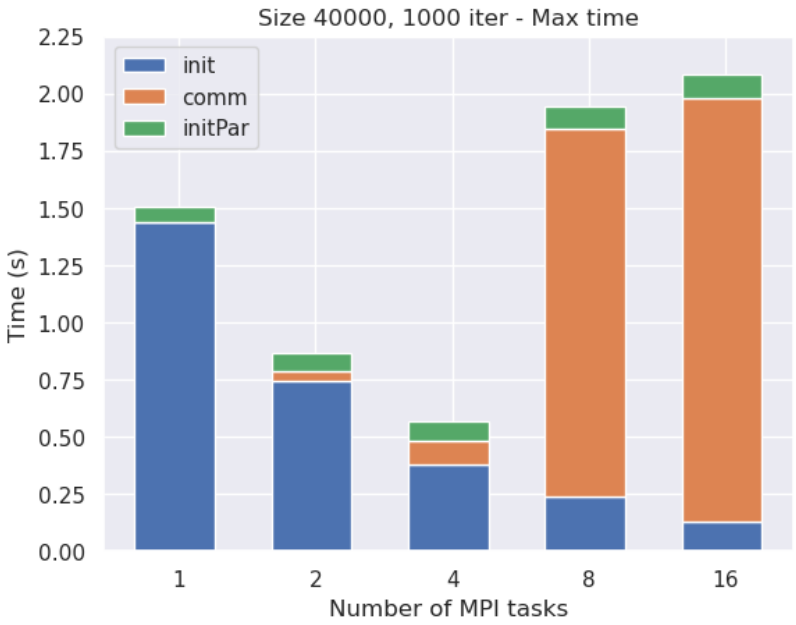
CPU, size 40000, 1000 iterations



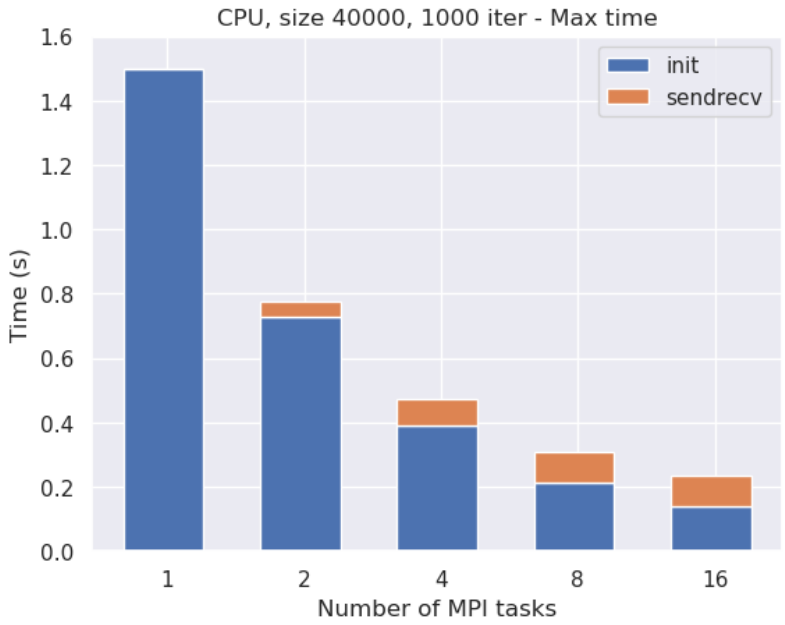
One-Sided comm

Send-Recv comm

CPU, size 40000, 1000 iterations

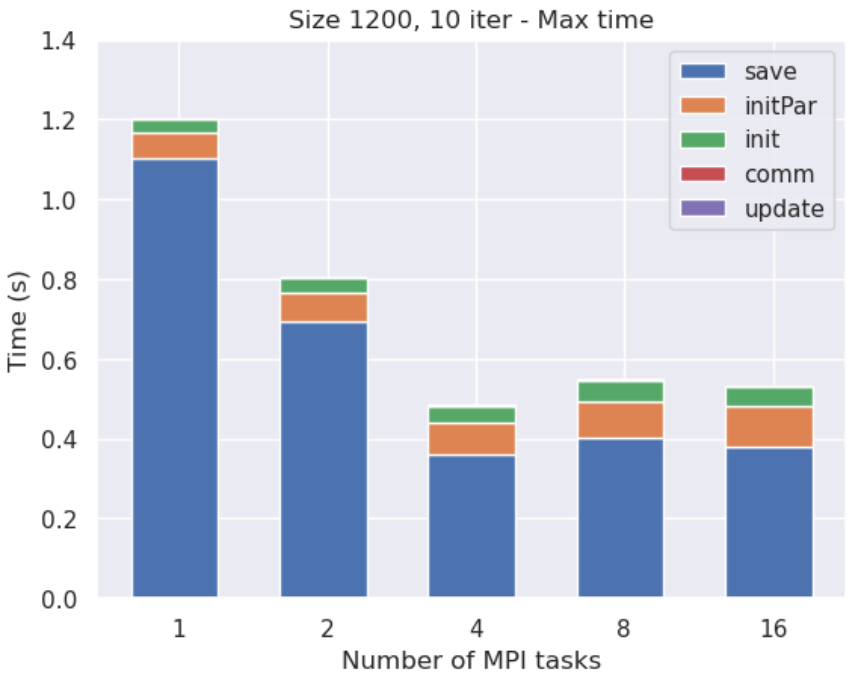


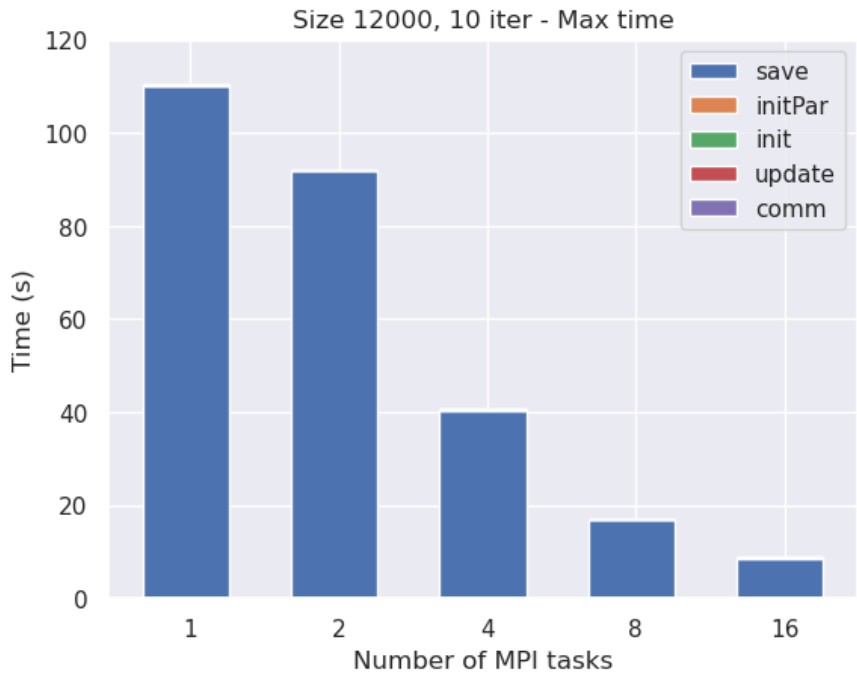
One-Sided comm



Send-Recv comm

Save time


Size 1200, 10 iter - Max time
Time (s)
Number of MPI tasks
save
initPar
init
comm
update
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1
2
4
8
16


Size 12000, 10 iter - Max time
Time (s)
Number of MPI tasks
save
initPar
init
update
comm
0
20
40
60
80
100
120
1
2
4
8
16

End