Theory and Practice of MPI Programming

In-Ho Lee (이인호)
Korea Research Institute of Standards and Science, Daejeon 34113, Korea
(한국표준과학연구원)

ihlee@kriss.re.kr
http://incredible.egloos.com

KIAS, June 28-30, 2017

Goal

- Parallel computing
- MPI based parallel computing
- Practical applications

효율적이고 범용적인 병렬 계산의 기본 원리를 이해한다.
실습을 통해서 병렬 문제 양식을 알아낸다. 양식 구별 능력을 함양한다.
다양한 병렬 컴퓨팅 적용 사례들을 습득한다.
최종적으로 각자 연구에 적용한다.

Contents

Brief introduction to MPI

MPI basics

MPI practice

It’s neither complicated nor bloated.

The 8th KIAS CAC Summer School

6/28 (Wed.)

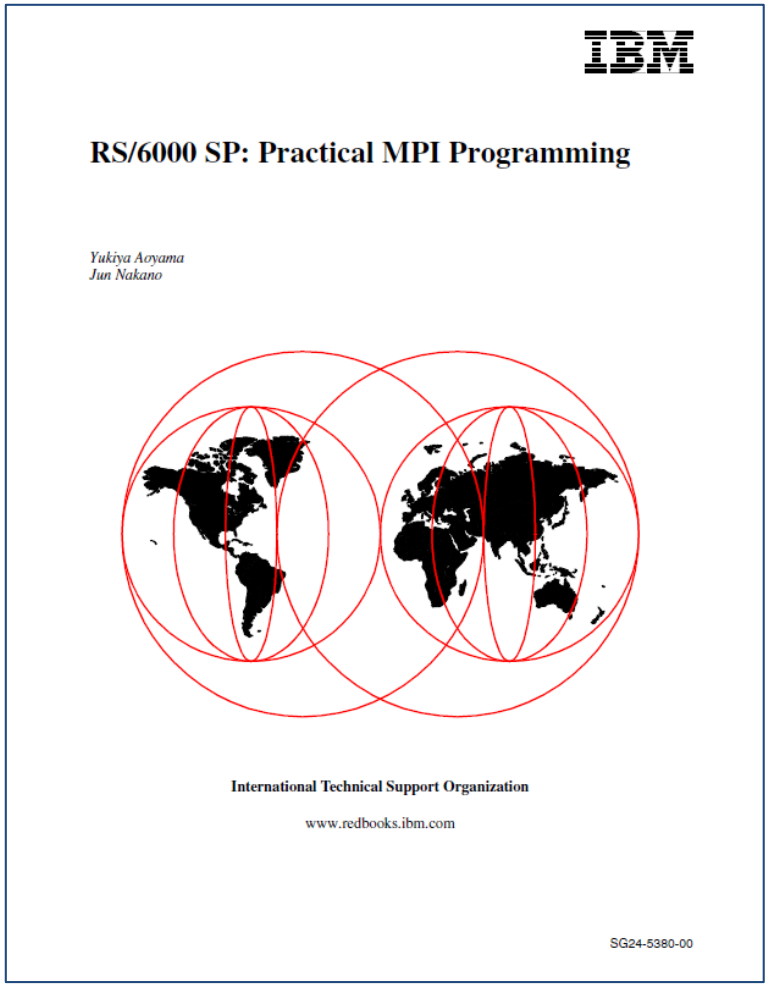
08:30 ~ 09:00	(30min.)	Registration	
09:00 ~ 09:10	(10min.)	Welcome address	CAC Director
09:10 ~ 09:40	(30min.)	Generative Adversarial Network in Machine Learning	안강헌 (충남대)
09:40 ~ 11:20	(100min.)	MPI Tutorial using Fortran/C	이인호 (KRISS)
11:20 ~ 11:35	(15min.)	Coffee break	
11:35 ~ 13:15	(100min.)	CUDA / OpenACC Programming	류현곤 (nVidia)
13:15 ~ 14:15	(60min.)	Lunch	
14:15 ~ 15:55	(100min.)	Python for Scientists	정인석 (KIAS)
15:55 ~ 16:30	(35min.)	Coffee Break & Team building	
16:30 ~ 18:10	(100min.)	Machine Learning	노영균 (SNU)
18:10 ~ 19:10	(60min.)	Banquet (Pizza)	
		Team projects	

6/29 (Thu.)

09:00 ~ 10:40	(100min.)	MPI Tutorial using Fortran/C	이인호 (KRISS)
10:40 ~ 10:55	(15min.)	Coffee Break	
10:55 ~ 12:35	(100min.)	CUDA / OpenACC Programming	류현곤 (nVidia)
12:35 ~ 12:50	(15min.)	Photo	
12:50 ~ 14:00	(70min.)	Lunch	
14:00 ~ 15:40	(100min.)	Python for Scientists	정인석 (KIAS)
15:40 ~ 15:55	(15min.)	Coffee Break	
15:55 ~ 17:35	(100min.)	Machine Learning	노영균 (SNU)
17:35 ~ 19:00	(85min.)	Dinner	
19:00 ~		Team Projects & Discussions	

Reference

가장 중요한 참고서적



Y. Aoyama and J. Nakano, 1999

References

MPI를 이용한 병렬 프로그래밍, KSC

MPI: A Message-Passing Interface Standard Version 3.0

MPI: The Complete Reference

MPI Subroutine Reference

Sourcebook of parallel computing

Algorithms and parallel computing

http://www.mpitutorial.com/

References

Message Passing Interface (MPI)
Blaise Barney, Lawrence Livermore National Laboratory

https://computing.llnl.gov/tutorials/mpi/
http://people.sc.fsu.edu/~jburkardt/f_src/f90_calls_c_and_mpi/f90_calls_c_and_mpi.html

C Language - Environment Management Routines Example

```c
#include "mpi.h"
#include <stdio.h>

int main(argc,argv)
int argc;
char *argv[]; {
int  numtasks, rank, rc;

rc = MPI_Init(&argc,&argv);
if (rc != MPI_SUCCESS) {
  printf ("Error starting MPI program. Terminating.\n");
  MPI_Abort(MPI_COMM_WORLD, rc);
  }

MPI_Comm_size(MPI_COMM_WORLD,&numtasks);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
printf ("Number of tasks= %d My rank= %d\n", numtasks,rank);

/*******  do some work *******/

MPI_Finalize();
}
```

Fortran - Environment Management Routines Example

```fortran
program simple
include 'mpif.h'

integer numtasks, rank, ierr, rc

call MPI_INIT(ierr)
if (ierr .ne. MPI_SUCCESS) then
   print *,'Error starting MPI program. Terminating.'
   call MPI_ABORT(MPI_COMM_WORLD, rc, ierr)
end if

call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)
print *, 'Number of tasks=',numtasks,' My rank=',rank

C ****** do some work ******

call MPI_FINALIZE(ierr)

end
```

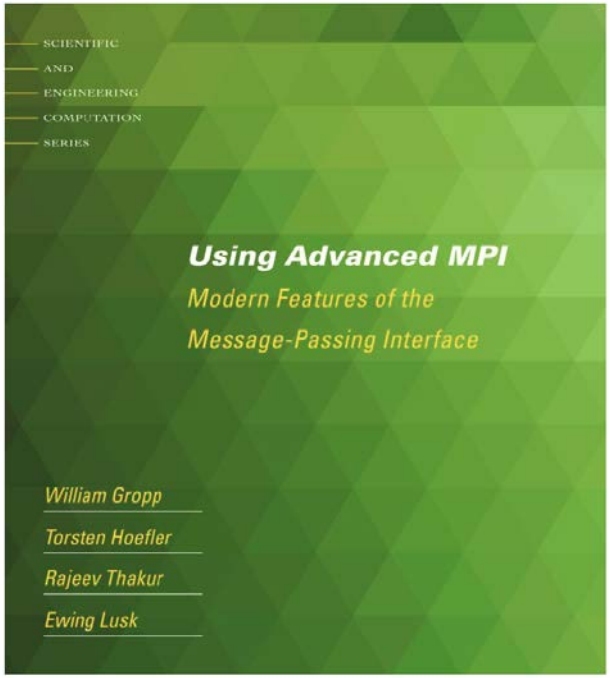
http://hpc-wiki.uni-graz.at/Wiki-Seiten/MPI%20Examples.aspx :set paste

References

http://www.mcs.anl.gov/research/projects/mpi/tutorial/

Google search :
Introduction to MPI – created by the PACS Training Group

Message Passing Fundamentals

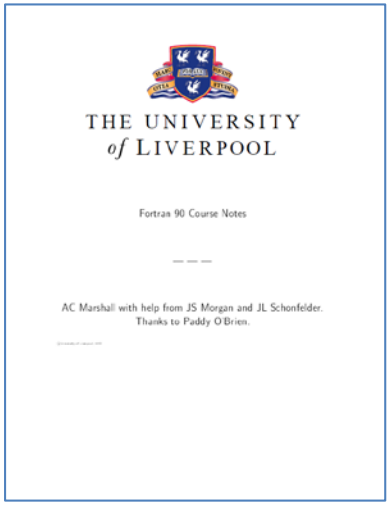


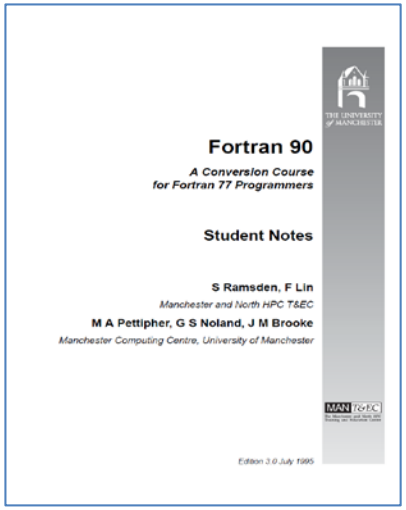
FORTRAN 90/ C

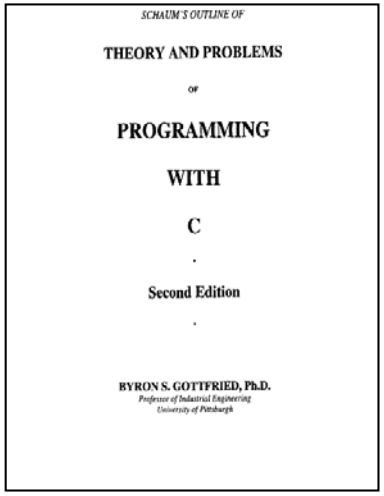
Fortran 90
A Conversion Course for Fortran 77 Programmers (The University of Manchester)

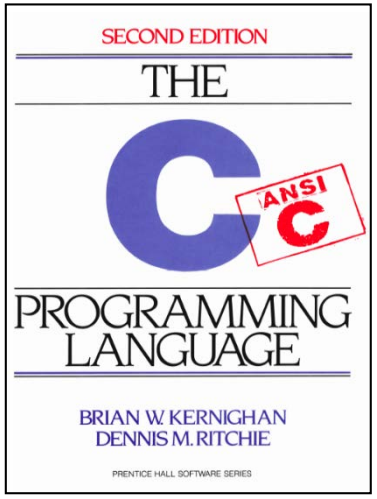
The University of Liverpool
Fortran 90 course notes

FORTRAN과 C 언어가 가장 빠르게 계산을 수행할 수 있는 컴퓨터 언어이다.
따라서, FORTRAN/C를 이용한 MPI 프로그래밍이 가장 널리 사용되는 병렬 프로그래밍이다.









두 개의 FORTRAN 90/C 레퍼런스 서적들, 인터넷: Stack Overflow

10,000,000 questions

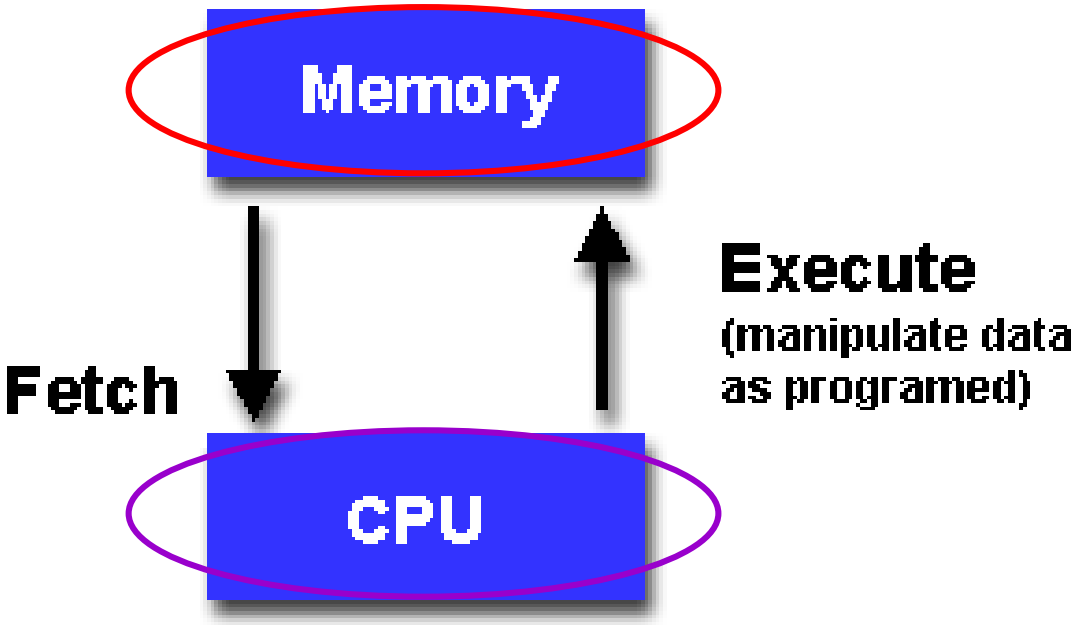
http://incredible.egloos.com

http://en.wikipedia.org/wiki/Parallel_computing

Supercomputer?
Why Parallel Computing?

- Large-scale calculations
- Fast calculations (optimization?)
- www.top500.org
- Save time - ***wall clock time*** (1 day *vs* 1 week)
- speed of light (30 cm/nanosecond)
- Performance/price

von Neumann computer



CPU gets instructions and/or data from memory,
decodes the instructions and then *sequentially* performs them.

Serial ←→ Parallel

associative property of addition

associative property of multiplication

commutative distributive

$(1+2)+3 = 1+(2+3)$

$(1+2)+3 \rightarrow 3+3 \rightarrow 6$

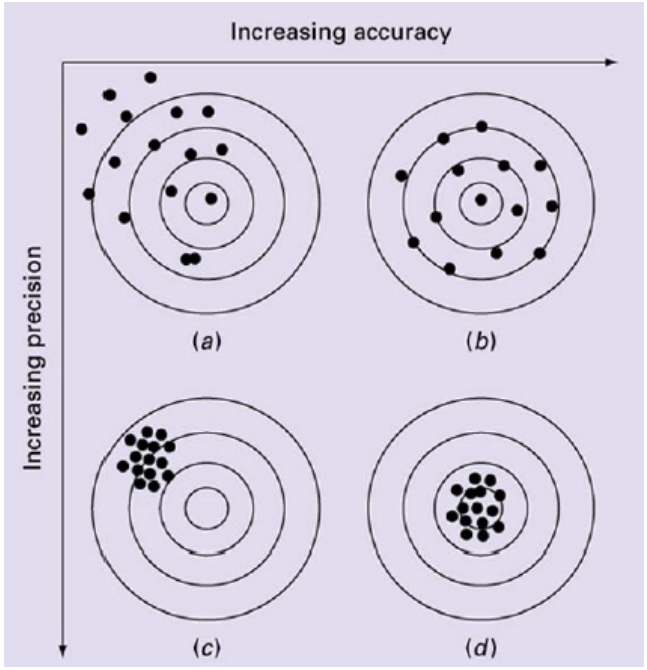
$1+(2+3) \rightarrow 1+5 \rightarrow 6$

$6 = 6$

SP : 10^{-38} 10^{39}
7 decimal precision
DP : 10^{-308} 10^{308}
15 decimal precision

Truncation Error

Roundoff Error

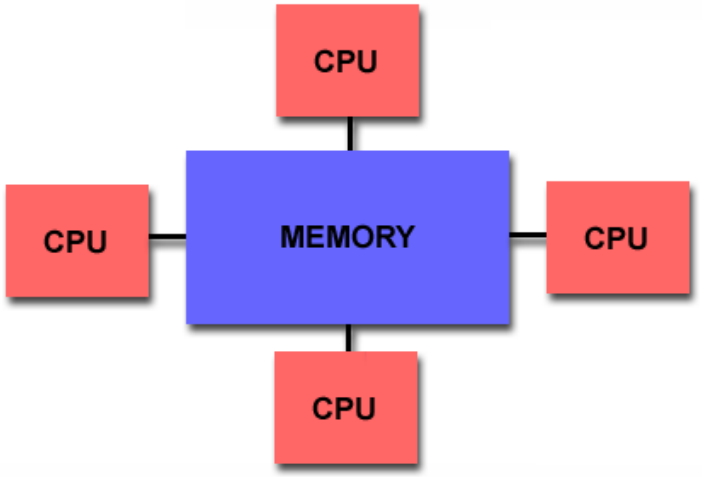


계산하는 순서가 다를 수 있다.
심지어 계산하는 CPU가 서로 다르다.

- Accuracy: how closely a computed or measured value agrees with the true values.
- Precision: how closely individual computed or measured values agree with each other.

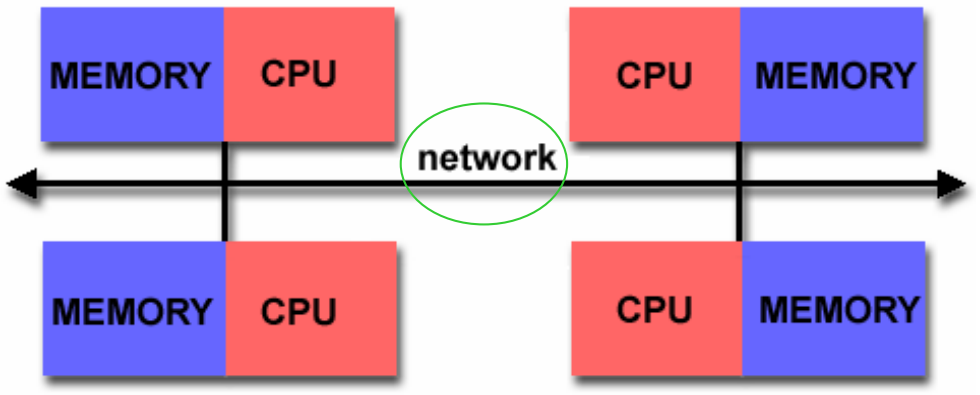
CPU & Memory

Shared Memory



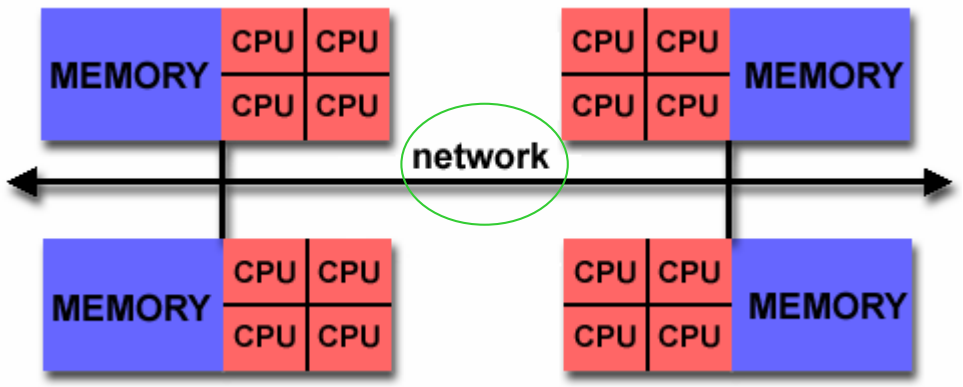
IBM SP Power3 Nodes, Regatta (Power4) servers,
SGI Power Challenge Series, Sun Enterprise Series

Distributed Memory



IBM SP (pre-Power3 nodes,
Clusters of uniprocessor nodes

Hybrid Distributed-Shared Memory



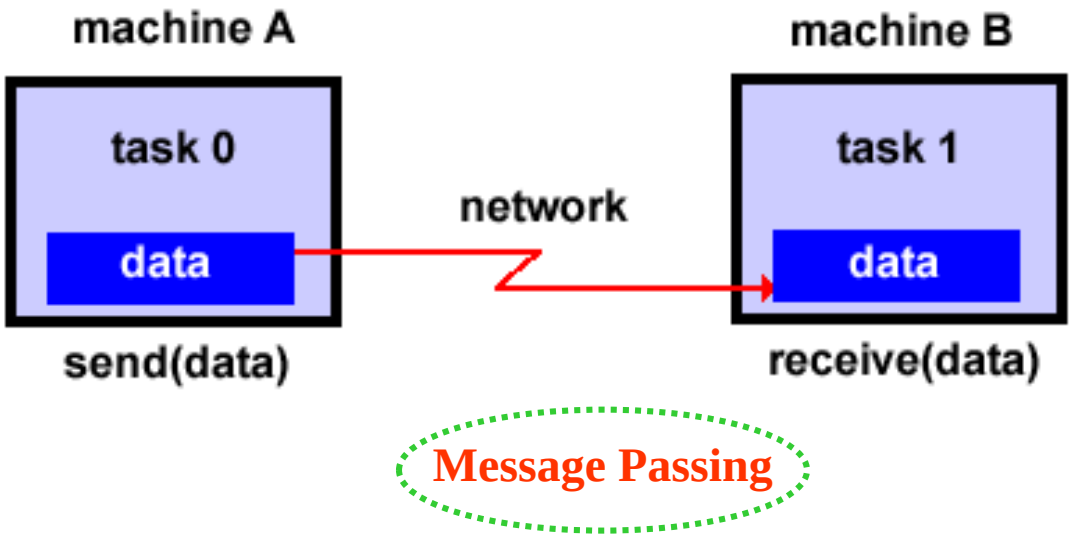
Clusters of SMPs,
IBM SP Series,
SGI Origin Series

Beowulf

- 1994 NASA, CESDIS에서 제작 **16 노드**(인텔DX4), *10 Mbps 이더넷*
- 지놈프로젝트, 세레라 지노믹스 사 (1200 대)

Home made?

고등과학원 cluster



1980년대 CRAY가 압도적 성능을 자랑함. 하지만 값싼 고성능 컴퓨터의 개발이 이루어짐.
여러 대의 값싸고 성능 좋은 컴퓨터들의 연결이 필수 불가결해짐. 새로운 이식이 가능한 소프트웨어가 필요해짐.

