

CheckMPI-Documentation

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1 Introduction

This code was developed to exploit MPI communication pattern and to built a *template* to check mpi performance using different HW.

It implements a simple 3D domain decomposition for a periodic domain. It was intended to check different communication patterns and their issues/performance. In detail we will (try to) explore

- `sendrecv`
- Non-blocking comms
- `mpi datatype`
- handmade packing/unpacking data
- `OpenACC` directives
- `Cuda Aware MPI`
- Communication-Computation overlap

2 Code structure

The code is written in **Fortran90** and ask for only unix **make** utility and a Fortran compiler and a MPI library.
Dynamic allocation is used.

```
.  
|- DOC  
|- LICENSE  
|- README.md  
|- RUN  
|- SRC  
|- TEST  
'- UTIL
```

Where:

- **DOC**: this directory contains documentation.
- **RUN**: in this directory, the exe will be copied.
- **SRC**: this directory contains all the source files.
- **TEST**: in this directory are present some script for testing the different options.
- **UTIL**: this directory some script and input files are present.

2.1 Licence

This code is released under the MIT license.

It can be downloaded from https://github.com/gamati01/Check_MPI.

3 Test Case

The test case is a *synthetic* test case. The focus is on the efficiency of the communication pattern. It is a:

- 3D domain.
- Periodic boundary conditions.
- 3 different fields to *be propagated* (`field1,field2,field3`).
- The fields are initialized with a complete sinusoidal for each task.
- All the tests are done using single precision unless stated elsewhere.
- The default propagation is
 - from rear to front (direction x)
 - from left to right (direction y)
 - from bottom to right (direction z)
- a *reversed* propagation can be activated

Note that no flops are performed, only "rigid" data movement.

The default propagation is:

```
do k = n, 1, -1
  do j = m, 1, -1
    do i = l, 1, -1
      field1(i,j,k) = field1(i-1,j,k)
      field2(i,j,k) = field2(i,j-1,k)
      field3(i,j,k) = field3(i,j,k-1)
    end do
  end do
end do
```

The input file used for the test is the following:

```
&parameters
lx = 600
ly = 600
lz = 600
proc_x = 2
proc_y = 2
proc_z = 2
itfin=15000
icheck=1510  /
```

3.1 Validation

The initial condition, a sinusoidal wave, is the same for each task, so the profiles should be *exactly the same* independently for all the tests: this means that the UNIX command `md5sum` should return the same hash.

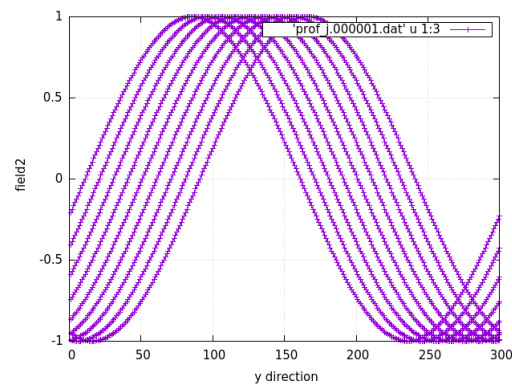


Figure 1: Validation for variable field2.

```
md5sum RUN_STEP*/prof_i*0.dat
3cdb4eef4d04a99e786046dead098237 RUN_STEP0/prof_i.000000.dat
3cdb4eef4d04a99e786046dead098237 RUN_STEP1/prof_i.000000.dat
3cdb4eef4d04a99e786046dead098237 RUN_STEP2/prof_i.000000.dat
3cdb4eef4d04a99e786046dead098237 RUN_STEP3/prof_i.000000.dat
3cdb4eef4d04a99e786046dead098237 RUN_STEP4/prof_i.000000.dat
...
```

In fig. 1 the value of `field2` is reported.

4 Code versions

At the moment 9 different versions are available. They can be selected at compile time via pre-processing flag syntax.