Levels of parallelism

Data parallel (*fine-grained* parallel)
OpenMP and HPF Directive-based data-parallel
Parallel execution of DO loops in FORTRAN

Task parallel (*coarse-grained* parallel)
MPI, PVM (message passing)

Inter-process communication

Very general model
Hardware platforms
Great control over data location and flow in a program
Higher performance level (scalability)

Programmer has to work hard to implement!

Some General Parallel Terminology

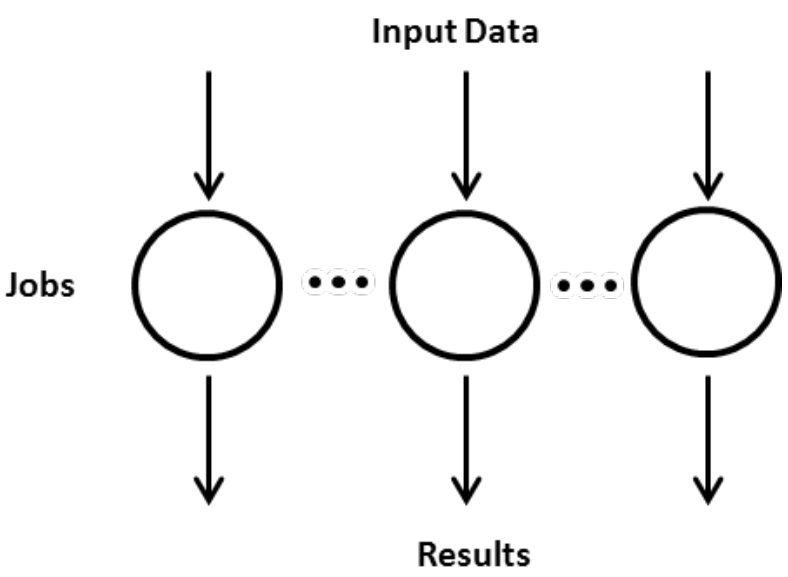
- **Observed Speedup** (WC-serial/WC-parallel)
  Scalability
- **Granularity** (coarse, fine)
  Computation / Communication Ratio
- **Synchronization**
- **Communications**

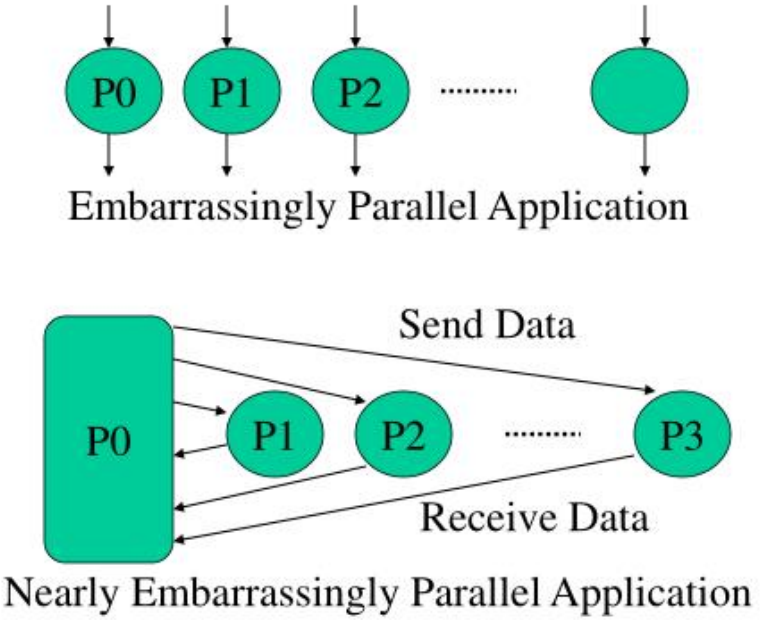
The purpose of parallelization is to reduce the time spent for computation. Ideally, the parallel program is *p times faster than the sequential program*, where *p is the number of processes involved in the parallel execution, but this* is not always achievable.

Embarrassingly parallel

- little or no communication of results between tasks

Rendering of computer graphics
Genetic algorithms



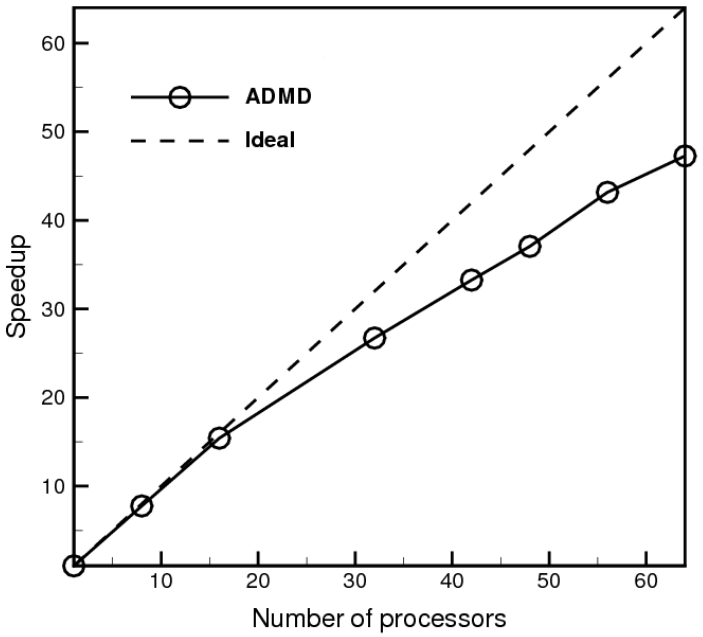


speedup

$$S_p = \frac{T_1}{T_p}$$

***p* is the number of processors.**
***T_p* is the execution time of the algorithm with *p* processors.**

Not CPU time, but wall-clock time reference

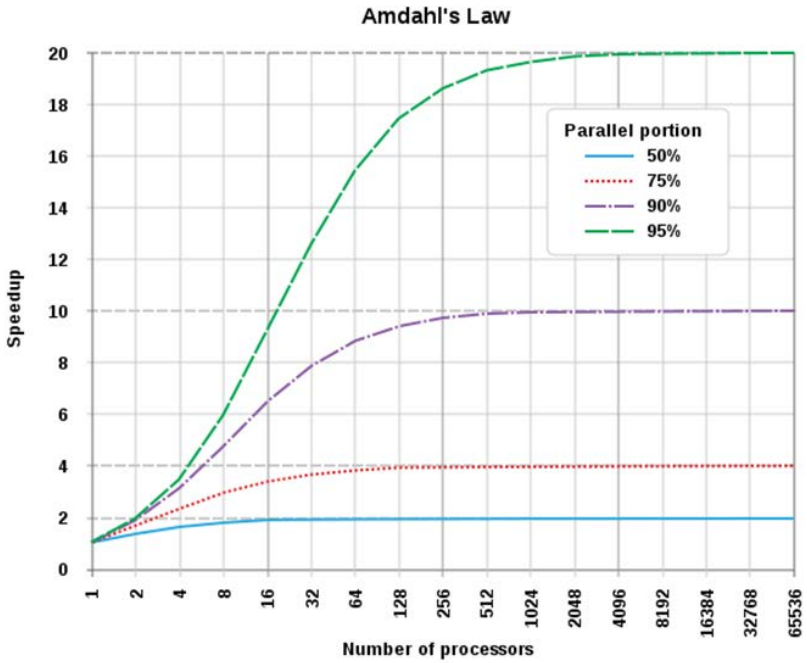


http://en.wikipedia.org/wiki/Speedup

Amdahl's law

The speedup is limited by the serial part of the program. For example, if 95% of the program can be parallelized, the theoretical maximum speedup using parallel computing would be 20 times.

병렬화 방법의 중요성.
병렬화를 시키는 방법들을 고려함.



Amdahl's law can be formulated the following way:

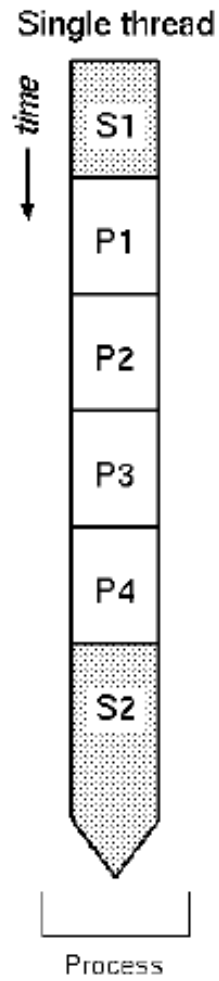
$$S_{\text{latency}}(s) = \frac{1}{(1-p) + \frac{p}{s}}$$

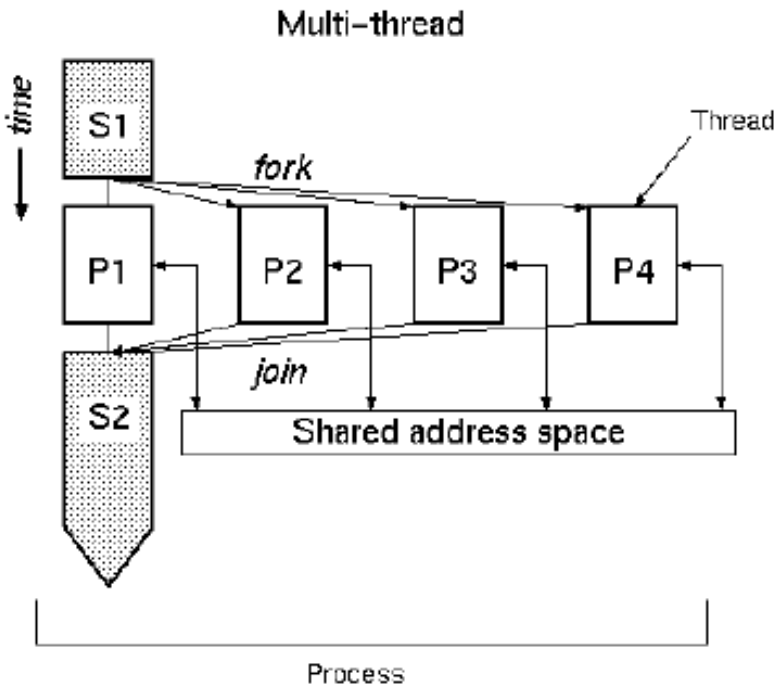
where

- S_{latency} is the theoretical speedup of the execution of the whole task;
- s is the speedup of the part of the task that benefits from improved system resources;
- p is the proportion of execution time that the part benefiting from improved resources originally occupied.

https://en.wikipedia.org/wiki/Amdahl%27s_law

SMP (Symmetric Multi-Processor)

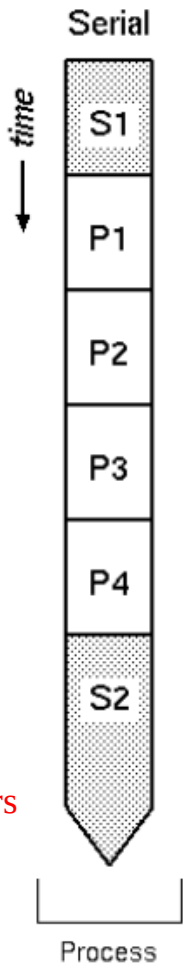


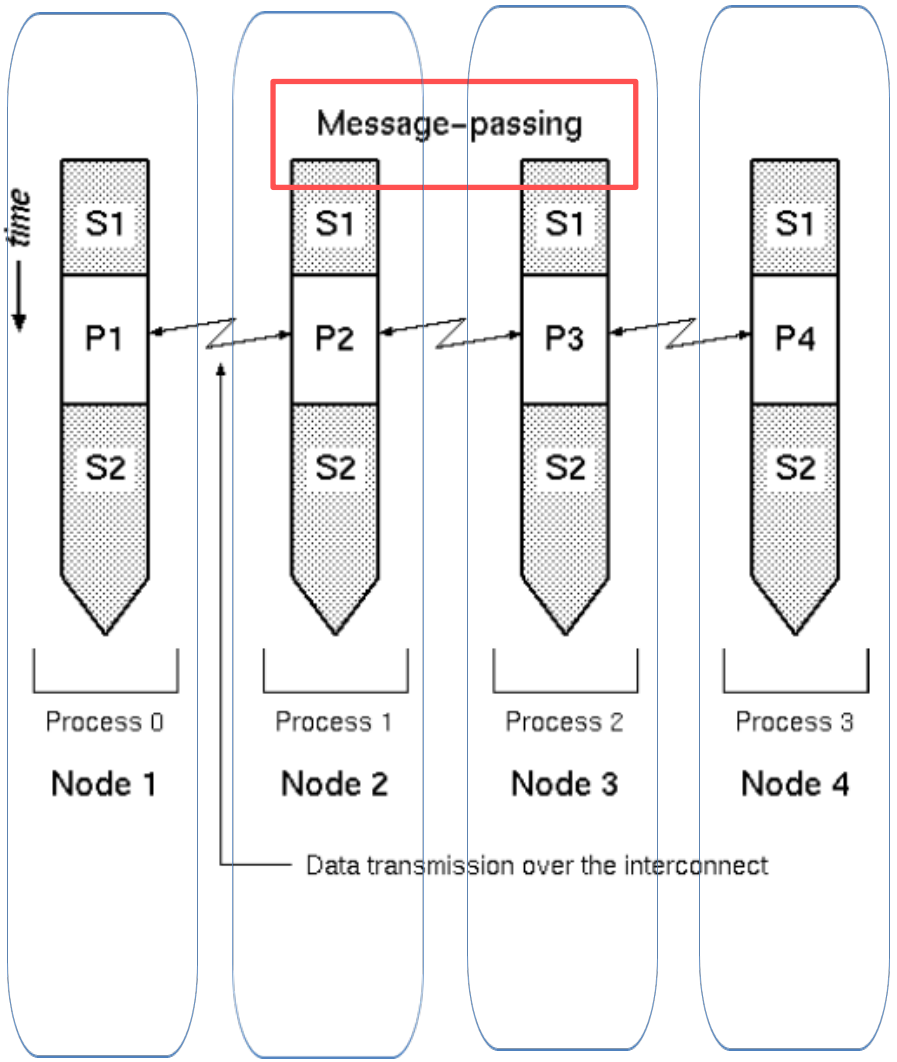


Cray YMP C/J 90
SGI Origin 200/2000
Sun E10000
SMP Intel-based computers (Dell, Unisys)

Y. Aoyama and J. Nakano

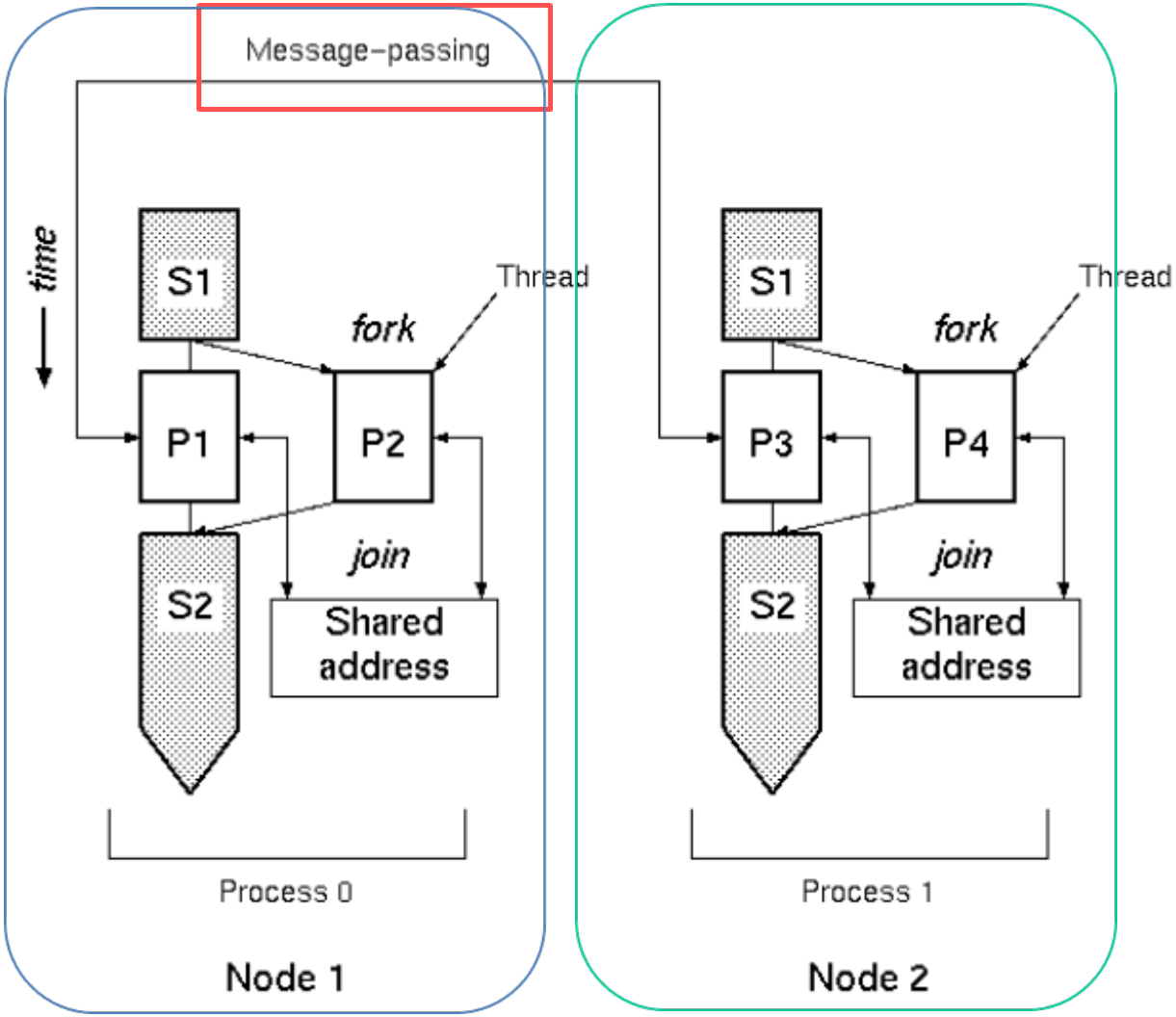
Message-Passing





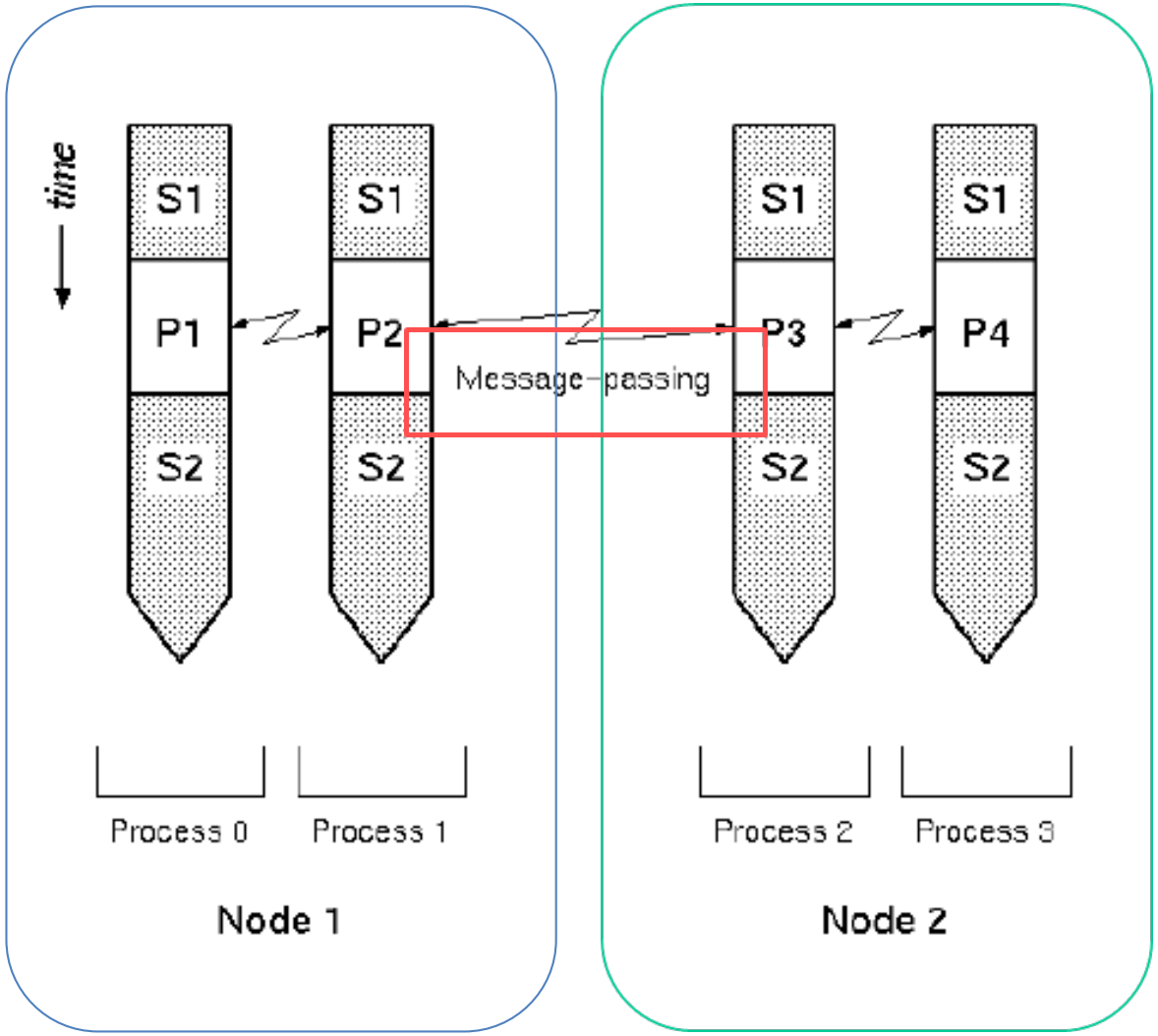
Cray T3E
Unix (Linux) clusters

Y. Aoyama and J. Nakano



Y. Aoyama and J. Nakano

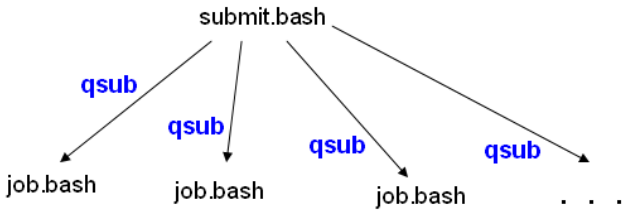
Multiple Single-Thread Processes Per Node



Y. Aoyama and J. Nakano

Non-MPI, master-slave, and data parsing (1/6)

- Master-slave mode
- More flexible (PBS script)
- One-serial but multiple directories
- Usual PBS-like job submission
- Data parsing over the directories



http://incredible.egloos.com/4842832

http://incredible.egloos.com/4836430

제3자의 컴퓨터 프로그램이 있고 그 내부를 잘 알지 못하는 경우,
제3자 프로그램을 새로 만들 필요가 없고 이용하기만 하면 될 경우,
또는 잘 병렬화 되어 있는 경우, 계산량이 충분히 큰 경우,
프로그램이 충분히 검정이 된 경우이고 반복적으로 사용할 수 있는 경우,
컴퓨터 자원을 독점적으로 사용하지 못할 경우,
여러 종류의 출력들을 동시에 활용하여 새로운 입력을 만들 경우,
하나의 순차 프로그램으로 사실상 병렬 프로그램이 가능하다.
유전 알고리듬과 같은 경우가 이 경우에 해당한다.
(목적함수 계산이 매우 복잡하고 시간적으로 오래 걸리는 경우)

Non-MPI, master-slave, and data parsing (2/6)

SOLDIER.pbs (job submission)
input_file (static input)
input_file (dynamic input)

Directory monitoring
Data parsing
Input generation
Job submission
call system()
inquire()

deposit/
0001/
0002/
0003/
….
0050/

하나의 시리얼 메인 프로그램이 여러 개의 디렉토리들을 만들고 각 디렉토리에서 적당히 시간이 걸리는 제3의 프로그램을 이용해서 계산들을 진행한다. PBS를 이용해서 job을 제출한다. 제출한 job들은 계산 중으로 판단한다. 계산이 끝나면, PBS 스크립트 마지막 부분에 있는 파일생성 신호를 이용하여 계산이 끝났음을 파일형식으로 알려준다. 메인 시리얼 프로그램은 각 디렉토리에서 계산 종료를 확인한다. 계산 종료를 확인한 경우 결과를 읽어 들이고, 그 자리에 또 다른 계산을 PBS로 제출한다. 물론, 해당 디렉토리에 인풋 파일을 만들어주어야 한다.

Non-MPI, master-slave, and data parsing (3/6)

```
#!/bin/sh
#PBS -l nodes=2:quad:ppn=8
#PBS -N csa_soldier

NPROCS=`wc -l < $PBS_NODEFILE`

hostname
date

cd $PBS_O_WORKDIR

# do not change file names, e.g., stdout.log, STOP

# normal
cp INCAR_rlx    INCAR
sleep 0.5
mpirun -genv I_MPI_DEBUG 5 -np $NPROCS /opt/VASP/bin/vasp.5.2.12_GRAPE_GRAPHENE_NORMAL.mpi.x > stdout.log
# accurate   550 eV
cp INCAR_rlxall INCAR
cp CONTCAR      POSCAR
sleep 0.5
mpirun -genv I_MPI_DEBUG 5 -np $NPROCS /opt/VASP/bin/vasp.5.2.12_GRAPE_GRAPHENE_NORMAL.mpi.x > stdout.log
cp OUTCAR out.out1
cp CONTCAR      POSCAR
sleep 0.5
mpirun -genv I_MPI_DEBUG 5 -np $NPROCS /opt/VASP/bin/vasp.5.2.12_GRAPE_GRAPHENE_NORMAL.mpi.x > stdout.log
cp OUTCAR out.out2
cp CONTCAR      POSCAR
sleep 0.5
mpirun -genv I_MPI_DEBUG 5 -np $NPROCS /opt/VASP/bin/vasp.5.2.12_GRAPE_GRAPHENE_NORMAL.mpi.x > stdout.log
cp OUTCAR out.out3
cp CONTCAR      POSCAR
# accurate   550 eV
#cp INCAR_bs     INCAR
#cp CONTCAR      POSCAR
#sleep 0.5
#mpirun -genv I_MPI_DEBUG 5 -np $NPROCS /opt/VASP/bin/vasp.5.2.12_GRAPE_GRAPHENE_NORMAL.mpi.x > stdout.log

STAMP=$(date +%Y%m%d_%H%M%S)_$RANDOM
echo $STAMP
cp CONTCAR   /home/ihlee/csa_vasp/B28_in/deposit/CONTCAR_$STAMP
cp OUTCAR    /home/ihlee/csa_vasp/B28_in/deposit/OUTCAR_$STAMP
cp EIGENVAL  /home/ihlee/csa_vasp/B28_in/deposit/EIGENVAL_$STAMP
cp DOSCAR    /home/ihlee/csa_vasp/B28_in/deposit/DOSCAR_$STAMP

sleep 0.5
touch STOP
echo "DONE" >> STATUS
```

한 디렉토리에서 계산이 끝날 때 그 디렉토리에 계산 종료와 관련된 정보를 적어준다.
메인 프로그램은 수시로 계산 종료를 체크한다. 파일을 읽어서 판단한다.

동일한 형식의 파일들은 시간-랜덤 넘버를 사용한 태그를 붙여서 한 곳에 보관한다.
물론, 입력, 출력 파일에 입력과 출력을 확인할 수 있는 태그가 있어야 편리하다.

Non-MPI, master-slave, and data parsing (4/6)

```
!     Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine send_exe(mm,ndir,loccupied,kcmd,nwork,iseq)
      USE csa_application, ONLY : natom,lpbc
      implicit none
      integer mm,ndir,kcmd,nwork,iseq(nwork)
      logical loccupied(ndir)
      integer jd,i,ish
      real*8 r6(6),cmatrix(3,3),a1(3),a2(3),a3(3),ddg
      character*80 file_names(20),tmpname
      character*280 cmd
      real ranmar

      do jd=1,ndir
      if(.not. loccupied(jd))then
      call iofilearray(jd,file_names)
      call csa_rnd_lattice_basis(mm,nwork,iseq)
      ish=ndeg-6
      if(lpbc)then
      do i=1,6
      r6(i)=qosi0(ish+i)
      enddo
      call lat2matrix(r6,cmatrix,1)
      a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
            endif
      if(lpbc)then
      call direct_pbc(qosi0)
            else
      call centering(qosi0)
            endif
      call write_poscar(mm,file_names(3))
      ddg=0.12d0 ; tmpname=trim(file_names(5))//'_012'
      call write_kpoints(ddg,a1,a2,a3,tmpname)
      ddg=0.06d0 ; tmpname=trim(file_names(5))//'_006'
      call write_kpoints(ddg,a1,a2,a3,tmpname)
      ddg=0.03d0 ; tmpname=trim(file_names(5))//'_003'
      call write_kpoints(ddg,a1,a2,a3,tmpname)
      ddg=0.02d0 ; tmpname=trim(file_names(5))//'_002'
      call write_kpoints(ddg,a1,a2,a3,tmpname)
      ddg=0.00d0 ; tmpname=trim(file_names(5))//'_000'
      call write_kpoints(ddg,a1,a2,a3,tmpname)
!     call sleep(1)
      call system('sleep 0.1')
      cmd='cp '//trim(file_names(3))//' '//trim(file_names(3))//'_'
      cmd=trim(cmd) ; call system(cmd)
!
      cmd='cd ./'//trim(file_names(1))//' ; '//'qsub ./CSA_SOLDIER.pbs'
      cmd=trim(cmd) ; call system(cmd)
      loccupied(jd)=.true.
      call system('sleep 0.1')
      exit
                  endif
      enddo
      end subroutine send_exe
```

만들어진 디렉토리들에 새로운 인풋 파일 만들어주기
(기본적인 파일들은 미리 복사 해 둠)
동적으로 인풋 파일들을 만들어줌
물론, 인풋 파일에 태그를 붙여준다 출력에도 동일한 태그가 있으면 좋다
특정 디렉토리가 계산 중인지 그렇지 않은지 표시하여 둠(계산 가능, 불가능)
PBS job 제출함
제출한 job는 무조건 계산 중으로 취급한다
계산이 종료 되면 특정한 정보를 해당 디렉토리에 표시한다
메인 루틴은 이 정보를 수시로 확인하고 계산 종료를 확인한다
계산이 종료된 디렉토리는 즉각 다른 계산을 할 수 있도록 지정된다

Non-MPI, master-slave, and data parsing (5/6)

```
!     Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine gen_directories(ndir)
      implicit none
      integer ndir
      character*80 string
      character*280 cmd
      integer isize,i

      isize=4
      if(ndir > 0)then
      do i=1,ndir
      call xnumeral(i,string,isize) ; string=trim(string)
      cmd='mkdir '//trim(string)                    ; cmd=trim(cmd) ; call system(cmd)
      cmd='cp ./CSA_SOLDIER.pbs '//trim(string)//'/' ; cmd=trim(cmd) ; call system(cmd)
      cmd='cp INCAR_rlx '//trim(string)//'/'         ; cmd=trim(cmd) ; call system(cmd)
      cmd='cp INCAR_rlxall '//trim(string)//'/'      ; cmd=trim(cmd) ; call system(cmd)
      cmd='cp INCAR_bs '//trim(string)//'/'          ; cmd=trim(cmd) ; call system(cmd)
      cmd='cp POTCAR  '//trim(string)//'/'           ; cmd=trim(cmd) ; call system(cmd)
      enddo
              endif
      if(ndir < 0)then
      ndir=iabs(ndir)
      do i=1,ndir
      call xnumeral(i,string,isize) ; string=trim(string)
      cmd='rm -rf '//trim(string)//'/' ; cmd=trim(cmd)
      call system(cmd)
      call sleep(1)
      enddo
              endif
      call sleep(1)
      return
      end
!
```

디렉토리들 만들기
0001/
0002/
….
그리고 그곳에 필요한 파일들 복사해 두기

Non-MPI, master-slave, and data parsing (6/6)

```
!     Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine jobstatus(fname,i)
      implicit none
      character*80 fname
      integer i
      logical lexist
      character*20 ch

      i=0
      inquire(file=trim(fname),exist=lexist)
      if(lexist)then
      open(77,file=trim(fname),form='formatted')
      do
      read(77,*,end=999) ch
      enddo
  999  continue
      close(77)
      if(trim(ch) == 'DONE' .or. trim(ch) == 'done') i=1
      if(trim(ch) == 'Done' .or. trim(ch) == 'DOne') i=1
      if(trim(ch) == 'DONe'                        ) i=1
            endif
      return
      end
!
!     Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine jobstatus0(fname)
      implicit none
      character*80 fname
      character*200 cmd

!     open(77,file=trim(fname),form='formatted')
!     write(77,*) 'ING'
!     close(77)
      cmd='echo "ING" >> '//trim(fname) ; cmd=trim(cmd)
      call system(cmd)
      call system('sleep 0.1')
      return
      end
```

만들어진 디렉토리들 중에서 계산이 종료된 디렉토리를 수시로 확인한다

MPI (message passing interface)

- The Message Passing Interface Standard (MPI) is a message passing library standard based on the consensus of the MPI Forum.
- MPI is not an IEEE or ISO standard, but has in fact, become the "industry standard" for writing message passing programs on HPC platforms.
- Various architectures
- Free implementations: MPICH, LAM, CHIMP, openmpi

Intel MPI

InfiniBand, Myrinet, Quadrics

MPI (message passing interface)

- MPI 자체는 병렬 라이브러리들에 대한 표준규약이다. (125개의 서브 프로그램들로 구성되어 있다.) MPI는 약 40개 기관이 참여하는 MPI forum에서 관리되고 있으며, 1992년 MPI 1.0 을 시작으로 현재 MPI 3.0까지 버전 업된 상태이다.
- Various architectures
- Free implementations: MPICH, LAM, CHIMP, openmpi

FLUENT (Fluid Dynamics and Heat transfer)
GASP (Gas Dynamics)
AMBER (Molecular dynamics)
NAMD (Molecular dynamics)
GROMACS (Molecular dynamics)
VASP (Electronic structure)
….

MPI (message passing interface)

The MPI-1 standard was defined in Spring of 1994.

1 This standard specifies the names, calling sequences, and results of subroutines and functions to be called from Fortran 77 and C, respectively. All implementations of MPI must conform to these rules, thus ensuring portability. MPI programs should compile and run on any platform that supports the MPI standard.

2 The detailed implementation of the library is left to individual vendors, who are thus free to produce optimized versions for their machines.

3 Implementations of the MPI-1 standard are available for a wide variety of platforms.

An MPI-2 standard has also been defined. It provides for additional features not present in MPI-1, including tools for parallel I/O, C++ and Fortran 90 bindings, and dynamic process management. At present, some MPI implementations include portions of the MPI-2 standard but the full MPI-2 is not yet available.

MPI-3.0 is a major update to the MPI standard.
Intel MPI
IBM GB/Q Clusters

data is moved from the address space of one process to that of another process

Top 10 Reasons to Prefer MPI Over PVM

1. MPI has more than one freely available, quality implementation.
2. MPI defines a 3rd party profiling mechanism.
3. MPI has full asynchronous communication.
4. MPI groups are solid and efficient.
5. MPI efficiently manages message buffers.
6. MPI synchronization protects 3rd party software.
7. MPI can efficiently program MPP and clusters.
8. MPI is totally portable.
9. MPI is formally specified.
10. MPI is a de facto **standard.**

Advantages of Message Passing

- Universality : MP model fits well on separate processors connected by fast/slow network. Matches the hardware of most of today's parallel supercomputers as well as network of workstations (NOW)
- Expressivity : MP has been found to be a useful and complete model in which to express parallel algorithms. It provides the control missing from data parallel or compiler based models
- Ease of debugging : Debugging of parallel programs remain a challenging research area. Debugging is easier for MPI paradigm than shared memory paradigm (even if it is hard to believe)

Implementations of MPI

There are a number of freely available implementations of MPI that run on a variety of platforms:

The MPICH implementation runs on a wide range of platforms and operating systems including Unix/Linux, Windows NT, and Windows 2000/XP Professional.
The LAM implementation runs on networks of Unix/Posix workstations.
MP-MPICH runs on Unix systems, Windows NT and Windows 2000/XP Professional.
The WMPI implementation runs on Windows platforms running Windows 95/98, ME, NT and 2000.
MacMPI is a partial implementation of MPI for Macintosh computers.
openmpi
Intel MPI

Most parallel machine vendors have optimized versions.

MPICH_GM
MPICH_G2

http://www.mpi.nd.edu/MPI/Mpich
http://www-unix.mcs.anl.gov/mpi/mpich/indexold.html
GLOBUS:
http://www.globus.org/mpi/
http://exodus.physics.ucla.edu/appleseed/

Official implementations

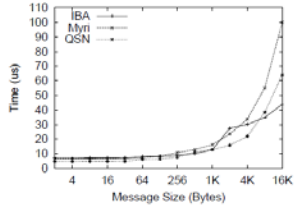
Most current MPI implementations are supported :

MPICH/p4 : over ethernet devices
MPICH/gm : Myrinet
MVAPICH : InfiniBand
MPICH/shmem : a single-node multi-processor machine
MPICH2/PMI :
Intel MPI :
EMP :
Open MPI :
LAM :

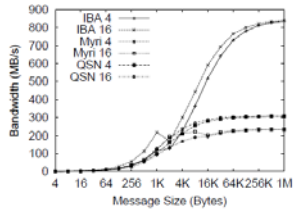
The initial implementation of the MPI 1.x standard was MPICH, from Argonne National Laboratory (ANL) and Mississippi State University.
IBM
LAM/MPI from Ohio Supercomputer Center
Open MPI

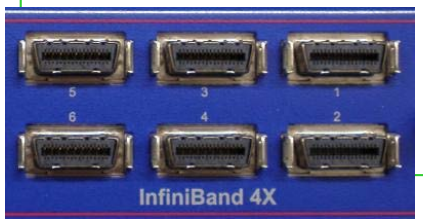
Latency and Bandwidth

- *latency* is the time it takes to send a minimal (0 byte) message from point A to point B. ~120,~120,~7,~0.5 microsecond



- *bandwidth* is the amount of data that can be communicated per unit time. ~100 Mbps, ~1 Gbps, ~1.98 Gbps, ~1 Gb/sec





높은 스루풋, 낮은 레이턴시

Cf. CPU time Fast ethernet, Gigbit ethernet, Myrinet, Quadrics 2, InfiniBand

Computation *vs* communication

연결을 위해서 기본적으로 걸리는 시간 (잠복, 잠재)

Communication time ← latency, throughput

연결이 된 후 할당된 데이터 전송에 걸리는 시간 : 단위시간당 처리량

Latency를 줄이기 위해서는 한 번의 연결에 집중적으로 통신하는 것이 좋다.

데이터 통신에 걸리는 시간 *vs* CPU를 이용한 계산시간

InfiniBand is a computer-networking communications standard used in high-performance computing that features very high throughput and very low latency.

	Fast Ethernet	Gigabit Ethernet	Myrinet	Quadrics 2
latency	120 microsecond	120 microsecond	7 microsecond	0.5 microsecond
bandwidth	100 Mbps	1 Gbps	1.98 Gbps	1 Gbyte/second

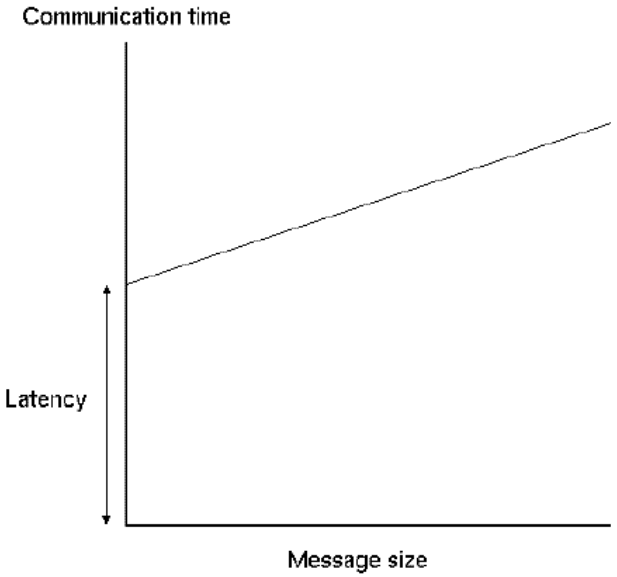
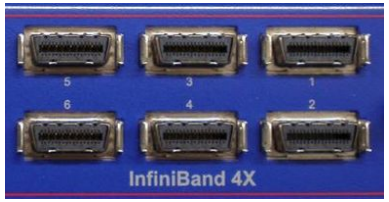


Figure 32. The Communication Time

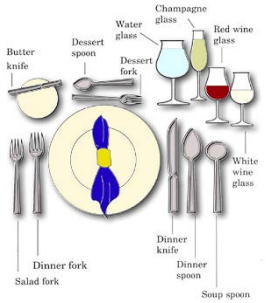


	SDR	DDR	QDR	FDR10	FDR	EDR	HDR	NDR	XDR
Signaling rate (Gbit/s)	2.5	5	10	10.3125	14.0625[6]	25	50	100	250
Theoretical effective throughput, Gbs, per 1x[7]	2	4	8	10	13.64	24.24			
Speeds for 4x links (Gbit/s)	8	16	32	40	54.54	96.97			
Speeds for 8x links (Gbit/s)	16	32	64	80	109.08	193.94			
Speeds for 12x links (Gbit/s)	24	48	96	120	163.64	290.91			
Encoding (bits)	8/10	8/10	8/10	64/66	64/66	64/66	64/66		
Adapter latency (microseconds)[8]	5	2.5	1.3	0.7	0.7	0.5			
Year[9]	2001, 2003	2005	2007	2011	2011	2014[7]	2017[7]	after 2020	future

InfiniBand

SPMD

Start parallel job on *N* processors



Message passing between processors

Each processor does some calculations (*processor dependent codes are run*)

Message passing between processors

End parallel job

/usr/local/mpich/

/usr/local/mpich/bin/mpif90 a.f90

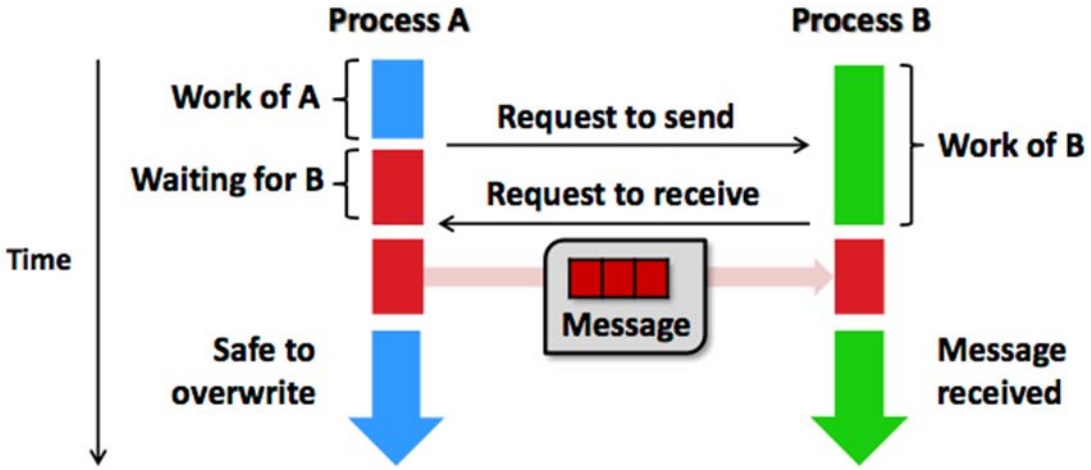
mpirun –np 8 a.out

bin/ etc/ include/ man/ share/
doc/ examples/ lib/ sbin/ www/

The 6 basic MPI routines

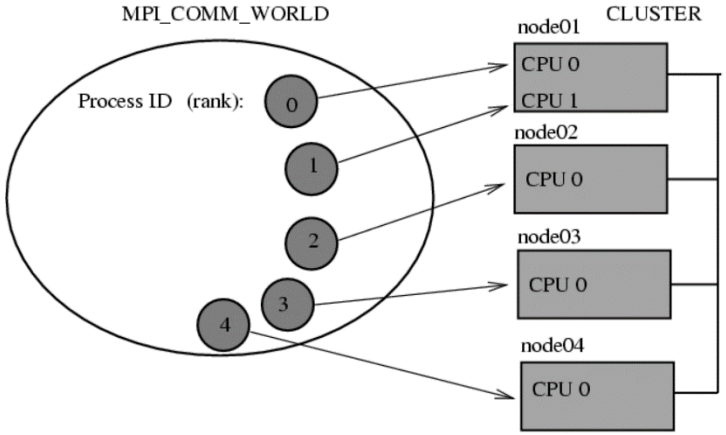
- MPI is used to create parallel programs based on message passing
- Usually the same program is run on multiple processors
- The 6 basic calls in MPI are:
  - MPI_INIT(ierr)
  - MPI_COMM_RANK(MPI_COMM_WORLD, **myid**, ierr)
  - MPI_COMM_SIZE(MPI_COMM_WORLD, **numprocs**, ierr)
  - MPI_Send(**buffer**, **count**, MPI_INTEGER, *destination*, tag, MPI_COMM_WORLD, ierr)
  - MPI_Recv(**buffer**, **count**, MPI_INTEGER, *source*, tag, MPI_COMM_WORLD, status, ierr)
  - call MPI_FINALIZE(ierr)