The syntax, e.g. to choose **Step6** version, is:

```
make STEP6=1
```

In detail, these are the different options to choose from, for each task and for each timestep:

- **Step0**: $3 \times 2 \times$ `sendrecv` calls per direction and using `mpi datatype`.
- **Step1**: $3 \times 2 \times$ `sendrecv` calls and explicit pack-unpack (only for x direction), development step.
- **Step2**: $2 \times$ `sendrecv` calls and explicit pack-unpack (all directions).
- **Step3**: $2 \times$ `sendrecv` calls and explicit pack-unpack (all directions) with `kernel OpenACC` directive.
- **Step4**: $2 \times$ `sendrecv` calls and explicit pack-unpack (all directions) with `kernel OpenACC` directive and using `CUDAWARE` MPI calls.
- **Step5**: $2 \times$ `isend` and `recv` calls only for x direction and explicit pack-unpack with `kernel OpenACC` directive and using `CUDAWARE` MPI calls (development step).
- **Step6**: like **Step5** but with `isend` and `recv` for all the three directions (development step).
- **Step7**: like **Step6** but with `isend` and `irecv` for all the three directions (development step).
- **Step8**: like **Step7** with communication-computation overlap.
- **Step9**: like **Step7** with communication-computation overlap and `asyn` clause.

In tab. 3 is reported for each step which device is supported and if it is a *develop* version or a production one.

Table 1: GPU/CPU support for different versions

version	CPU	GPU	production ver.
Step0	yes	no	yes
Step1	yes	no	no
Step2	yes	no	yes
Step3	yes*	yes	yes
Step4	yes*	yes	yes
Step5	yes*	yes	no
Step6	yes*	yes	no
Step7	yes*	yes	no
Step8	yes*	yes	yes
Step9	yes*	yes	yes

4.1 Step0

It is the starting point version: it uses one different single `sendrecv` call for each population to propagate information. It calls `bcond_comm_step0` subroutine. It means 3 calls to `sendrecv` for each direction (+/-) and each decomposition along x, y, z . In total for each timestep and task 6 calls are required. In the following the calls for positive propagation are shown.

```

tag = 04
call mpi_sendrecv(field1(0,0,n), 1, xyplane, up(2), tag,      &
                  field1(0,0,0), 1, xyplane, down(2), tag,    &
                  lbcomm, status, ierr)

tag = 06
call mpi_sendrecv(field2(0,0,n), 1, xyplane, up(2), tag,      &
                  field2(0,0,0), 1, xyplane, down(2), tag,    &
                  lbcomm, status, ierr)

tag = 07
call mpi_sendrecv(field3(0,0,n), 1, xyplane, up(2), tag,      &
                  field3(0,0,0), 1, xyplane, down(2), tag,    &
                  lbcomm, status, ierr)

```

It use explicitly `mpi datatype`

```

! yz plane is composed by single points (stride.ne.1)
call MPI_type_vector((n+2)*(m+2),1,1+2, MYMPIREAL,yzplane,ierr)
call MPI_type_commit(yzplane,ierr)
!
! xz plane is composed by arrays (the single vector has stride.eq.1)
call MPI_type_vector(n+2,1+2,(m+2)*(1+2), MYMPIREAL,xzplane,ierr)
call MPI_type_commit(xzplane,ierr)
!
! xy plane is a contiguous array (stride.eq.1)
call MPI_type_contiguous((1+2)*(m+2),MYMPIREAL,xyplane,ierr)
call MPI_type_commit(xyplane,ierr)

```

These are the options activated with the command `make`

```
# default (NVIDIAcompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
OPT = -fast -Mcontiguous -Mnodepchk
VER = step0
```

This version is a CPU-only.

4.2 Step1

In this version, data for the x direction are explicitly packed/unpacked using a do loop. It calls `bcond_comm_step1` subroutine.

```
!  
  do k = 0,n+1  
    do j = 0,m+1  
      bufferXIN(j,k)=field1(1,j,k)  
    enddo  
  enddo  
!  
  call mpi_sendrecv(bufferXIN(0,0),msgsizeX,MYMPIREAL,front(2),tag,&  
                    bufferXOUT(0,0),msgsizeX,MYMPIREAL,rear(2),tag,&  
                    lbcomm,status,ierr)  
!  
  do k = 0,n+1  
    do j = 0,m+1  
      field1(0,j,k) = bufferXOUT(j,k)  
    enddo  
  enddo  
!
```

These are the options activated with the command `make STEP1=1`

```
# default (NVIDIAcompiler)  
CC = mpicc  
FC = mpifort  
FIX = -DPGI  
FOPT = -fast -Mcontiguous -Mnodepchk  
COPT =  
OPT = -fast -Mcontiguous -Mnodepchk  
ifdef STEP1  
  FIX=-DSTEP1  
  VER=step1  
endif
```

This version is a CPU-only.