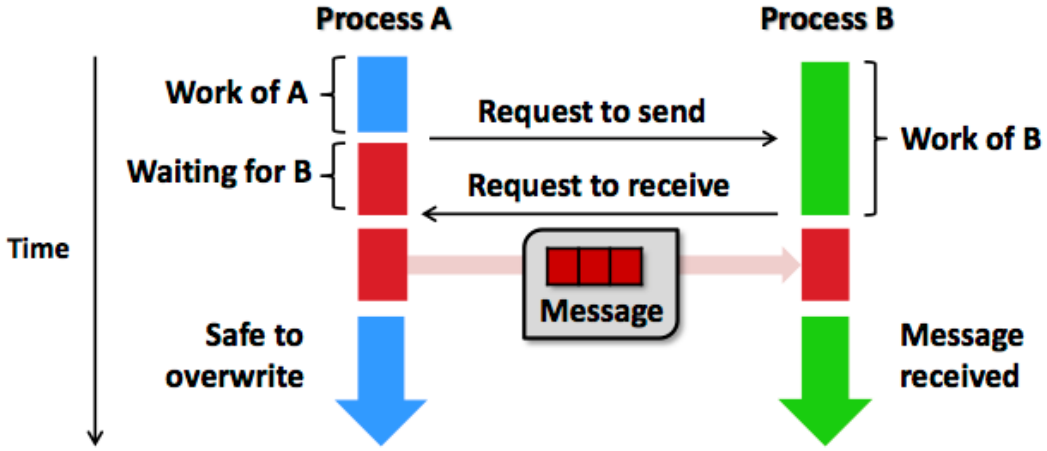
C Binding	
Format:	`rc = MPI_Xxxxx(parameter, ... )`
Example:	`rc = MPI_Bsend(&buf,count,type,dest,tag,comm)`
Error code:	Returned as "rc". MPI_SUCCESS if successful
Fortran Binding	
Format:	`CALL MPI_XXXXX(parameter,..., ierr)` `call mpi_xxxxx(parameter,..., ierr)`
Example:	`CALL MPI_BSEND(buf,count,type,dest,tag,comm,ierr)`
Error code:	Returned as "ierr" parameter. MPI_SUCCESS if successful



Communicators

- Communicators
  - A parameter for most MPI calls
  - A collection of processors working on some part of a parallel job
  - MPI_COMM_WORLD is defined in the MPI include file as all of the processors in your job
  - Can create subsets of MPI_COMM_WORLD
  - Processors within a communicator are assigned numbers 0 to n-1





communicators

Communicator is a group of processors that can communicate with each other.
There can be many communicators.
MPI_COMM_WORLD is a **pre-defined communicator** encompassing all of the processes.

MPI_INIT: MPI 환경 초기화하기 : *유저 수준에서 바꿀 것이 사실상 없음.*
MPI_COMM_SIZE: 사용 중인 processor 숫자 반환 : 유저 수준에서 바꿀 것이 사실상 없음.
MPI_COMM_RANK: 현 CPU의 번호 (rank라도 함. processor 갯수가 nproc일 때, 가능한 rank 값은0,1,2,3....nproc-1이다.) : *유저 수준에서 바꿀 것이 사실상 없음.*
두 개의 processor 간 통신: rank값들을 사용하여서 현재 processor 번호를 확인하고 준비된 데이터를 원하는 processor로 전송한다. 마찬 가지로 현재의 processor번호를 확인하고 전송되어 올 데이터를 받는다. 물론, 우리는 어떤 processor로 부터 데이터가 오는지 그리고 어떤 processor가 이 데이터를 받아야 하는지 다 알고 있다.
MPI_SEND: 원하는 processor에게 데이터 전송시 사용 : 유저의 구체적인 목적이 적용됨 (원하는 데이터 형, 사이즈,...)
MPI_RECV: 원하는 processor로부터 데이터 전송받을 때 사용 : 유저의 구체적인 목적이 적용됨 (원하는 데이터 형, 사이즈,...)

MPI_FINALIZE: MPI 환경 종료하기: *유저 수준에서 바꿀 것이 사실상 없음.*

Include files

- The MPI include file
  - C: mpi.h
  - Fortran: mpif.h (a f90 module is a good place for this)
- Defines many constants used within MPI programs
- In C, defines the interfaces for the functions
- Compilers know where to find the include files

```
#include "mpi.h"
#include <stdio.h>
#include <math.h>
```

```
program main
implicit none
include 'mpif.h'
```

/usr/local/mpich/include

basex11.h	mpeexten.h	mpi_fortdefs.h
f90base/	mpef.h	mpidefs.h
f90choice/	mpetools.h	mpif.h
mpe.h	mpi.h	mpio.h
mpe_graphics.h	mpi2c++/	mpiof.h
mpe_log.h	mpi_errno.h	protofix.h

```
include "mpif.h"     ! Constants used by MPI, e.g. constant integer value MPI_COMM_WORLD
integer istatus(MPI_STATUS_SIZE)     !   MPI_STATUS_SIZE는 위에서 선언한 include문으로 불러들인 내용에서 이미 정의된 것들이다.


integer nproc, me, ierr, idestination, isource, n_array_length, itag


  call MPI_Init(ierr)
  call MPI_Comm_size(MPI_COMM_WORLD, nproc, ierr)
  call MPI_Comm_rank(MPI_COMM_WORLD, me, ierr)
```

```
itag=19
idestination=1
call MPI_Send(real_array_user,n_array_length,MPI_REAL8,idestination,itag,MPI_COMM_WORLD,ierr)
```

real*8 형태의 데이터가 가야할 곳 지정해주어야 한다. 물론, 이 데이터의 크기도 보내는 곳에서 지정해줘야 한다. 특정 노드에서 정보를 보내기 때문에 위 함수는 특정 노드에서 불려져야 한다.

```
itag=19
isource=0
call MPI_Recv(real_array_user,n_array_length,MPI_REAL8,isource,itag,MPI_COMM_WORLD,istatus,ierr)
```

데이터를 받는 쪽에서는 그 형태와 크기를 알고 있어야 하며, 어디에서부터 출발했는지를 알아야 한다.

user-defined tags provided in MPI for user convenience in organizing application

Standard, Blocking Send

- MPI_Send: Sends data to another processor
- Use MPI_Receive to "get" the data
- C
  - MPI_Send(&buffer, count, datatype, *destination*, tag, communicator);
- Fortran
  - Call MPI_Send(buffer, count, datatype, *destination*, tag, communicator, ierr)
- Call blocks until message on the way

Basic C Datatypes in MPI

MPI Datatype	C datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED_INT	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	
MPI_PACKED	

MPI_COMPLEX

MPI_DOUBLE_COMPLEX

Language	Script Name	Underlying Compiler
C	mpicc	gcc
	mpigcc	gcc
	mpiicc	icc
	mpipgcc	pgcc
C++	mpiCC	g++
	mpig++	g++
	mpiicpc	icpc
	mpipgCC	pgCC
Fortran	mpif77	g77
	mpigfortran	gfortran
	mpiifort	ifort
	mpipgf77	pgf77
	mpipgf90	pgf90

-fast
-C

ifort

-CB
-check all

Compiler	Option	Example
Intel	-v	ifort -v
PGI	-v	pgf90 -v
GNU	-v --version	g++ --version

C/MPI version of “Hello, World”

```
#include <stdio.h>
#include <mpi.h>
int main(argc, argv)
int argc;
char *argv[ ];
{
        int myid, numprocs;

        MPI_Init (&argc, &argv) ;
        MPI_Comm_size(MPI_COMM_WORLD, &numprocs) ;
        MPI_Comm_rank(MPI_COMM_WORLD, &myid) ;
        printf(“Hello from %d₩n”, myid) ;
        printf(“Numprocs is %d₩n”, numprocs) ;
        MPI_finalize():
}
```

Fortran/MPI version of “Hello, World”

```
program  hello
include ‘mpif.h’
integer myid, ierr, numprocs

call MPI_INIT( ierr)
call MPI_COMM_RANK( MPI_COMM_WORLD, myid, ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

write (*,*) “Hello from “, myid
write (*,*) “Numprocs is”, numprocs
call MPI_FINALIZE(ierr)
stop
end
```

Minimal MPI program

- Every MPI program needs these…
  - C version

```
#include <mpi.h>                    /* the mpi include file */
                                        /* Initialize MPI */
ierr=MPI_Init(&argc, &argv);
                           /* How many total PEs are there */
ierr=MPI_Finalize();
```

- Commonly Used…
  - C version

```
ierr=MPI_Comm_size(MPI_COMM_WORLD, &nPEs);
                        /* What node am I (what is my rank?) */
ierr=MPI_Comm_rank(MPI_COMM_WORLD, &iam);
...
```

In C MPI routines are functions and return an error value.

Minimal MPI program

- Every MPI program needs these…
  - Fortran version

```
 include 'mpif.h'  ! MPI include file
c     Initialize MPI
      call MPI_Init(ierr)
c     Find total number of PEs
      call MPI_Comm_size(MPI_COMM_WORLD, nPEs, ierr)
c     Find the rank of this node
      call MPI_Comm_rank(MPI_COMM_WORLD, iam, ierr)
      ...
      call MPI_Finalize(ierr)
```

In Fortran, MPI routines are subroutines, and last parameter is an error-handling value.

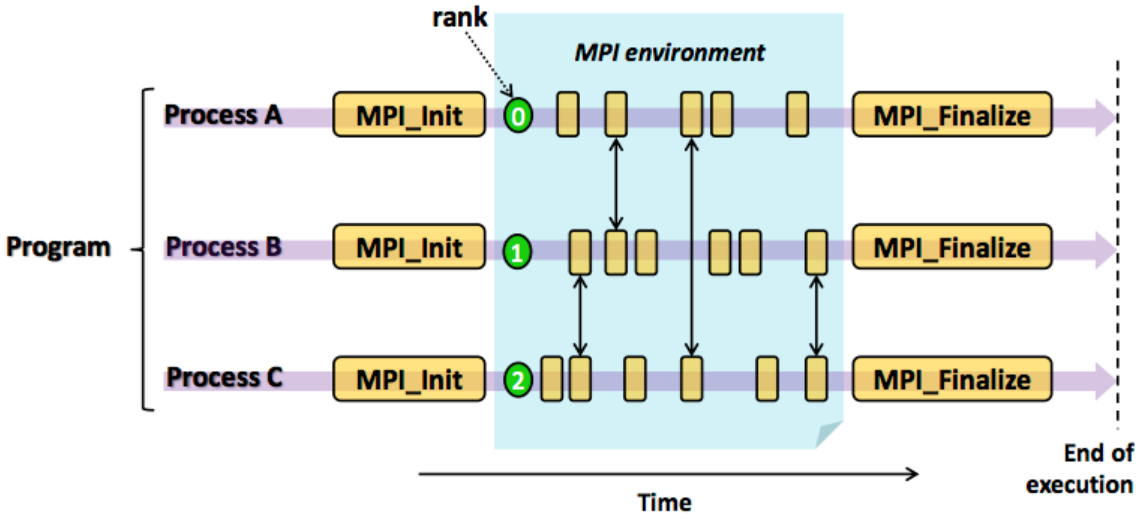
MPI "Hello, World"

- A parallel hello world program
  - Initialize MPI
  - Have each node print out its node number
  - Quit MPI

myid=0 : special

1 node calculation : 0
2 node calculation : 0, 1
3 node calculation,.....,. : 0, 1, 2

At least one node is involved.



Advantages of Message Passing

- Performance:
  - This is the most compelling reason why MP will remain a permanent part of parallel computing environment
  - As modern CPUs become faster, management of their caches and the memory hierarchy is the key to getting most out of them
  - MP allows a way for the programmer to explicitly associate specific data with processes and allows the compiler and cache management hardware to function fully
  - Memory bound applications can exhibit superlinear speedup when run on multiple PEs compare to single PE of MP machines

Background on MPI

- MPI - Message Passing Interface
  - Library standard defined by committee of vendors, implementers, and parallel programmer
  - Used to create parallel SPMD programs based on message passing
- Available on almost all parallel machines in C and Fortran
- About 125 routines including advanced routines
- 6 basic routines

Key Concepts of MPI

- Used to create parallel SPMD programs based on message passing
- Normally the same program is running on several different nodes
- Nodes communicate using message passing

Data types

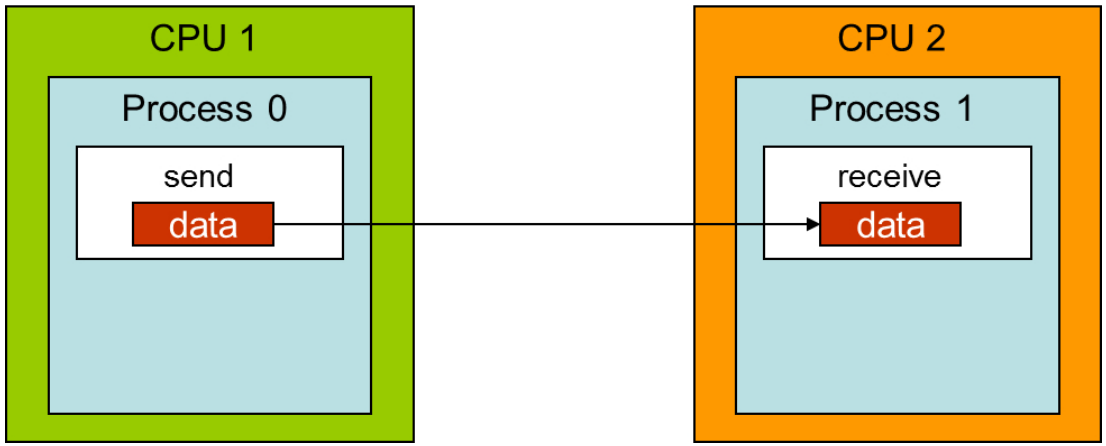
- Data types
  - When sending a message, it is given a data type
  - Predefined types correspond to "normal" types
    - MPI_REAL , MPI_FLOAT -Fortran and C real
    - MPI_DOUBLE_PRECISION, (mpi_real8), MPI_DOUBLE – Fortran and C double
    - MPI_INTEGER and MPI_INT - Fortran and C integer
  - Can create user-defined types

Basic Communications in MPI

- Data values are transferred from one processor to another
  - One process sends the data
  - Another receives the data
- Standard, Blocking
  - Call does not return until the message buffer is free to be reused
- Standard, Nonblocking
  - Call indicates a start of send or received, and another call is made to determine if finished

Basic MPI Send and Receive

- A parallel program to send & receive data
  - Initialize MPI
  - Have processor 0 send an integer to processor 1
  - Have processor 1 receive an integer from processor 0
  - Both processors print the data
  - Quit MPI



Simple Send & Receive Program

```
      program send_recv
      include "mpif.h"
! This is MPI send - recv program
      integer myid, ierr,numprocs
      integer itag,isource,idestination,kount
      integer buffer
      integer istatus(MPI_STATUS_SIZE)

      call MPI_INIT( ierr )
      call MPI_COMM_RANK( MPI_COMM_WORLD, myid, ierr )
      call MPI_COMM_SIZE( MPI_COMM_WORLD, numprocs, ierr )
      itag=1234
      isource=0
      idestination=1
      kount=1
     if(myid .eq. isource)then
        buffer=5678
        Call MPI_Send(buffer, kount, MPI_INTEGER,idestination, itag, MPI_COMM_WORLD, ierr)
        write(*,*)"processor ",myid," sent ",buffer
      endif
      if(myid .eq. idestination)then
        Call MPI_Recv(buffer, kount, MPI_INTEGER,isource, itag, MPI_COMM_WORLD, istatus, ierr)
        write(*,*)"processor ",myid," got ",buffer
      endif


      call MPI_FINALIZE(ierr)
      stop
      end
```

MPI_ANY_TAG
MPI_ANY_SOURCE

Simple Send & Receive Program

```
      PROGRAM simple_send_and_receive
      INCLUDE 'mpif.h'
      INTEGER myrank, ierr, istatus(MPI_STATUS_SIZE)
      REAL a(100)
C Initialize MPI:
      call MPI_INIT(ierr)
C Get my rank:
      call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
C Process 0 sends, process 1 receives:
      if( myrank.eq.0 )then
      call MPI_SEND( a, 100, MPI_REAL, 1, 17, MPI_COMM_WORLD, ierr)
      else if ( myrank.eq.1 )then
call MPI_RECV( a, 100, MPI_REAL, 0, 17, MPI_COMM_WORLD, istatus, ierr)
                              endif
C Terminate MPI:
      call MPI_FINALIZE(ierr)
      END
```

istatus(MPI_SOURCE), status(MPI_TAG) and status(MPI_ERROR) contain, respectively, the source, tag and error code of the received message.

```
call mpi_probe(0,mytag,MPI_COM_WORLD,istatus,ierr)
call mpi_get_count(istatus,MPI_REAL,icount,ierr)
write(*,*)"getting ", icount," values"
call mpi_recv(iray,icount,MPI_REAL,0,mytag,MPI_COMM_WORLD,istatus,ierr)
```

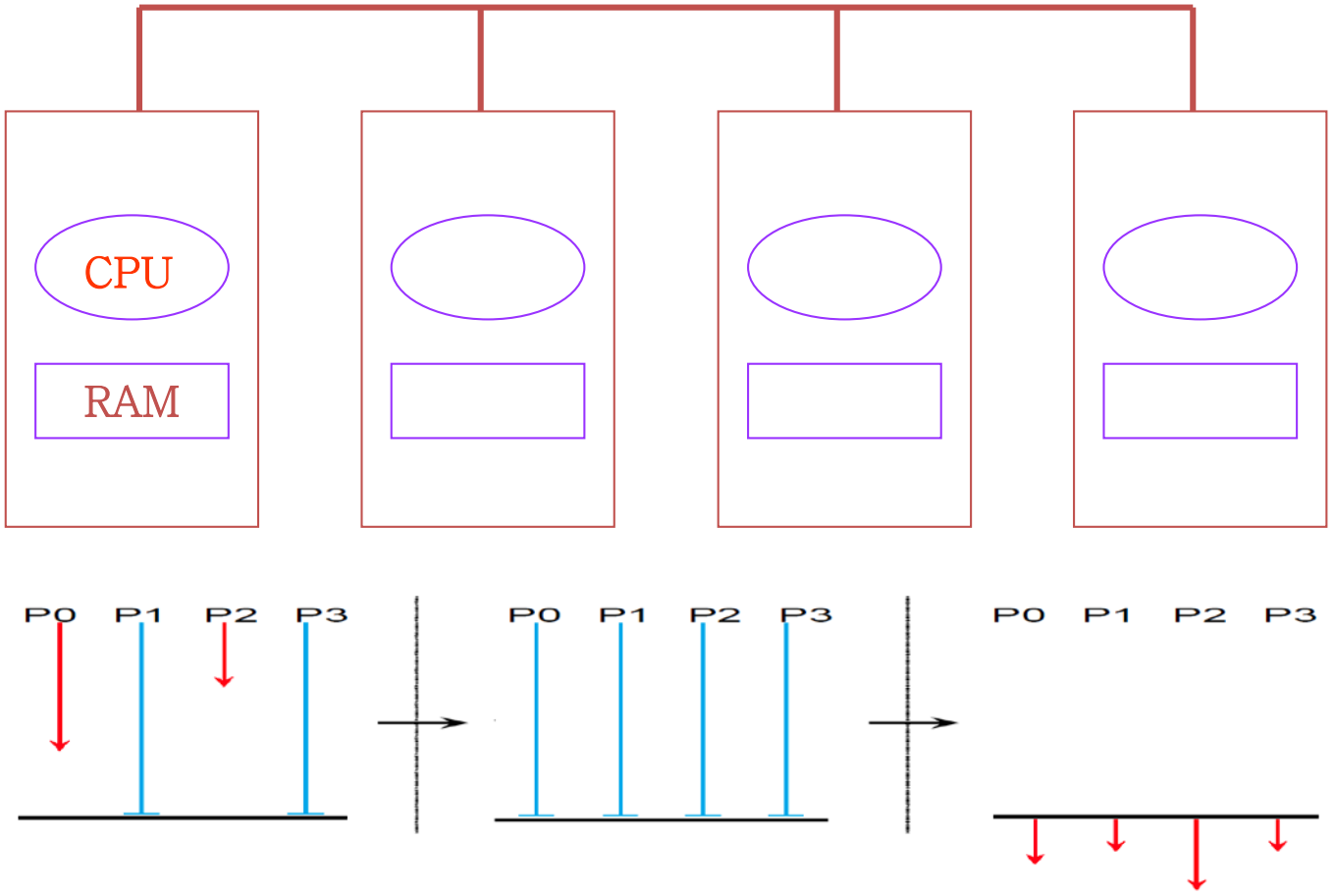
MPI_ANY_TAG
MPI_ANY_SOURCE

Simple Send & Receive Program

```
                                                        /* simple send and receive */
#include <stdio.h>
#include <mpi.h>

void main (int argc, char **argv) {
int myrank;
MPI_Status status;
double a[100];

MPI_Init(&argc, &argv);                                 /* Initialize MPI */
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);                 /* Get rank */
if( myrank == 0 )                                       /* Send a message */
MPI_Send( a, 100, MPI_DOUBLE, 1, 17, MPI_COMM_WORLD );
else if( myrank == 1 )                                  /* Receive a message */
MPI_Recv( a, 100, MPI_DOUBLE, 0, 17, MPI_COMM_WORLD, &status );
MPI_Finalize();                                         /* Terminate MPI */
}
```

Messages can be screened at the receiving end by specifying a specific tag, or not screened by specifying MPI_ANY_TAG as the tag in a receive.