4.3 Step2

In this version, the data for the three directions is explicitly packed/unpacked using a do loop and a single `sendrecv` is used for all the 3 fields to be propagated. It calls `bcond_comm_step2` subroutine.

```
do k = 0,n+1
  do i = 0,l+1
    bufferYIN(i,k,1)=field1(i,1,k)
    bufferYIN(i,k,2)=field2(i,1,k)
    bufferYIN(i,k,3)=field3(i,1,k)
  enddo
enddo
!
call mpi_sendrecv(bufferYIN(0,0,1),msgsizeY,MYMPIREAL,left(2),tag,&
                  bufferYOUT(0,0,1),msgsizeY,MYMPIREAL,right(2),tag,&
                  lbcomm,status,ierr)
!
do k = 0,n+1
  do i = 0,l+1
    field1(i,m+1,k)=bufferYOUT(i,k,1)
    field2(i,m+1,k)=bufferYOUT(i,k,2)
    field3(i,m+1,k)=bufferYOUT(i,k,3)
  enddo
enddo
```

These are the options activated with the command `make STEP2=1`

```
# default (NVIDIAcompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
COPT =
OPT = -fast -Mcontiguous -Mnodepchk
ifdef STEP2
  FIX=-DSTEP2
  VER=step2
endif
```

This version is a CPU-only.

4.4 Step3

In this version OpenACC directives are use for

- loop inside `do_somethingGPU` subroutine pack and unpack fields to propagate

It calls `bcond_comm_step3` subroutine. For the loop inside `do_somethingGPU` subroutine, an explicit copy has to be done to exploit GPU parallelism, it is activated by `FAST` pre-processing flags.

```
ifdef FAST
!$acc kernels
    do k = 0, n+1
        do j = 0, m+1
            do i = 0, l+1
                temp1(i,j,k) = field1(i,j,k)
                temp2(i,j,k) = field2(i,j,k)
                temp3(i,j,k) = field3(i,j,k)
            end do
        end do
    end do
!$acc end kernels
!
!$acc kernels
    do k = 1, n
        do j = 1, m
            do i = 1, l
                field1(i,j,k) = temp1(i-1,j,k)
                field2(i,j,k) = temp2(i,j-1,k)
                field3(i,j,k) = temp3(i,j,k-1)
            end do
        end do
    end do
!$acc end kernels
#else
....
endif
```

For the pack/unpack section these are the `kernels` directives were used

```
!$acc kernels
    do k = 0,n+1
        do j = 0,m+1
            bufferXIN(j,k,1)=field1(1,j,k)
            bufferXIN(j,k,2)=field2(1,j,k)
            bufferXIN(j,k,3)=field3(1,j,k)
        enddo
    enddo
!$acc end kernels
!
    call mpi_sendrecv(bufferXIN(0,0,1),msgsizeX,MYMPIREAL,front(2),tag,&
                      bufferXOUT(0,0,1),msgsizeX,MYMPIREAL,rear(2),tag,&
                      lbcomm,status,ierr)
!
!$acc kernels
```

```

do k = 0,n+1
  do j = 0,m+1
    field1(0,j,k) = bufferXOUT(j,k,1)
    field2(0,j,k) = bufferXOUT(j,k,2)
    field3(0,j,k) = bufferXOUT(j,k,3)
  enddo
enddo
!$acc end kernels

```

These are the options activated with the command `make STEP3=1`

```

# default (NVIDIAcompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
COPT =
OPT = -fast -Mcontiguous -Mnodepchk
ifdef STEP3
  FIX=-DSTEP3 -acc -Minfo=acc -DOPENACC -DFAST
  VER=step3
endif