A set of computing nodes connected via networks



MPI_Send

Call MPI_Send(buffer, count, datatype, *destination*, tag, communicator, ierr)

- buffer: The data
- count : Length of source array (in elements, 1 for scalars)
- datatype : Type of data, for example : MPI_DOUBLE_PRECISION, MPI_INT, etc
- *destination* : Processor number of destination processor in communicator
- tag : Message type (arbitrary integer)
- communicator : Your set of processors
- ierr : Error return (Fortran only)

Standard, Blocking Receive

- Call blocks until message is in buffer
- C
  - MPI_Recv(&buffer,count, datatype, *source*, tag, communicator, & status);
- Fortran
  - Call MPI_ RECV(buffer, count, datatype, *source*, tag, communicator, istatus, ierr)
- Status - contains information about incoming message
  - C
    - MPI_Status status;
  - Fortran
    - Integer istatus(MPI_STATUS_SIZE)

MPI_Recv

Call MPI_Recv(buffer, icount, datatype, *isource*, itag, &
communicator, istatus, ierr)

- buffer: The data
- icount : Max. number of elements that can be received
- datatype : Type of data, for example :
  MPI_DOUBLE_PRECISION, MPI_INT, etc
- *isource* : Processor number of source processor in communicator
- itag : Message type (arbitrary integer)
- communicator : Your set of processors
- istatus: Information about message
- ierr : Error return (Fortran only)

```
call MPI_RECV(ind,nid,MPI_INTEGER,MPI_ANY_SOURCE,itag,MPI_COMM_WORLD,istatus,ierr)
man=istatus(MPI_SOURCE)
```

istatus(MPI_SOURCE), istatus(MPI_TAG) and istatus(MPI_ERROR) contain, respectively, the source, tag and error code of the received message.

```
program hello
  implicit none
  include "mpif.h"
  character(LEN=12) :: inmsg, message
  integer i, ierr, me, nproc, itag,kount
  integer istatus(MPI_STATUS_SIZE)

  call MPI_Init(ierr)
  call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
  call MPI_Comm_rank(MPI_COMM_WORLD,me,ierr)
  itag = 100 ; kount=12

  if (me == 0) then
    message = "Hello, world"
    do i = 1,nproc-1
      call MPI_Send(message,kount,MPI_CHARACTER,i,itag,MPI_COMM_WORLD,ierr)
    end do
    write(*,*) "process", me, ":", message
  else
    call MPI_Recv(inmsg,kount,MPI_CHARACTER,0,itag,MPI_COMM_WORLD,istatus,ierr)
    write(*,*) "process", me, ":", inmsg

  end if
  call MPI_Finalize(ierr)
end program hello
```

Simple Send & Receive Program

```
#include <stdio.h>
#include "mpi.h"
int main(argc,argv)
int argc;
char *argv[];
{
      int myid;
      int tag,source,destination,count;
      int buffer;
      MPI_Status status;
    MPI_Init(&argc,&argv);
      MPI_Comm_rank(MPI_COMM_WORLD,&myid);
tag=1234;
   source=0;
   destination=1;
   count=1;
   if(myid == source){
     buffer=5678;
    MPI_Send(&buffer,count,MPI_INT,destination,tag,MPI_COMM_WORLD);
     printf("processor %d  sent %d\n",myid,buffer);
   }
   if(myid == destination){
MPI_Recv(&buffer,count,MPI_INT,source,tag,MPI_COMM_WORLD,&status);
       printf("processor %d  got %d\n",myid,buffer);
   }
   MPI_Finalize();
 }
```

status.MPI_SOURCE, status.MPI_TAG, and status.MPI_ERROR contain the source, tag, and error code respectively of the received message

```
      subroutine Get_data(a, b, n, myid, nproc)
      IMPLICIT NONE
      real*8 a, b
      integer   n, myid,  nproc
C
      INCLUDE 'mpif.h'
      integer source, dest, tag, istatus(MPI_STATUS_SIZE), ierr
      data source /0/
C
      if (myid == 0) then
      print *, 'Enter a, b and n'
      read *, a, b, n
C
       do dest = 1 , nproc-1
        tag = 0
        call MPI_SEND(a, 1, MPI_REAL8 , dest, tag, MPI_COMM_WORLD, ierr )
        tag = 1
        call MPI_SEND(b, 1, MPI_REAL8 , dest, tag, MPI_COMM_WORLD, ierr )
        tag = 2
        call MPI_SEND(n, 1, MPI_INTEGER, dest, tag, MPI_COMM_WORLD, ierr )
       end do
                    else
        tag = 0
        call MPI_RECV(a, 1, MPI_REAL8 , source, tag, MPI_COMM_WORLD, istatus, ierr )
        tag = 1
        call MPI_RECV(b, 1, MPI_REAL8 , source, tag, MPI_COMM_WORLD, istatus, ierr )
        tag = 2
        call MPI_RECV(n, 1, MPI_INTEGER, source, tag, MPI_COMM_WORLD, istatus, ierr )
                    end if
      return
      end
```

istatus(MPI_SOURCE), istatus(MPI_TAG), istatus(MPI_ERROR) contain respectively the source, the tag, and the error code of the received message.

```
int recvd_tag, recvd_from, recvd_count;
MPI_Status status; MPI_Recv(..., MPI_ANY_SOURCE, MPI_ANY_TAG, ..., &status)
recvd_tag= status.MPI_TAG; recvd_from= status.MPI_SOURCE;
MPI_Get_count( &status, datatype, &recvd_count);
```

MPI User Guide in Fortran, P. S. Pacheco *et al.*

```
      PROGRAM simple_send_and_receive
      INCLUDE 'mpif.h'
      INTEGER myid, ierr, istatus(MPI_STATUS_SIZE)
      REAL  a(100)
C Initialize MPI:
      call MPI_INIT(ierr)
C Get my rank:
      call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
C Process 0 sends, process 1 receives:
       if( myid .eq. 0 )then
       call MPI_SEND( a, 100, MPI_REAL, 1, 17, MPI_COMM_WORLD, ierr)
       else if ( myid .eq. 1 )then
       call MPI_RECV( a, 100, MPI_REAL, 0, 17, MPI_COMM_WORLD, istatus, ierr )
       endif
C Terminate MPI:
       call MPI_FINALIZE(ierr)
       END
```

Process 0 sends a message to process 1, and process 1 receives it.

istatus(MPI_SOURCE), istatus(MPI_TAG) and istatus(MPI_ERROR) contain, respectively, the source, tag and error code of the received message.

```
include 'mpif.h'
integer myid, numprocs, ierr, ntemp
integer istatus (MPI_STATUS_SIZE)
real*8 sum
call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)
sum=myid
if(myid == 0)then
do i=1,numprocs-1
call MPI_RECV(ntemp,1,MPI_INTEGER, i,i, MPI_COMM+WORLD, istatus, ierr)
sum=sum+ntemp
enddo
average=sum/numprocs ; write(6,*) 'the average is ', average
else
call MPI_SEND(myid,1,MPI_INTEGER,0,myid,MPI_COMM_WORLD, ierr)
endif
call MPI_FINALIZE(ierr)
end
```

istatus - contains information about incoming message

```
subroutine get_input(aa,bb,nn)
include “mpif.h”
real*8 aa,bb
integer nn,myid
integer ierr

call MPI_COMM_RANK(MPI_COMM_WORLD,myid,ierr)

if(myid == 0)then
print *, ‘Enter aa, bb, nn’
read *, aa,bb,nn
endif

call MPI_BCAST(aa,1, MPI_REAL8,  0, MPI_COMM_WORLD, ierr)
call MPI_BCAST(bb,1, MPI_REAL8, 0, MPI_COMM_WORLD,  ierr)
call MPI_BCAST(nn,1, MPI_INTEGER, 0, MPI_COMM_WORLD,  ierr)

end subroutine get_input
```

```
implicit none
integer n, np, i, j, ierr, master,num
real*8 h, result, a, b, integral, pi, my_a, my_range, MPI_WTime,start_time,end_time, my_result
include "mpif.h"
integer Iam, source, dest, tag, istatus(MPI_STATUS_SIZE)
data master/0/
call MPI_Init(ierr)   ;    call MPI_Comm_rank(MPI_COMM_WORLD, Iam, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, np, ierr)
   pi = acos(-1.0d0)  ;     a = 0.0d0   ;  b = pi*1.d0/2.d0   ;  dest = 0    ;  tag = 123
    if(Iam  ==  master) then
print *,'The requested number of processors =',p ;  print *,'Enter total number of increments across all processors'
     read(*,*) n
     start_time = MPI_Wtime()
    endif
     call MPI_Bcast(n, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, ierr)
    h = (b-a)/n    ;    num = n/np ;  my_range = (b-a)/np ;  my_a = a+ Iam*my_range
    my_result = integral(my_a, num, h)
    write(*,"('Process ',i2,' has the partial result of',f10.6)")   Iam,my_result
    call MPI_Reduce(my_result, result, 1, MPI_REAL8, MPI_SUM, dest, MPI_COMM_WORLD, ierr)
    if(Iam  == master) then
     print *,'The result =',result
     end_time = MPI_Wtime() ;  print *, 'elapsed time is ',end_time-start_time,' seconds'
    endif
    call MPI_Finalize(ierr)  ; stop ;  end
```

Status

- In C
  - status is a structure of type MPI_Status which contains three fields MPI_SOURCE, MPI_TAG, and MPI_ERROR
  - status.MPI_SOURCE, status.MPI_TAG, and status.MPI_ERROR contain the source, tag, and error code respectively of the received message
- In Fortran
  - status is an array of INTEGERS of length MPI_STATUS_SIZE, and the 3 constants MPI_SOURCE, MPI_TAG, MPI_ERROR are the indices of the entries that store the source, tag, & error
  - status(MPI_SOURCE), status(MPI_TAG), and status(MPI_ERROR) contain respectively the source, the tag, and the error code of the received message.

status.MPI_SOURCE, status.MPI_TAG, and status.MPI_ERROR contain the source, tag, and error code respectively of the received message

```
! Program hello.ex1.f
! Parallel version using MPI calls
! Modified from basic version so that workers send back
! a message to the master, who prints out a message for each worker
program hello
implicit none
integer, parameter:: DOUBLE=kind(1.0d0), SINGLE=kind(1.0)
include "mpif.h"
character(LEN=12) :: inmsg,message
integer :: i,ierr,me,nproc,itag,iwrank
integer, dimension(MPI_STATUS_SIZE) :: istatus
!
call MPI_Init(ierr)
call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
call MPI_Comm_rank(MPI_COMM_WORLD,me,ierr)
itag = 100
!
if (me == 0) then
message = "Hello, world"
do i = 1,nproc-1
call MPI_Send(message,12,MPI_CHARACTER,i,itag,MPI_COMM_WORLD,ierr)
end do
write(*,*) "process", me, ":", message
do i = 1,nproc-1
call MPI_Recv(iwrank,1,MPI_INTEGER,MPI_ANY_SOURCE,itag,MPI_COMM_WORLD, istatus, ierr)
write(*,*) "process", iwrank, ":Hello, back"
end do
else
call MPI_Recv(inmsg,12,MPI_CHARACTER,0,itag,MPI_COMM_WORLD,istatus,ierr)
call MPI_Send(me,1,MPI_INTEGER,0,itag,MPI_COMM_WORLD,ierr)
end if
call MPI_Finalize(ierr)
end program hello
```

http://www.dartmouth.edu/~rc/classes/

```
Program Example1
implicit none
integer n, p, i, j,num
real h, result, a, b, integral, pi
real my_a,my_range
pi = acos(-1.0)                    ! = 3.141592...
a = 0.0                            ! lower limit of integration
b = pi*1./2.                       ! upper limit of integration
p = 4 !! number of processes (partitions)
n = 100000 !! total number of increments
h = (b-a)/n                        ! length of increment
num= n/p                           ! number of calculations done by each process
result = 0.0                       ! stores answer to the integral
do i=0,p-1                         ! sum of integrals over all processes
my_range = (b-a)/p
my_a = a + i*my_range
result = result + integral(my_a,num,h)
enddo
print *,'The result =',result
stop
end

real function integral(a,n,h)
implicit none
integer n, i, j
real h, h2, aij, a
real fct, x
fct(x) = cos(x)                    ! kernel of the integral
integral = 0.0                     ! initialize integral
h2 = h/2.
do j=0,n-1                         ! sum over all "j" integrals
aij = a+j*h                        ! lower limit of "j" integral
integral = integral + fct(aij+h2)*h
enddo
return
end
```

Buffer and Deadlock

safe

```
if (rank == 0 )then
call mpi_send(sbuff,kount,MPI_REAL8, 1, itag, MPI_COMM_WORLD, ierr)
call mpi_recv(rbuff,kount,MPI_REAL8, 1, itag, MPI_COMM_WORLD, istatus,ierr)
else if (rank ==1 )then
call mpi_recv(rbuff,kount,MPI_REAL8, 0, itag, MPI_COMM_WORLD, istatus,ierr)
call mpi_send(sbuff, kount, MPI_REAL8, 0, itag, MPI_COMM_WORLD, ierr)
endif
```

Deadlock; 수렁, 교착

```
if (rank == 0 )then
call mpi_recv(rbuff,kount,MPI_REAL8, 1, itag, MPI_COMM_WORLD, istatus,ierr)
call mpi_send(sbuff,kount,MPI_REAL8, 1, itag, MPI_COMM_WORLD, ierr)
else if (rank ==1 )then
call mpi_recv(rbuff,kount,MPI_REAL8, 0, itag, MPI_COMM_WORLD, istatus, ierr)
call mpi_send(sbuff, kount, MPI_REAL8, 0, itag, MPI_COMM_WORLD, ierr)
endif
```

Buffering dependent

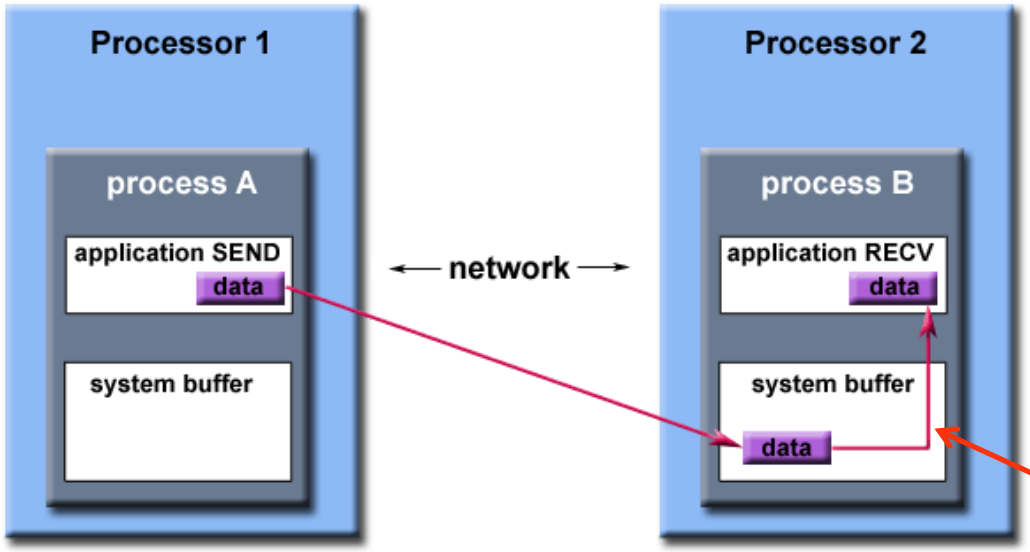
```
if (rank == 0 )then
call mpi_send(sbuff,kount,MPI_REAL8, 1, itag, MPI_COMM_WORLD, ierr)
call mpi_recv(rbuff,kount,MPI_REAL8, 1, itag, MPI_COMM_WORLD, istatus,ierr)
else if (rank ==1 )then
call mpi_send(sbuff, kount, MPI_REAL8, 0, itag, MPI_COMM_WORLD, ierr)
call mpi_recv(rbuff,kount,MPI_REAL8, 0, itag, MPI_COMM_WORLD, istatus, ierr)
endif
```

kount is large→ deadlock occurs

Non-blocking communications

The programmer should be able to explain why the program does not (or does) deadlock.

Note that increasing array dimensions and message sizes have no effect on the safety of the protocol.



Path of a message buffered at the receiving process

https://computing.llnl.gov/tutorials/mpi/

System buffer size

Deadlock (C)

```
                                                        /* simple deadlock */
#include <stdio.h>
#include <mpi.h>
void main (int argc, char **argv) {
int myrank;
MPI_Status status;
double a[100], b[100];
MPI_Init(&argc, &argv);                                 /* Initialize MPI */
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);                 /* Get rank */
if( myrank == 0 ) {
                                                        /* Receive, then send a message */
MPI_Recv( b, 100, MPI_DOUBLE, 1, 19, MPI_COMM_WORLD, &status );
MPI_Send( a, 100, MPI_DOUBLE, 1, 17, MPI_COMM_WORLD );
}
else if( myrank == 1 ) {
                                                        /* Receive, then send a message */
MPI_Recv( b, 100, MPI_DOUBLE, 0, 17, MPI_COMM_WORLD, &status );
MPI_Send( a, 100, MPI_DOUBLE, 0, 19, MPI_COMM_WORLD );
}
MPI_Finalize();                                         /* Terminate MPI */
}
```

Deadlock (FORTRAN)

```
        PROGRAM simple_deadlock
        INCLUDE 'mpif.h'
        INTEGER myrank, ierr, istatus(MPI_STATUS_SIZE)
        REAL a(100), b(100)
C Initialize MPI:
        call MPI_INIT(ierr)
C Get my rank:
        call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
C Process 0 receives and sends; same for process 1
if( myrank.eq.0 )then
   call MPI_RECV( b, 100, MPI_REAL, 1, 19, MPI_COMM_WORLD, istatus, ierr )
   call MPI_SEND( a, 100, MPI_REAL, 1, 17, MPI_COMM_WORLD, ierr)
else if ( myrank.eq.1 )then
   call MPI_RECV( b, 100, MPI_REAL, 0, 17, MPI_COMM_WORLD, istatus, ierr )
   call MPI_SEND( a, 100, MPI_REAL, 0, 19, MPI_COMM_WORLD, ierr)
endif
C Terminate MPI:
        call MPI_FINALIZE(ierr)
        END
```

```
      PROGRAM safe_exchange
      INCLUDE 'mpif.h'
      INTEGER myrank, ierr, istatus(MPI_STATUS_SIZE)
      REAL  a(100), b(100)
C Initialize MPI:
      call MPI_INIT(ierr)
C Get my rank:
      call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
C Process 0 receives and sends; process 1 sends and receives
      if( myrank .eq. 0 )then
      call MPI_RECV( b, 100, MPI_REAL, 1, 19, MPI_COMM_WORLD, istatus, ierr )
      call MPI_SEND( a, 100, MPI_REAL, 1, 17, MPI_COMM_WORLD, ierr)
      else if ( myrank .eq. 1 )then
      call MPI_SEND( a, 100, MPI_REAL, 0, 19, MPI_COMM_WORLD, ierr )
      call MPI_RECV( b, 100, MPI_REAL, 0, 17, MPI_COMM_WORLD, istatus, ierr)
      endif
C Terminate MPI:
      call MPI_FINALIZE(ierr)
      END
```

```
                                                    /* safe exchange */
#include <stdio.h>
#include <mpi.h>
void main (int argc, char **argv) {
int myrank;
MPI_Status status;
double a[100], b[100];
MPI_Init(&argc, &argv);                    /* Initialize MPI */
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);    /* Get rank */
if( myrank == 0 ) {
                                           /* Receive a message, then send one */
MPI_Recv( b, 100, MPI_DOUBLE, 1, 19, MPI_COMM_WORLD, &status );
MPI_Send( a, 100, MPI_DOUBLE, 1, 17, MPI_COMM_WORLD );
}
else if( myrank == 1 ) {
                                            /* Send a message, then receive one */
MPI_Send( a, 100, MPI_DOUBLE, 0, 19, MPI_COMM_WORLD );
MPI_Recv( b, 100, MPI_DOUBLE, 0, 17, MPI_COMM_WORLD, &status );
}
MPI_Finalize();                                          /* Terminate MPI */
}
```

status.MPI_SOURCE, status.MPI_TAG, and status.MPI_ERROR contain the source, tag, and error code respectively of the received message

status.MPI_SOURCE 자료를 보낸 노드의 아이디를 알아 낼 수 있다.

```
      PROGRAM depends_on_buffering
      INCLUDE 'mpif.h'
      INTEGER myrank, ierr, istatus(MPI_STATUS_SIZE)
      REAL*8  a(100), b(100)
C Initialize MPI:
      call MPI_INIT(ierr)
C Get my rank:
      call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
C Process 0 sends and receives; same for process 1
      if( myrank .eq. 0 )then
      call MPI_SEND( a, 100, MPI_REAL8, 1, 17, MPI_COMM_WORLD, ierr)
      call MPI_RECV( b, 100, MPI_REAL8, 1, 19, MPI_COMM_WORLD, istatus, ierr )
      else if ( myrank .eq. 1 )then
      call MPI_SEND( a, 100, MPI_REAL8, 0, 19, MPI_COMM_WORLD, ierr )
      call MPI_RECV( b, 100, MPI_REAL8, 0, 17, MPI_COMM_WORLD, istatus, ierr)
      endif
C Terminate MPI:
      call MPI_FINALIZE(ierr)
      END
```

REAL*8 → DOUBLE PRECISION
MPI_REAL8 → MPI_DOUBLE_PRECISION

Again, process 0 attempts to exchange messages with process 1. This time, both processes send first, then receive. Success depends on the availability of buffering in MPI.

If the message sizes are increased, sooner or later the program will deadlock.

```
      PROGRAM probable_deadlock
      INCLUDE 'mpif.h'
      INTEGER myrank, ierr, istatus(MPI_STATUS_SIZE)
      INTEGER n
      PARAMETER (n=100000000)
      REAL  a(n), b(n)
C Initialize MPI:
      call MPI_INIT(ierr)
C Get my rank:
      call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
C Process 0 sends, then receives; same for process 1
      if( myrank.eq.0 )then
      call MPI_SEND( a, n, MPI_REAL, 1, 17, MPI_COMM_WORLD, ierr)
      call MPI_RECV( b, n, MPI_REAL, 1, 19, MPI_COMM_WORLD, istatus, ierr )
      else if ( myrank.eq.1 )then
      call MPI_SEND( a, n, MPI_REAL, 0, 19, MPI_COMM_WORLD, ierr )
      call MPI_RECV( b, n, MPI_REAL, 0, 17, MPI_COMM_WORLD, istatus, ierr)
      endif
C Terminate MPI:
      call MPI_FINALIZE(ierr)
      END
```

This program will deadlock under the default configuration of nearly all available MPI implementations.

Asynchronous communication

MPI_Wait used to complete communication

```
      PROGRAM simple_deadlock_avoided
      INCLUDE 'mpif.h'
      INTEGER myrank, ierr, istatus(MPI_STATUS_SIZE)
      INTEGER irequest
      REAL  a(100), b(100)
C Initialize MPI:
      call MPI_INIT(ierr)
C Get my rank:
      call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
C Process 0 posts a receive, then sends; same for process 1
      if( myrank.eq.0 )then
      call MPI_IRECV( b, 100, MPI_REAL, 1, 19, MPI_COMM_WORLD, irequest, ierr )
      call MPI_SEND( a, 100, MPI_REAL, 1, 17, MPI_COMM_WORLD, ierr)
      call MPI_WAIT( irequest, istatus, ierr )
      else if ( myrank.eq.1 )then
      call MPI_IRECV( b, 100, MPI_REAL, 0, 17, MPI_COMM_WORLD, irequest, ierr )
      call MPI_SEND( a, 100, MPI_REAL, 0, 19, MPI_COMM_WORLD, ierr)
      call MPI_WAIT( irequest, istatus, ierr )
                  endif
C Terminate MPI:
      call MPI_FINALIZE(ierr)
      END
```

This is a race condition, which can be very difficult to debug.

```
int i=123; MPI_Request myRequest; MPI_Isend(&i, 1, MPI_INT, 1,
MY_LITTLE_TAG,MPI_COMM_WORLD, &myRequest);
i=234;
```

```
int i=123; MPI_Request myRequest;
MPI_Isend(&i, 1, MPI_INT, 1, MY_LITTLE_TAG, MPI_COMM_WORLD, &myRequest);
// do some calculations here // Before we re-use variable i, we need to wait until the asynchronous function call is complete
MPI_Status myStatus; MPI_Wait(&myRequest, &myStatus);
i=234;
```

MPI_Wait blocks until the message specified by “request” completes.

```
                                                                    /* deadlock avoided */
#include
#include
void main (int argc, char **argv) {
int myrank;
MPI_Request request;
MPI_Status status;
double a[100], b[100];
MPI_Init(&argc, &argv);                                              /* Initialize MPI */
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);                              /* Get rank */
if( myrank == 0 ) {
                                                          /* Post a receive, send a message, then wait */
MPI_Irecv( b, 100, MPI_DOUBLE, 1, 19, MPI_COMM_WORLD, &request );
MPI_Send( a, 100, MPI_DOUBLE, 1, 17, MPI_COMM_WORLD );
MPI_Wait( &request, &status );
}
else if( myrank == 1 ) {
                                                           /* Post a receive, send a message, then wait */
MPI_Irecv( b, 100, MPI_DOUBLE, 0, 17, MPI_COMM_WORLD, &request );
MPI_Send( a, 100, MPI_DOUBLE, 0, 19, MPI_COMM_WORLD );
MPI_Wait( &request, &status );
}
MPI_Finalize();                                                      /* Terminate MPI */
}
```

It is always safe to order the calls of MPI_(I)SEND and MPI_(I)RECV so that a send subroutine call at one process and a corresponding receive subroutine call at the other process appear in matching order.

```
IF (myrank==0) THEN
  CALL MPI_SEND(sendbuf, ...)
  CALL MPI_RECV(recvbuf, ...)
ELSEIF (myrank==1) THEN
  CALL MPI_RECV(recvbuf, ...)
  CALL MPI_SEND(sendbuf, ...)
ENDIF
```

In this case, you can use either blocking or non-blocking subroutines.

Considering the previous options, performance, and the avoidance of deadlocks, it is recommended to use the following code.

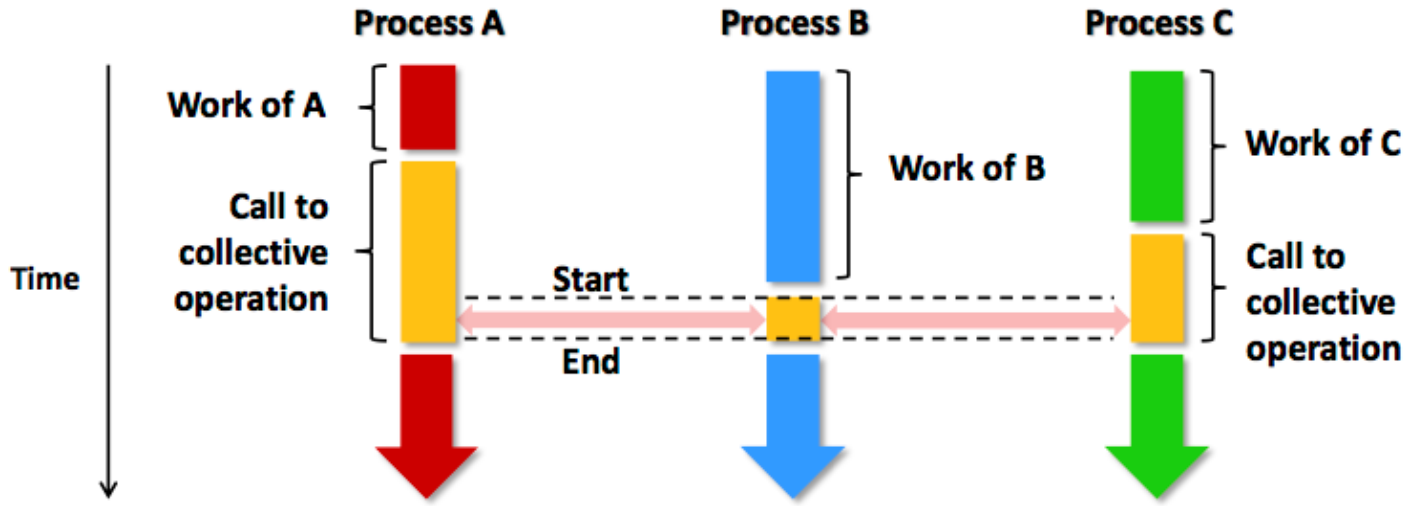
```
IF (myrank==0) THEN
  CALL MPI_ISEND(sendbuf, ..., ireq1, ...)
  CALL MPI_IRECV(recvbuf, ..., ireq2, ...)
ELSEIF (myrank==1) THEN
  CALL MPI_ISEND(sendbuf, ..., ireq1, ...)
  CALL MPI_IRECV(recvbuf, ..., ireq2, ...)
ENDIF
CALL MPI_WAIT(ireq1, ...)
CALL MPI_WAIT(ireq2, ...)
```

Y. Aoyama and J. Nakano p. 28

Blocking send/receive

A **blocking send or receive does not return from the subroutine call until the** operation has actually completed. Thus it insures that the relevant completion criteria have been satisfied before the calling process is allowed to proceed.

You are sure that the data has actually arrived and is ready for use.



210.98.30.18

210.98.30.28

xmanager 연결할 때, 아래와 같이 하면 큰 폰트로 글씨를 표시할 수 있다.
/usr/bin/xterm -ls -display $DISPLAY -fn 12x24

/usr/bin/xterm -ls -display $DISPLAY -fn 12x24 -fg gray -bg black

guest

kias!guest

:set background=light

:set background=dark

:set paste

:syntax off

:syntax on

ls

ls –ltra

예를 들어 프로그램 실행 전후,
파일들의 생성 순서가 중요할 경우

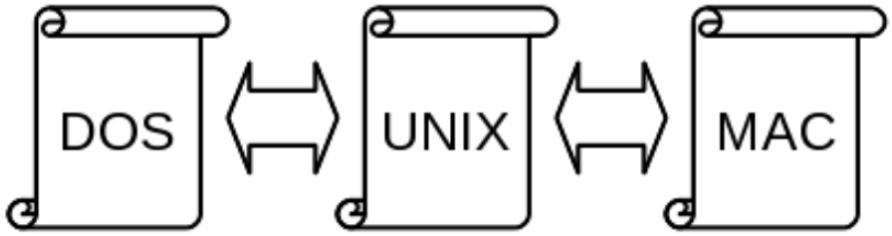
Editors
Vi
Emacs
Pico

mkdir abc
cd abc
ls

mv aa aa1

cp aa bb

Dos2Unix / Unix2Dos - Text file format converters



Convert text files with DOS or Mac line breaks to Unix line breaks and vice versa.

:set showmatch
:set paste
텍스트 복사할 때 제대로 문자들 배열이 되도록 해주는 옵션

SGE: Sun Grid Engine

```
#!/bin/bash
#$ -V
#$ -cwd
#$ -S /bin/bash
#$ -N sge_run_test

### Total used process count numbers on cpu_openmpi
#$ -pe cpu_openmpi 4

### Total used process count numbers on gpu_openmpi
### $ -pe gpu_openmpi 4

### Queue Name
### To use cpu => cpu
### To use gpu => gpu
#$ -q cpu

#$ -R yes

# This job's working directory
echo Working directory is $SGE_CWD_PATH
cd $SGE_CWD_PATH

echo Running on host `hostname`
echo Time is `date`
echo Directory is `pwd`
echo This jobs runs on the following processors:
echo `cat $PE_HOSTFILE`
# Define number of processors
NPROCS=`wc -l < $PE_HOSTFILE`
echo "nprocs=$NPROCS"
NPROCS=$NSLOTS

# your job
mpirun -np $NPROCS ./a.out > output1
```

pestat

Portable Batch System (PBS)

- Process and Resource Management
- Torque, openpbs
  - http://www.clusterresources.com/products/torque-resource-manager.php
- Commands (실습)

```
% qstat          (Status)
% man qstat
% qstat -a
% qstat -u newton
% qstat -an
% qstat -q
% qstat -s
% qstat -f
% pestat         (Node Status)
% qsub
% qdel
```

- PBS script (실습과 함께)

From Dr. K. Joo (KIAS), The 2nd CAC Summer School on Parallel Computing

PBS Scripts

```
#!/bin/sh
### Job name
#PBS -N JOB_NAME
### Declare job non-rerunable
#PBS -r n
### Output files
#PBS -j oe
### Mail to user
#PBS -m ae
### Queue name (n2, n4, n16, n32, n64)
#PBS -q n32
### Walltime limit (hh:mm:ss)
#PBS -l walltime=168:00:00

# This job's working directory
echo Working directory is $PBS_O_WORKDIR
cd $PBS_O_WORKDIR

echo Running on host `hostname`
echo Time is `date`
echo Directory is `pwd`
echo This jobs runs on the following processors:
echo `cat $PBS_NODEFILE`
# Define number of processors
NPROCS=`wc -l < $PBS_NODEFILE`
```

```
## your parallel job

mpiexec -np $NPROCS a.out
```

```
* PBS interactive mode
% qsub -I -q n8 -N job_name
% qsub -I -q n16 -N job_name

% echo $PBS_O_WORKDIR
% echo $PBS_NODEFILE
% cat $PBS_NODEFILE
% export | grep PBS

* PBS commands
% cat start.mat
% qsub start.mat
% qdel 57480
```

From Dr. K. Joo (KIAS), The 2nd CAC Summer School on Parallel Computing

Point to Point Communication (Fortran)

Call MPI_SEND(buf, count, datatype, dest, tag, comm, ierr);

- buf : Send buffer
- count : Number of sent elements
- datatype : MPI datatype

- dest : Destination Process ID
- tag : Message tag
- comm : Communicator

Call MPI_RECV(buf, count,datatype,source, tag, comm,status, ierr);

- buf : Receive Buffer
- source : Source Process ID
- status : Receive status

From Dr. K. Joo (KIAS), The 2nd CAC Summer School on Parallel Computing

Point to Point Communication (C)

MPI_Send(buf, count, datatype, dest, tag, comm);

- buf : Send buffer
- count : Number of sent elements
- datatype : MPI datatype

- dest : Destination Process ID
- tag : Message tag
- comm : Communicator

MPI_Recv(buf, count,datatype,source, tag, comm,&status);

- buf : Receive Buffer
- source : Source Process ID
- status : Receive status

From Dr. K. Joo (KIAS), The 2nd CAC Summer School on Parallel Computing

```
mpif90 hello.f90
mpicc hello.c
```

```
mpiexec –np 2 ./a.out
```

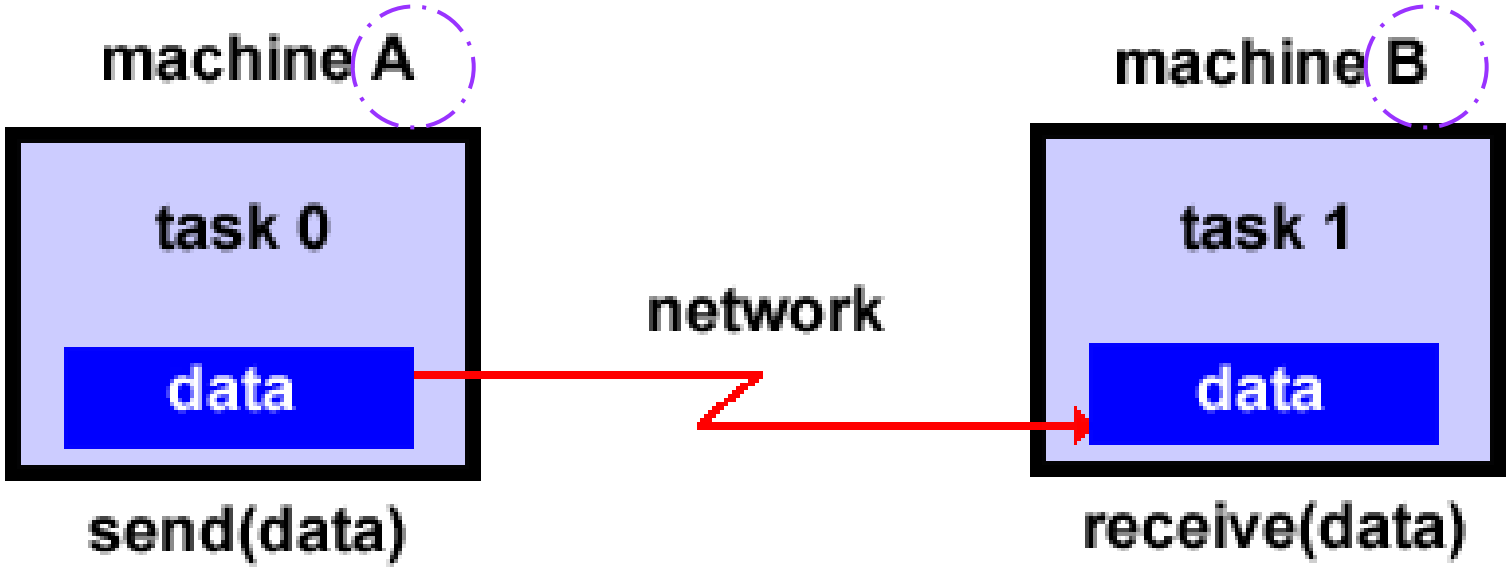
```
mpirun –np 3 ./a.out
```

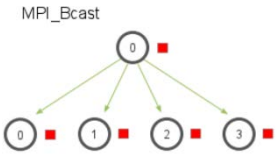
```
qsub start.mat
pestat
qstat –a
```

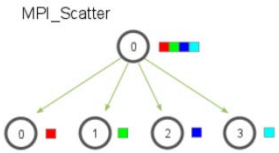
```
DOUBLE PRECISION :: start, end
 start = MPI_Wtime()

 ! code to be timed

 end   = MPI_Wtime()
 print*,'That took ',end-start,' seconds'
```

```
foreach num (`seq -s" " 41 42`)
ssh c${num} ps -ef | grep  program_name | awk '{print $2}' | xargs kill -9
end
```

Point-to-point communications

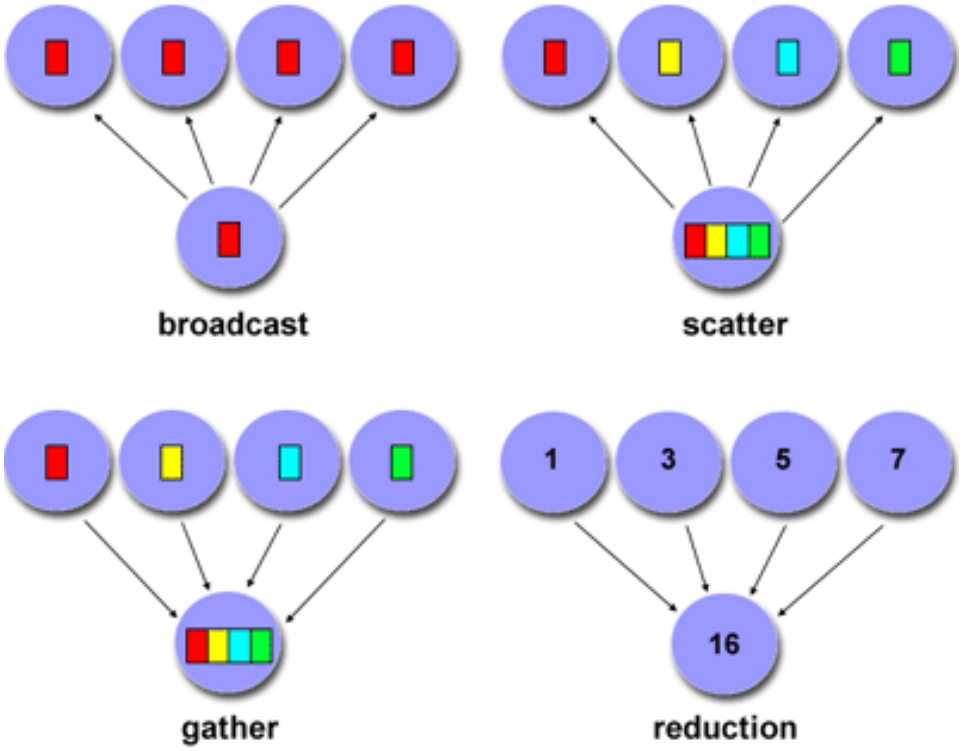




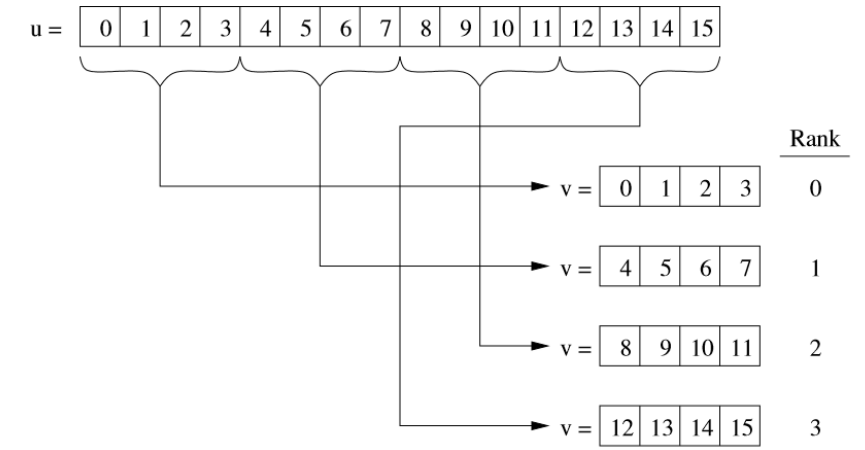


Collective communications

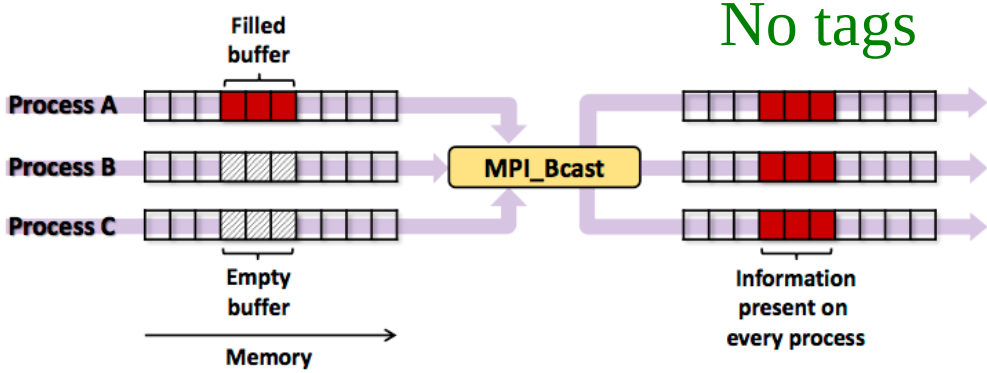
No tags

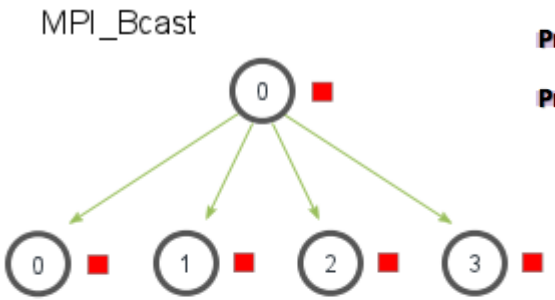


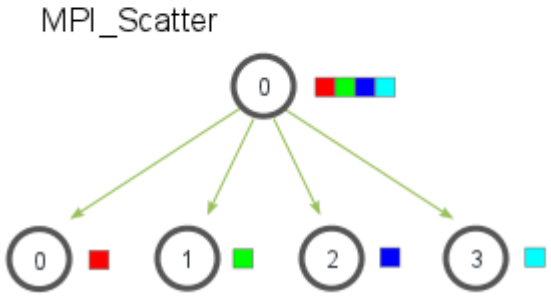

```
MPI_Scatter(u, 4, MPI_INT, v, 4, MPI_INT, 0, MPI_COMM_WORLD);
```



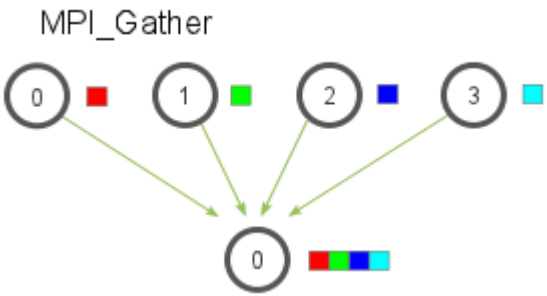
No tags

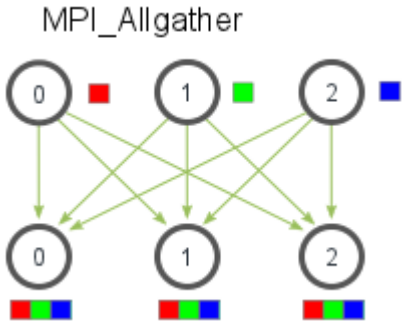






MPI_Bcast() – Broadcast (one to all)
MPI_Reduce() – Reduction (all to one)
MPI_Allreduce() – Reduction (all to all)
MPI_Scatter() – Distribute data (one to all)
MPI_Gather() – Collect data (all to one)
MPI_Alltoall() – Distribute data (all to all)
MPI_Allgather() – Collect data (all to all)