```

By default only the CPU version is compiled. To activate the GPU version the correct compile line is:

```
make STEP3=1 GPUENABLE=1
```

4.5 Step4

In this version OpenACC directives are used to exploit Cuda-aware MPI comms. It calls `bcond_comm_step4` subroutine.

```
...
!$acc host_data use_device(bufferZIN,bufferZOUT)
    call mpi_sendrecv(bufferZIN(0,0,1),msgsizeZ,MYMPIREAL,up(2),tag,&
                      bufferZOUT(0,0,1),msgsizeZ,MYMPIREAL,down(2),tag,&
                      lbcomm,status,ierr)
!$acc end host_data
....
```

These are the options activated with the command `make STEP4=1`

```
# default (NVIDIACompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
OPT = -fast -Mcontiguous -Mnodepchk
ifdef STEP4
    FIX=-DSTEP4 -acc -Minfo=acc -DOPENACC -DFAST
    VER=step4
endif
```

By default, only the CPU version is compiled. To activate the GPU version the compile line is:

```
make STEP4=1 GPUENABLE=1
```

4.6 Step5

This is a development step.

It calls `bcond_comm_step5` subroutine. It is like Step4 but using `isend` and `recv` subroutines only for the x direction.

```
! First pack data.....
!$acc kernels
  do k = 0,n+1
    do j = 0,m+1
! x+ direction
      bufferXINP(j,k,1)=field1(1,j,k)
      bufferXINP(j,k,2)=field2(1,j,k)
      bufferXINP(j,k,3)=field3(1,j,k)
!
! x- direction
      bufferXINM(j,k,1)=field1(1,j,k)
      bufferXINM(j,k,2)=field2(1,j,k)
      bufferXINM(j,k,3)=field3(1,j,k)
    enddo
  enddo
!$acc end kernels
!
! Second send pack data.....
  tag = 11
!$acc host_data use_device(bufferXINP)
  call mpi_isend(bufferXINP(0,0,1),msgsizeX,MYMPIREAL,front(2), &
    tag,lbecomm, reqs_front(1), ierr)
!$acc end host_data
  tag = 10
!$acc host_data use_device(bufferXINM)
  call mpi_isend(bufferXINM(0,0,1),msgsizeX,MYMPIREAL,rear(2), &
    tag,lbecomm, reqs_rear(1), ierr)
!$acc end host_data
!
  tag = 11
!Third receive data
!$acc host_data use_device(bufferXOUTP)
  call mpi_recv(bufferXOUTP(0,0,1),msgsizeX,MYMPIREAL,rear(2), &
    tag,lbecomm, status_front, ierr)
!$acc end host_data
  tag = 10
!$acc host_data use_device(bufferXOUTM)
  call mpi_recv(bufferXOUTM(0,0,1),msgsizeX,MYMPIREAL,front(2), &
    tag,lbecomm, status_rear, ierr)
!$acc end host_data
!
! Fourth unpack data
!$acc kernels
  do k = 0,n+1
    do j = 0,m+1
! x+ direction
      field1(0,j,k) = bufferXOUTP(j,k,1)
```



```

        field2(0,j,k) = bufferXOUTP(j,k,2)
        field3(0,j,k) = bufferXOUTP(j,k,3)
!
! x- direction
        field1(l+1,j,k) = bufferXOUTM(j,k,1)
        field2(l+1,j,k) = bufferXOUTM(j,k,2)
        field3(l+1,j,k) = bufferXOUTM(j,k,3)
    enddo
enddo
!$acc end kernels
!
! Fifth wait...
    call mpi_wait(reqs_rear(1), status_rear, ierr)
    call mpi_wait(reqs_front(1), status_front, ierr)
!