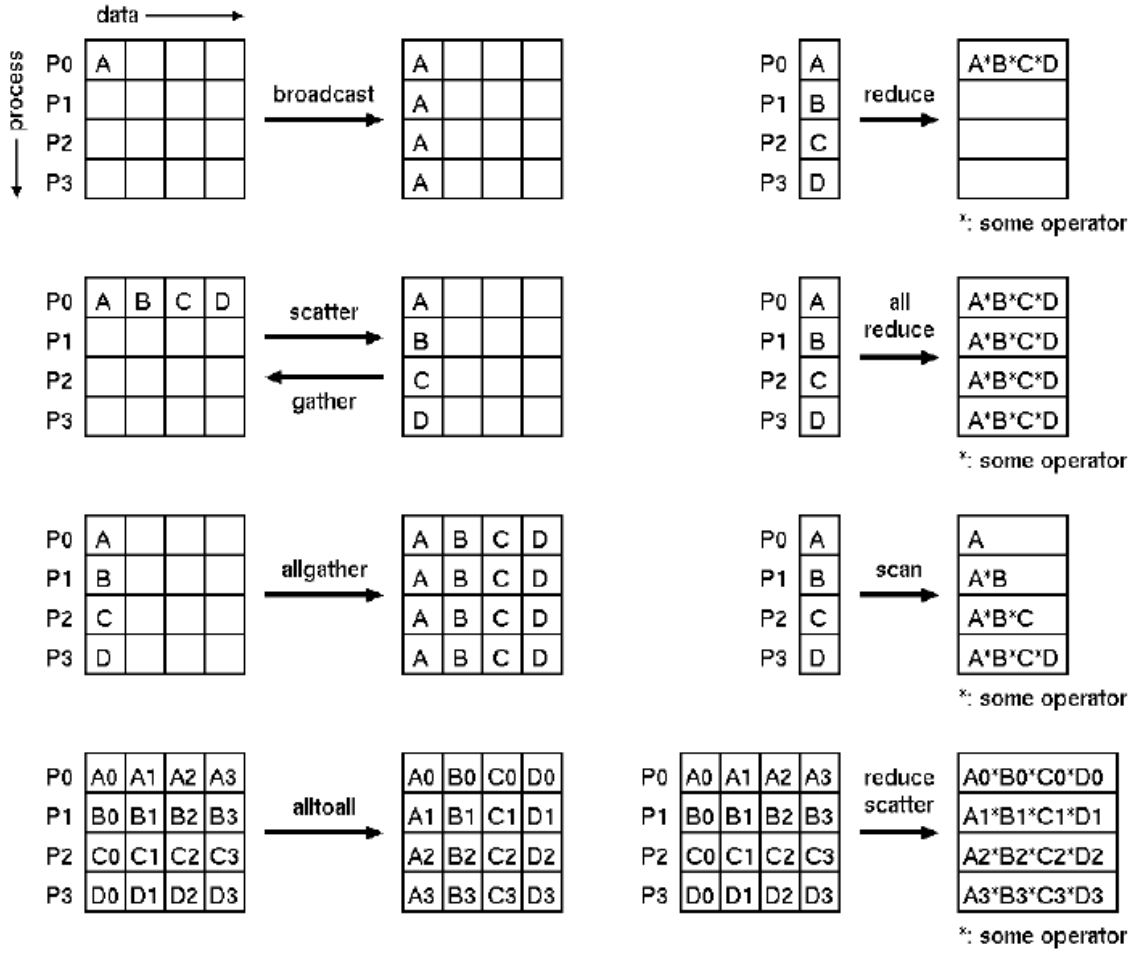


오류의 가능성이 현저히 적다.
이미 최적화된 통신 방법이다.

Collective communications

No tags

scatterv
gatherv



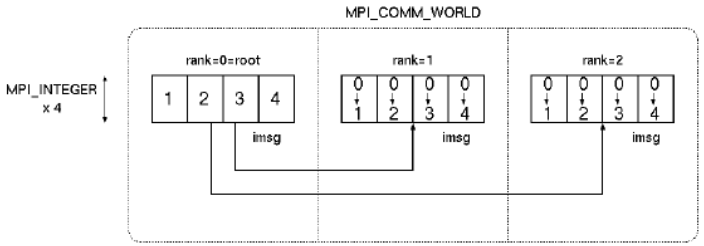
Y. Aoyama and J. Nakano

Collective communications

No tags

bcast.f

```
 1       PROGRAM bcast
 2       INCLUDE 'mpif.h'
 3       INTEGER imsg(4)
 4       CALL MPI_INIT(ierr)
 5       CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
 6       CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
 7       IF (myrank==0) THEN
 8         DO i=1,4
 9           imsg(i) = i
10         ENDDO
11       ELSE
12         DO i=1,4
13           imsg(i) = 0
14         ENDDO
15       ENDIF
16       PRINT *,'Before:',imsg
17       CALL MP_FLUSH(1)
18       CALL MPI_BCAST(imsg, 4, MPI_INTEGER,
19      &               0, MPI_COMM_WORLD, ierr)
20       PRINT *,'After :',imsg
21       CALL MPI_FINALIZE(ierr)
22       END
```



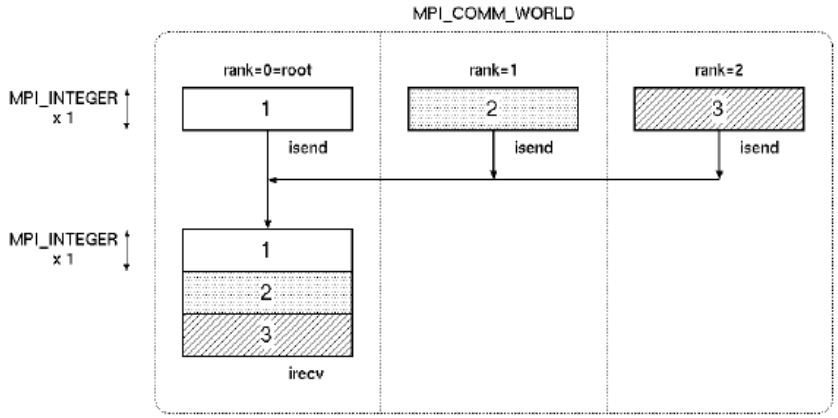
No tags

Collective communications

No tags

gather.f

```
 1       PROGRAM gather
 2       INCLUDE 'mpif.h'
 3       INTEGER irecv(3)
 4       CALL MPI_INIT(ierr)
 5       CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
 6       CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
 7       isend = myrank + 1
 8       CALL MPI_GATHER(isend, 1, MPI_INTEGER,
 9      &                irecv, 1, MPI_INTEGER,
10      &                0, MPI_COMM_WORLD, ierr)
11       IF (myrank==0) THEN
12         PRINT *,'irecv =',irecv
13       ENDIF
14       CALL MPI_FINALIZE(ierr)
15       END
```



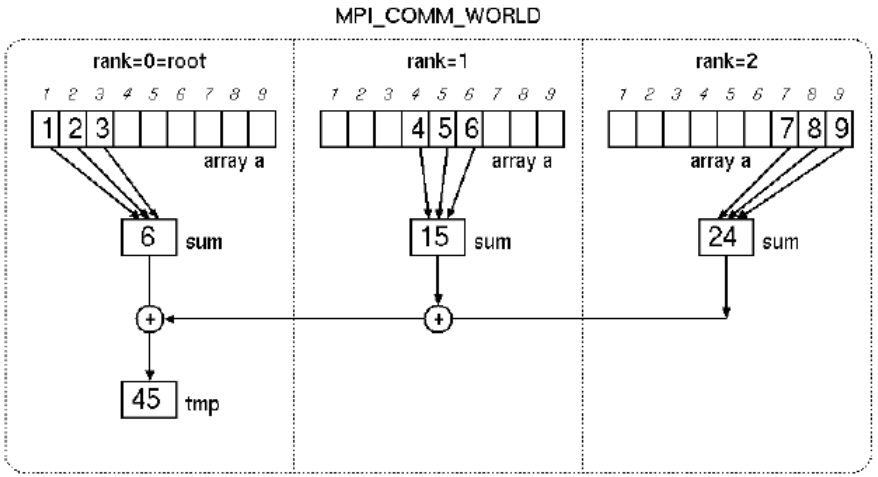
Y. Aoyama and J. Nakano

Collective communications

No tags

```
 1       PROGRAM reduce
 2       INCLUDE 'mpif.h'
 3       REAL a(9)
 4       CALL MPI_INIT(ierr)
 5       CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
 6       CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
 7       ista = myrank * 3 + 1
 8       iend = ista + 2
 9       DO i=ista,iend
10         a(i) = i
11       ENDDO
12       sum = 0.0
13       DO i=ista,iend
14         sum = sum + a(i)
15       ENDDO
16       CALL MPI_REDUCE(sum, tmp, 1, MPI_REAL, MPI_SUM, 0,
17      &                MPI_COMM_WORLD, ierr)
18       sum = tmp
19       IF (myrank==0) THEN
20         PRINT *,'sum =',sum
21       ENDIF
22       CALL MPI_FINALIZE(ierr)
23       END
```

No tags

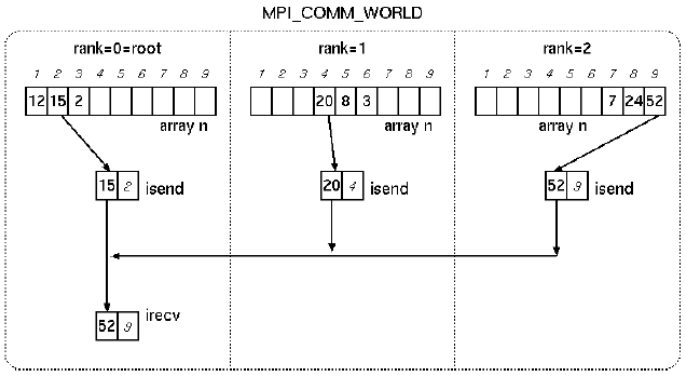


Y. Aoyama and J. Nakano

Collective communications

No tags

```
PROGRAM maxloc_p
INCLUDE 'mpif.h'
INTEGER n(9)
INTEGER isend(2), irecv(2)
DATA n /12, 15, 2, 20, 8, 3, 7, 24, 52/
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
ista = myrank * 3 + 1
iend = ista + 2
imax = -999
DO i = ista, iend
  IF (n(i) > imax) THEN
    imax = n(i)
    iloc = i
  ENDIF
ENDDO
isend(1) = imax
isend(2) = iloc
CALL MPI_REDUCE(isend, irecv, 1, MPI_2INTEGER,
&                MPI_MAXLOC, 0, MPI_COMM_WORLD, ierr)
IF (myrank == 0) THEN
  PRINT *, 'Max =', irecv(1), 'Location =', irecv(2)
ENDIF
CALL MPI_FINALIZE(ierr)
END
```



No tags

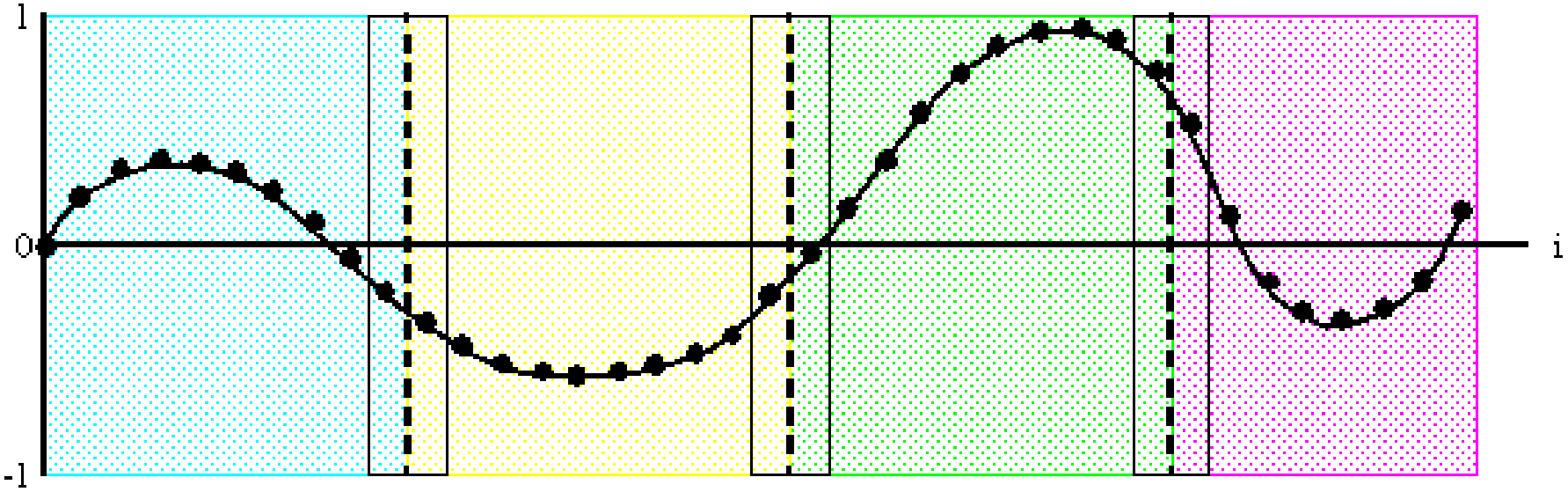
do not use a call such as `MPI_Reduce(&x, &x, 1, MPI_DOUBLE, 0, comm);`

Y. Aoyama and J. Nakano

Reduce operators

MPI Reduction Operation		C Data Types	Fortran Data Type
MPI_MAX	maximum	integer, float	integer, real, complex
MPI_MIN	minimum	integer, float	integer, real, complex
MPI_SUM	sum	integer, float	integer, real, complex
MPI_PROD	product	integer, float	integer, real, complex
MPI_LAND	logical AND	integer	logical
MPI_BAND	bit-wise AND	integer, MPI_BYTE	integer, MPI_BYTE
MPI_LOR	logical OR	integer	logical
MPI_BOR	bit-wise OR	integer, MPI_BYTE	integer, MPI_BYTE
MPI_LXOR	logical XOR	integer	logical
MPI_BXOR	bit-wise XOR	integer, MPI_BYTE	integer, MPI_BYTE
MPI_MAXLOC	max value and location	float, double and long double	real, complex,double precision
MPI_MINLOC	min value and location	float, double and long double	real, complex, double precision

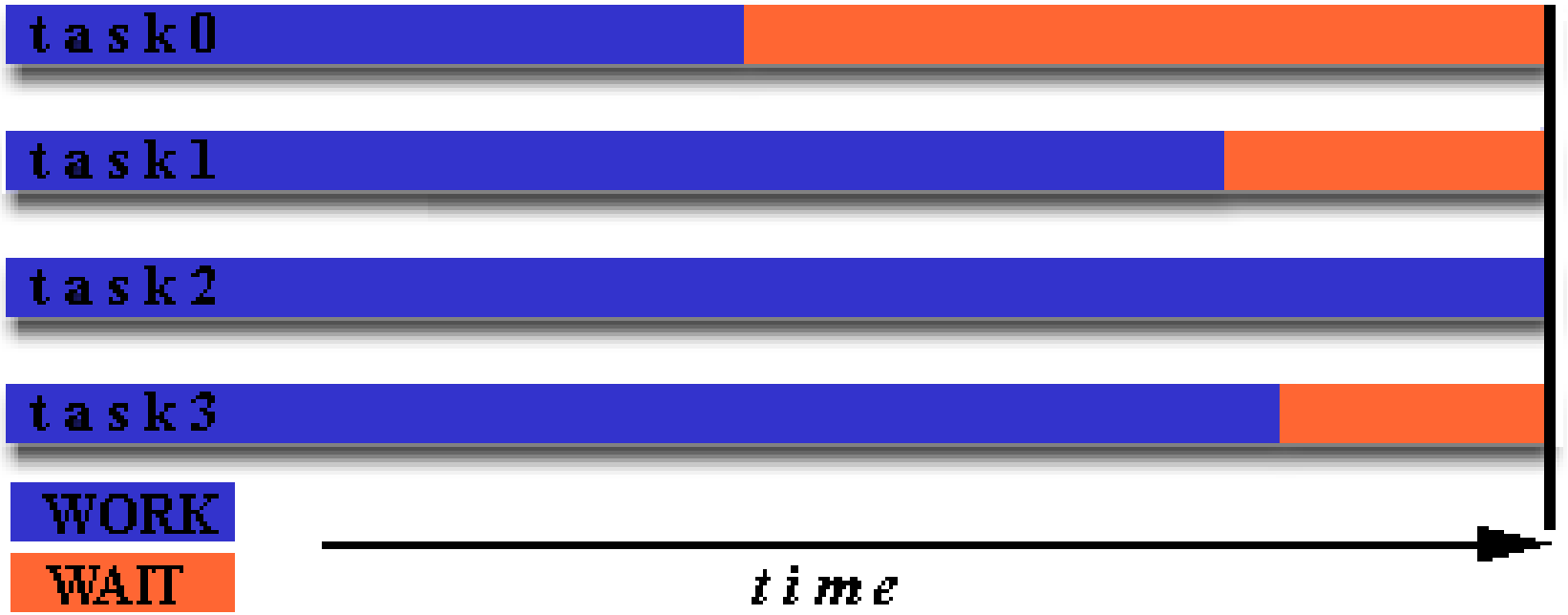
Communications?



FFT

FD

Load Balancing



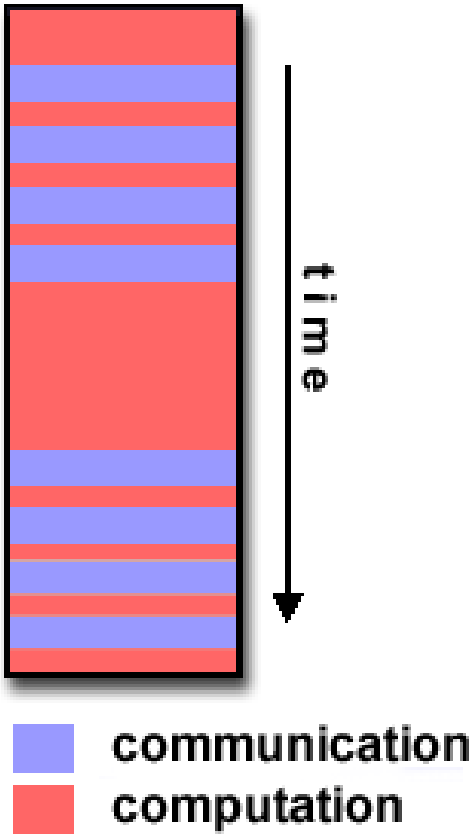
top, 각 노드에서 직접 확인, “평균하는 시간간격”을 조절함 (top→d).

Equally partition the work

Use dynamic work assignment

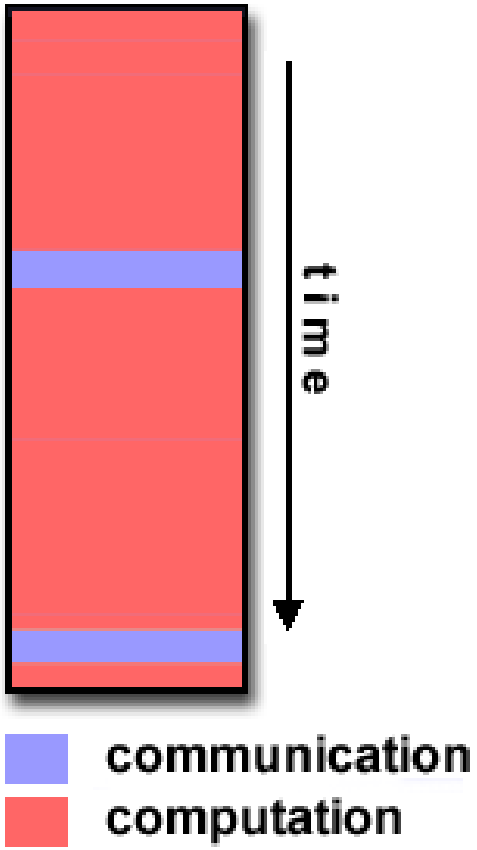
Granularity

Fine-grain Parallelism



새로운 알고리듬?

Coarse-grain Parallelism



Relatively **large amounts of computational work are done** between *communication/synchronization events*

Problem decomposition

- Domain decompostion
- Functional decomposition

★ 같은 방식의 계산인데 데이터가 서로 다른 경우

★ 서로 다른 노드의 데이터가 필요하고 노드 자체의 데이터와 연합하여 계산이 진행되는 경우

Parallel programming issues

★load balancing
★minimizing communication
★overlapping communication and computation

계산과 통신을 연합하여야 한다. 통신은 될 수 있으면 자주 하지 않아야 한다. (minimizing communication)
왜냐하면 통신은 매우 느리기 때문이다.
노드들이 거의 균등한 정도로 계산을 수행하면 아주 좋다. (load balancing)
이러한 계산을 충분히 오랬 동안 수행한 다음에 통신을 하는 방식이 좋다.

계속해서 계산할 인풋자료를 계산 노드들에 전달하는 경우가 있다. 물론, 계산된 결과는 계산 즉시 받아들인다. 또한, 다음에 계산할 추가 작업을 위한 인풋자료를 계속해서 나누는 경우가 있을 수 있다.
이 때, MPI_ANY_SOURCE를 이용해서 자료를 받아 들인다. 어느 계산노드에서 온 계산결과 자료인지 알 수 있다. 노드에서 계산하는 것들이 모두 동일한 컴퓨터 시간을 요구하지 않는 경우에 보다 더 적합한 방법이다.
예를 들면, 계속적인 방법으로 최소화 하는 작업을 하는 경우, 계산마다 최종 수렴 계산결과를 얻어내는 시간이 동일하지 않을 수 있다.