```

These are the options activated with the command `make STEP5=1`

```

# default (NVIDIAcompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
OPT = -fast -Mcontiguous -Mnodepchk
ifdef STEP5
    FIX=-DSTEP5 -acc -Minfo=acc -DOPENACC -DFAST
    VER=step5
endif

```

By default, only the CPU version is compiled. To activate the GPU version the compile line is:

```

make STEP5=1 GPUENABLE=1

```

4.7 Step6

This is a development step. It calls `bcond_comm_step6` subroutine. It is like **Step6** but with `isend` and `recv` subroutines for all the three directions. These are the options activated with the command `make STEP6=1`

```
# default (NVIDIAcompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
OPT = -fast -Mcontiguous -Mnodepchk
ifdef STEP6
    FIX=-DSTEP6 -acc -Minfo=acc -DOPENACC -DFAST
    VER=step6
endif
```

By default, only the CPU version is compiled. To activate the GPU version the compile line is:

```
make STEP6=1 GPUENABLE=1
```

4.8 Step7

This is a development step. It calls `bcond_comm_step7` subroutine.

It is like **Step6** but with `isend` and `irecv` for all three directions and restructured to allow computation and communication overlap.

It works correctly only if there is more than one task for each direction (i.e. total tasks ≥ 8). The structure is the following

```
!-----
! First pack data.....
      call time(tcountZ0)
!$acc kernels
      do j = 0,m+1
        do i = 0,l+1
          ...
        end do
      end do
!-----
! Second receive data
      tag = 34
!$acc host_data use_device(bufferZOUTP)
      call mpi_irecv(bufferZOUTP(0,0,1), msgsizeZ, MYMPIREAL, down(2), &
        tag, lbcomm, reqs_up(1), ierr)
!$acc end host_data
      ...
!-----
! Third send data.....
      tag = 34
!$acc host_data use_device(bufferZINP)
      call mpi_isend(bufferZINP(0,0,1), msgsizeZ, MYMPIREAL, up(2), &
        tag, lbcomm, reqs_up(2), ierr)
!$acc end host_data
      ...
!-----
! forth wait...
      call MPI_Waitall(2, reqs_up, MPI_STATUSES_IGNORE, ierr)
      ...
!-----
! fifth unpack data
      call time(tcountZ0)
!$acc kernels
      do j = 0,m+1
        do i = 0,l+1
          ! z+ direction
          temp1(i,j,0)=bufferZOUTP(i,j,1)
          temp2(i,j,0)=bufferZOUTP(i,j,2)
          ...
        end do
      end do
```

These are the options activated with the command `make STEP7=1`

```
# default (NVIDIA compiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
OPT = -fast -Mcontiguous -Mnodepchk
```

```
ifdef STEP7
    FIX=-DSTEP7 -acc -Minfo=acc -DOPENACC -DFAST
    VER=step7
endif
```

By default, only the CPU version is compiled. To activate the GPU version the compile line is:

```
make STEP7=1 GPUENABLE=1
```

4.9 Step8

In this version, the operations of `do_something` subroutine are split to allow the overlap. It calls `bcond_comm_step8` and `do_somethingGPU_overlap` subroutine.

It works correctly only if there is more than one task for each direction (e.b. total tasks ≥ 8).

The overlap is done putting the copy of temporary files between the section where data are sent and the wait section:

```
!-----
! Third send data....
      tag = 34
!$acc host_data use_device(bufferZINP)
      call mpi_isend(bufferZINP(0,0,1), msgsize, MYMPIREAL, up(2), &
                    tag,lbcomm,reqs_up(2),ierr)
!$acc end host_data
...
!-----
! overlap region
!$acc kernels
      do k = 1, n
        do j = 1, m
          do i = 1, l
            temp1(i,j,k) = field1(i,j,k)
            temp2(i,j,k) = field2(i,j,k)
            temp3(i,j,k) = field3(i,j,k)
          end do
        end do
      end do
!$acc end kernels
!-----
! forth wait...
      call MPI_Waitall(2,reqs_up, MPI_STATUSES_IGNORE, ierr)
...
```

These are the options activated with the command `make STEP8=1`

```
# default (NVIDIAcompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
OPT = -fast -Mcontiguous -Mnodepchk
ifdef STEP8
  FIX=-DSTEP8 -acc -Minfo=acc -DOPENACC -DFAST
  OBJ1= bcond.comm.step8.o do_somethingGPU_overlap.o
  VER=step8
endif
```

By default, only the CPU version is compiled. To activate the GPU version the compile line is:

```
make STEP8=1 GPUENABLE=1
```

4.10 Step9

This version is the same of Step8 with the use of `async` clause for `kernels` directives. It calls `bcond_comm_step8`.

It works correctly only if there is more than one task for each direction (e.b. total tasks ≥ 8).

```
! overlap region
....
!$acc kernels async
    do k = 0,n+1
        do i = 0,l+1
! y+ direction
            temp1(i,0,k)=bufferYOUTP(i,k,1)
            temp2(i,0,k)=bufferYOUTP(i,k,2)
            temp3(i,0,k)=bufferYOUTP(i,k,3)
!
! y- direction
            temp1(i,m+1,k)=bufferYOUTM(i,k,1)
            temp2(i,m+1,k)=bufferYOUTM(i,k,2)
            temp3(i,m+1,k)=bufferYOUTM(i,k,3)
        enddo
    enddo
!$acc end kernels
make STEP9=1 GPUENABLE=1
```

This implementation shows his efficiency for more than 64 tasks.

These are the options activated with the command `make STEP9=1`

```
# default (NVIDIAcompiler)
CC = mpicc
FC = mpifort
FIX = -DPGI
FOPT = -fast -Mcontiguous -Mnodepchk
OPT = -fast -Mcontiguous -Mnodepchk
ifdef STEP9
    FIX=-DSTEP9 -acc -Minfo=acc -DOPENACC -DFAST
    OBJ1= bcond.comm.step9.o do_somethingGPU_overlap.o
    VER=step9
endif
```

To activate the GPU version the compile line is:

```
make STEP9=1 GPUENABLE=1
```

Table 2: Figures for different versions (using single DGX node, with 8 tasks)

version	tot	%COLL	%MPI	x	y	z	type
Step0	661"	53%	47%	268"	15.4"	10.6"	CPU
Step1	484"	72%	28%	101"	15.4"	11.0"	CPU
Step2	488"	72%	28%	74"	19.1"	13.9"	CPU
Step7	680"	77%	23%	26.3"	23.8"	23.8"	CPU
Step8	1650"	77%	23%	26.3"	23.8"	23.8"	CPU
Step3	97.5"	16%	82%	26.3"	23.8"	23.8"	GPU
Step4	27.7"	59%	35%	3.52"	1.74"	3.62"	GPU
Step5	26.5"	61%	32%	2.51"	2.04"	3.25"	GPU
Step6	25.4"	64%	29%	2.46"	1.34"	3.02"	GPU
Step7	24.6"	-%	-%	-"	-"	-"	GPU
Step8	24.0"	-%	-%	-"	-"	-"	GPU
Step9	21.5"	-%	-%	-"	-"	-"	GPU

5 Performance Figures

For obtain the performance figures these HW has been used:

- DGX
 - CPU: AMD
 - GPU: Nvidia A100@40GB
- Leonardo
 - CPU: Intel
 - GPU: Nvidia A100@64GB

All the figures reported in the tables are obtained from file `task.000000.log`. In tab 2 are reported some performance figures for a 8-task run on DGX.

Each task uses a 300^3 gridpoint, 100'000 iterations were performed, and the decomposition was a $2 \times 2 \times 2$. Each task uses a 300^3 gridpoint, 100'000 iterations were performed, and the decomposition was a $2 \times 2 \times 2$.

In tab. 3 a scale-up using version STEP4, STEP8 and STEP9 are reported with respect to different number of tasks. Each task uses a 300^3 gridpoint, 100'000 iterations were performed, and a cubic decomposition was used.

Table 3: Figures for scale-up (using Leonardo, with 4 tasks per node

proc_x	proc_y	proc_x	STEP4	STEP8	STEP9
2	2	2	185"	159"	143"
3	3	3	267"	230"	196"
4	4	4	290"	280"	218"
5	5	5	404"	285"	224"
6	6	6	568"	291"	233"
7	7	7	621"	268"	232"
8	8	8	683"	285"	241"

5.1 Comments

6 To DO LIST

- MPIP
- Testy section