It is very difficult in practice to interleave communication with computation.

http://incredible.egloos.com/3755171

```
PROGRAM main
PARAMETER (n = 1000)
DIMENSION a(n)
DO i = 1, n
  a(i) = i
ENDDO
sum = 0.0
DO i = 1, n
  sum = sum + a(i)
ENDDO
PRINT *,'sum =',sum
END
```

나누어서 더할 수 있다!

```
SUBROUTINE para_range(n1, n2, nprocs, irank, ista, iend)
iwork1 = (n2 - n1 + 1) / nprocs
iwork2 = MOD(n2 - n1 + 1, nprocs)
ista = irank * iwork1 + n1 + MIN(irank, iwork2)
iend = ista + iwork1 - 1
IF (iwork2 > irank) iend = iend + 1
END
```

Iteration	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Rank	0	0	0	0	1	1	1	1	2	2	2	3	3	3

```
SUBROUTINE para_range(n1, n2, nprocs, irank, ista, iend)
iwork = (n2 - n1) / nprocs + 1
ista = MIN(irank * iwork + n1, n2 + 1)
iend = MIN(ista + iwork - 1, n2)
END
```

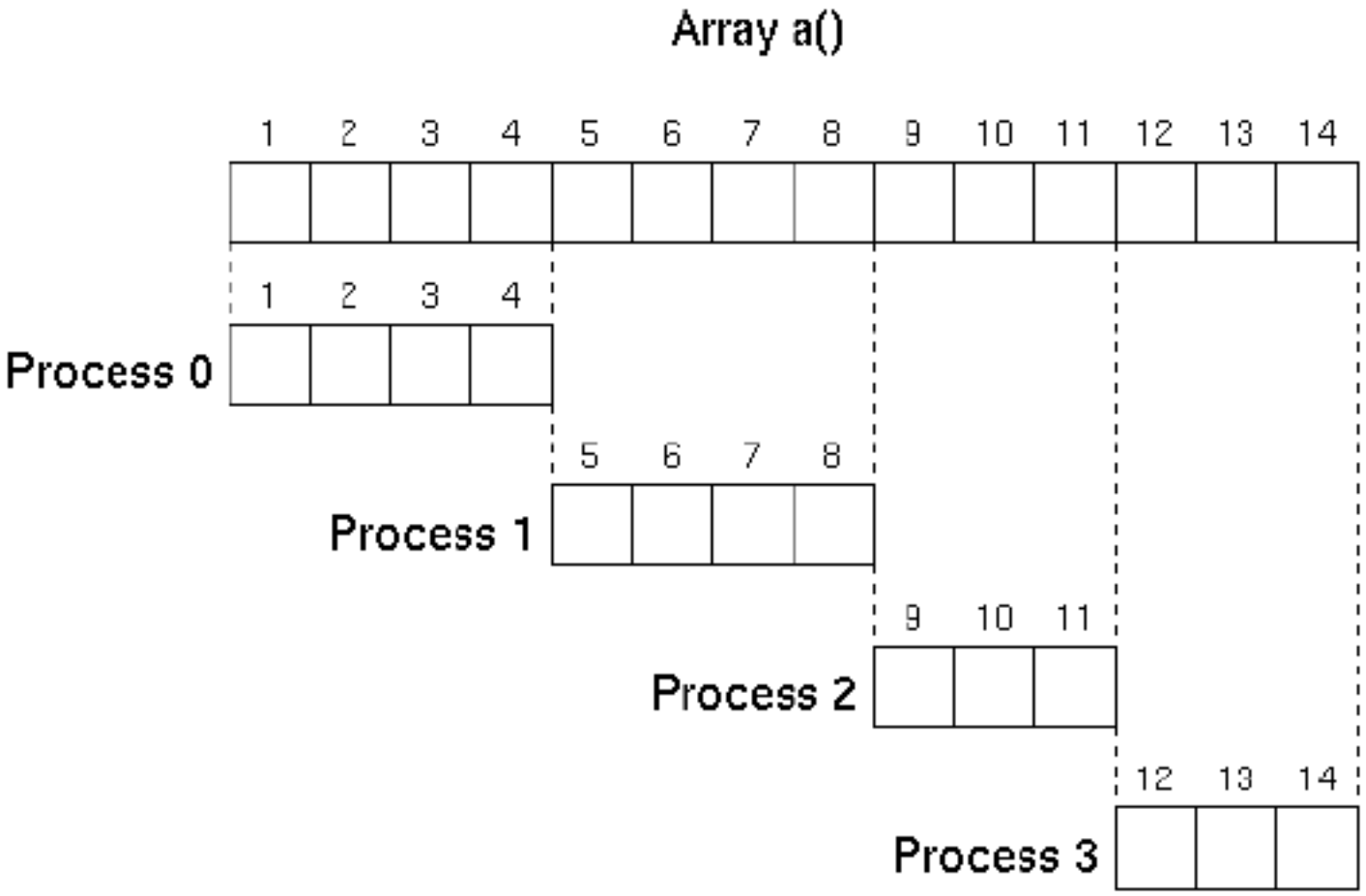
Iteration	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Rank	0	0	0	0	1	1	1	1	2	2	2	2	3	3

```
      subroutine equal_load(n1,n2,nproc,myid,istart,ifinish)
      implicit none
      integer nproc,myid,istart,ifinish,n1,n2
      integer iw1,iw2
      iw1=(n2-n1+1)/nproc ; iw2=mod(n2-n1+1,nproc)
      istart=myid*iw1+n1+min(myid,iw2)
      ifinish=istart+iw1-1 ; if(iw2 > myid) ifinish=ifinish+1
!     print*, n1,n2,myid,nproc,istart,ifinish
      if(n2 < istart) ifinish=istart-1
      return
      end
```

```
      PROGRAM main
      INCLUDE 'mpif.h'
      PARAMETER (n = 1000)
      DIMENSION a(n)
      CALL MPI_INIT(ierr)
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
      CALL para_range(1, n, nprocs, myrank, ista, iend)
      DO i = ista, iend
        a(i) = i
      ENDDO
      sum = 0.0
      DO i = ista, iend
        sum = sum + a(i)
      ENDDO
      CALL MPI_REDUCE(sum, ssum, 1, MPI_REAL,
     &                MPI_SUM, 0, MPI_COMM_WORLD, ierr)
      sum = ssum
      IF (myrank == 0) PRINT *,'sum =',sum
      CALL MPI_FINALIZE(ierr)
      END
```

계산하는 노드별로 다른 시작, 종료 지점을 알려 준다.

노드별로 시작, 종료점이 다르다는 것을 알려준다. 잘 나누어서 알려준다.



Y. Aoyama and J. Nakano

가장 많이 사용되는 do loop 병렬화의 방식을 아래에 표시했다.
do loop 병렬화 (3가지 방식)

1/3. block distribution

```
do i=n1,n2
.....
end do
-------------> 아래와 같이 serial에서 parallel로 바뀝니다.
do i=ista,iend
.....
end do
```

여기에서 ista, iend는 노드별(irank)로 다른값이 할당된다.

```
subroutine para_range(n1,n2,nprocs,irank,ista,iend)
implicit none
integer n1,n2,nprocs,irank,ista,iend
integer iwork1,iwork2
iwork1=(n2-n1+1)/nprocs
iwork2=mod(n2-n1+1,nprocs)
ista=irank*iwork1+n1+min(irank,iwork2)
iend=ista+iwork1-1
if(iwork2> irank) iend=iend+1
end
```

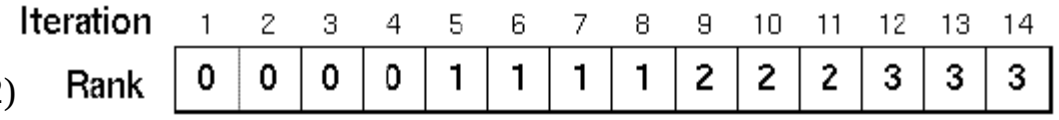


Figure 49. Block Distribution

2/3. cyclic distribution

round-robin fashion

do i=n1,n2
.....
end do
----------> 아래와 같이 serial에서 parallel로 바뀝니다.
do i=n1+irank, n2, nprocs
.....
end do

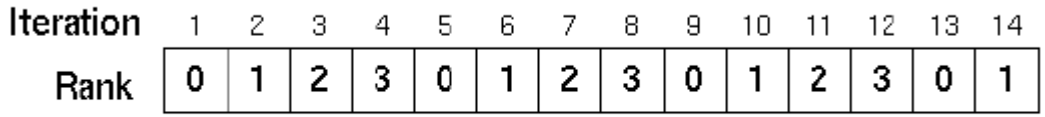


Figure 51. Cyclic Distribution

3/3. block-cyclic distribution

```
do i=n1,n2
.....
end do
----------> 아래와 같이 serial에서 parallel로 바뀝니다.
do ii=n1+irank*iblock, n2, nprocs*iblock
do i=ii,min(ii+iblock-1,n2)
.....
end do
end do
```

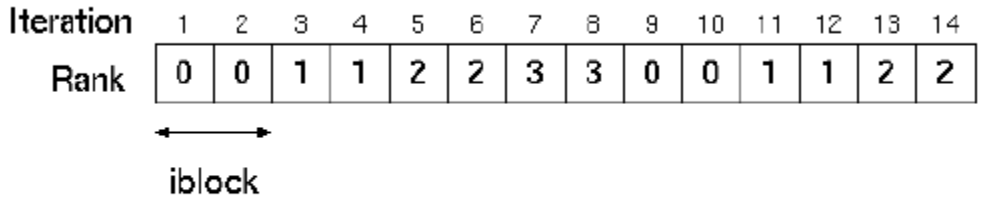


Figure 52. Block-Cyclic Distribution

```
      PROGRAM main
      implicit none
      real sum1,ssum
      integer i,ista,iend
      integer ierr,n1,n2,nprocs,myrank
      INCLUDE 'mpif.h'
      PARAMETER (n1 = 1, n2 = 1000)
      REAL, ALLOCATABLE :: a(:)

      CALL MPI_INIT(ierr)
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
      CALL para_range(n1, n2, nprocs, myrank, ista, iend)
      ALLOCATE (a(ista:iend))
      DO i = ista, iend
      a(i) = i
      ENDDO
!     sum1 = 0.0
!     DO i = ista, iend
!     sum1 = sum1 + a(i)
!    ENDDO
     sum1=sum(a)
      DEALLOCATE (a)
     CALL MPI_REDUCE(sum1, ssum, 1, MPI_REAL,MPI_SUM, 0, MPI_COMM_WORLD, ierr)
     sum1 = ssum
     PRINT *,'sum1 =',sum1, myrank
     CALL MPI_FINALIZE(ierr)
     END
```

real*8

MPI_REAL8
MPI_DOUBLE_PRECISION

```
      PROGRAM main
      INCLUDE 'mpif.h'
      PARAMETER (n1 = 1, n2 = 1000)
      REAL, ALLOCATABLE :: a(:)
      CALL MPI_INIT(ierr)
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
      CALL para_range(n1, n2, nprocs, myrank, ista, iend)
      ALLOCATE (a(ista:iend))
      DO i = ista, iend
        a(i) = i
      ENDDO
      sum = 0.0
      DO i = ista, iend
        sum = sum + a(i)

      ENDDO
      DEALLOCATE (a)
      CALL MPI_REDUCE(sum, ssum, 1, MPI_REAL,
     &                MPI_SUM, 0, MPI_COMM_WORLD, ierr)
      sum = ssum
      PRINT *,'sum =',sum
      CALL MPI_FINALIZE(ierr)
      END
```

real*8 sum, ssum

real*8, allocatable ::

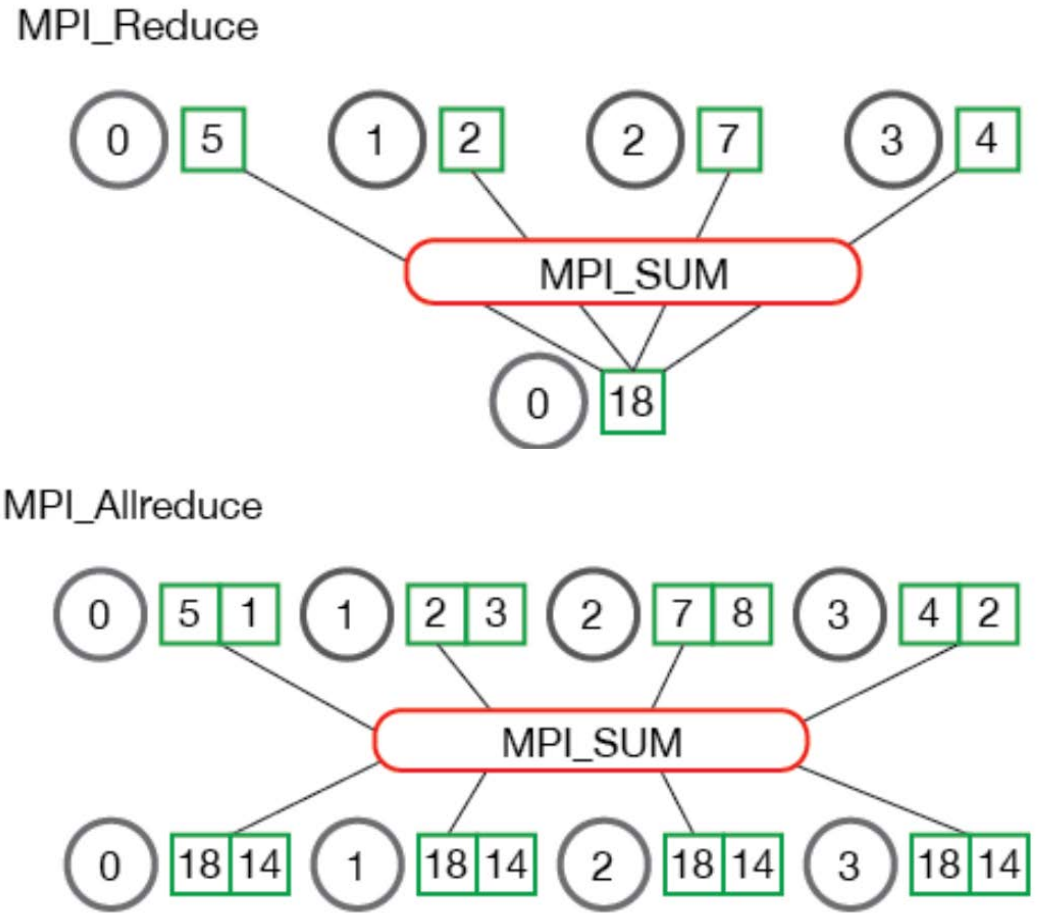
MPI_DOUBLE_PRECISION
MPI_REAL8

One-sided communication이 아닌 collective communication 이 매우 유용하다.
예를 들어, 노드별로 흩어져 있는 결과들을 종합하거나
특정 데이터를 노드별로 나누고자 할 때 collective communication 방법이 유용하다.

Processors Memory

CPU

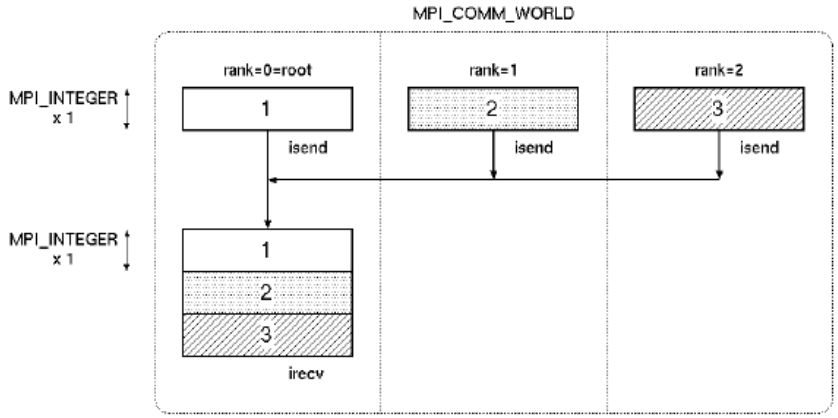
top



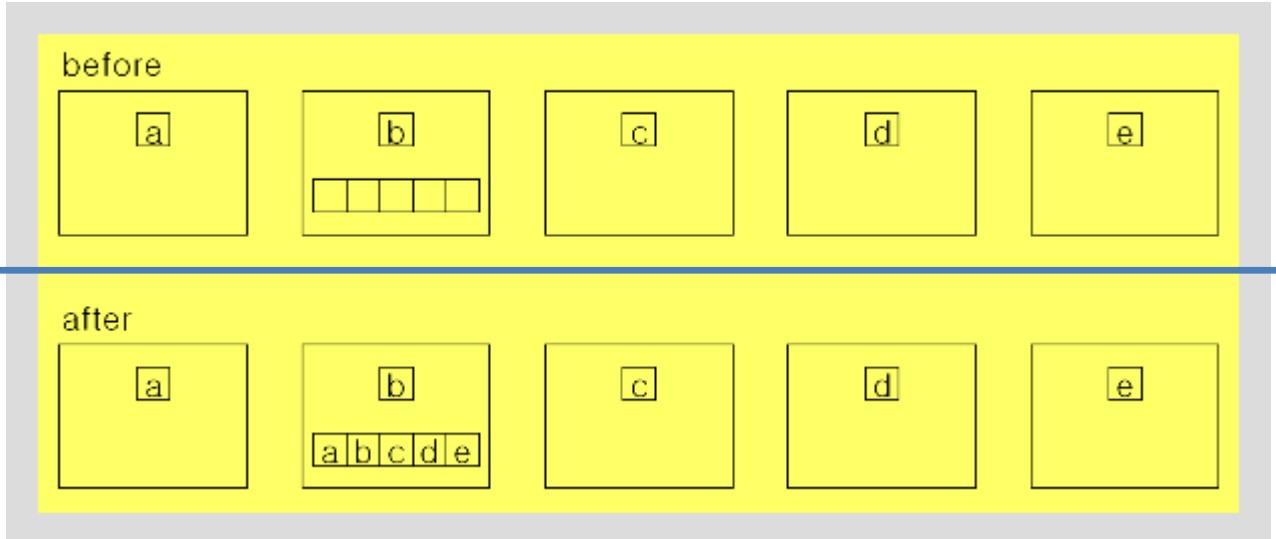
Collective communications

gather.f

```
 1       PROGRAM gather
 2       INCLUDE 'mpif.h'
 3       INTEGER irecv(3)
 4       CALL MPI_INIT(ierr)
 5       CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
 6       CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
 7       isend = myrank + 1
 8       CALL MPI_GATHER(isend, 1, MPI_INTEGER,
 9      &                irecv, 1, MPI_INTEGER,
10      &                0, MPI_COMM_WORLD, ierr)
11       IF (myrank==0) THEN
12         PRINT *,'irecv =',irecv
13       ENDIF
14       CALL MPI_FINALIZE(ierr)
15       END
```



gatherv



각 노드에 할당된 특정 크기(M)의 자료들을 특정 노드(0 노드)에 모두 모으고자 할 때가 있을 수 있다. 이 때, 특정 노드(0 노드)에서는 노드수(nproc)에 비례하는 배열 할당(M * nproc)이 필요하게 된다.

http://www.cac.cornell.edu/Ranger/MPIcc/scatterv.aspx

gaps allowed between messages in source data

irregular message sizes allowed

data can be distributed to processes in any order

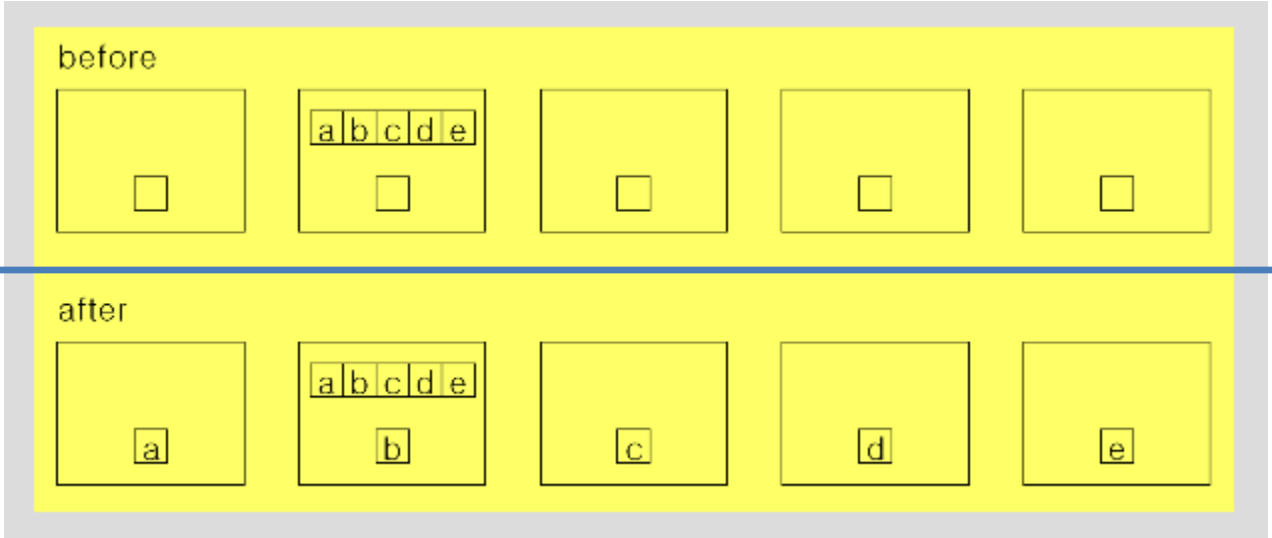
http://incredible.egloos.com/4086075

gatherv

```
!234567890
implicit none
include 'mpif.h'
integer, allocatable :: isend(:), irecv(:)
integer, allocatable :: ircnt(:), idisp(:)
integer ierr,nproc,myid
integer i,iscnt,  ndsize
call MPI_INIT(ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD,nproc,ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD,myid,ierr)
ndsize=10
allocate(isend(ndsize),irecv(nproc*ndsize))
allocate(ircnt(0:nproc-1),idisp(0:nproc-1))
ircnt=ndsize
idisp(0)=0
do i=1,nproc-1
idisp(i)=idisp(i-1)+ircnt(i)
enddo
do i=1,ndsize ! node specific data with a data-size ndsize
isend(i)=myid+1
enddo
iscnt=ndsize
call MPI_GATHERV(isend, iscnt, MPI_INTEGER, irecv, ircnt, idisp, MPI_INTEGER,0, MPI_COMM_WORLD, ierr)
if(myid == 0)then
print*, 'irecv= ',irecv
endif
deallocate(ircnt,idisp)  ;   deallocate(isend,irecv)
call MPI_FINALIZE(ierr)  ;  stop  ;  end
```

scatterv

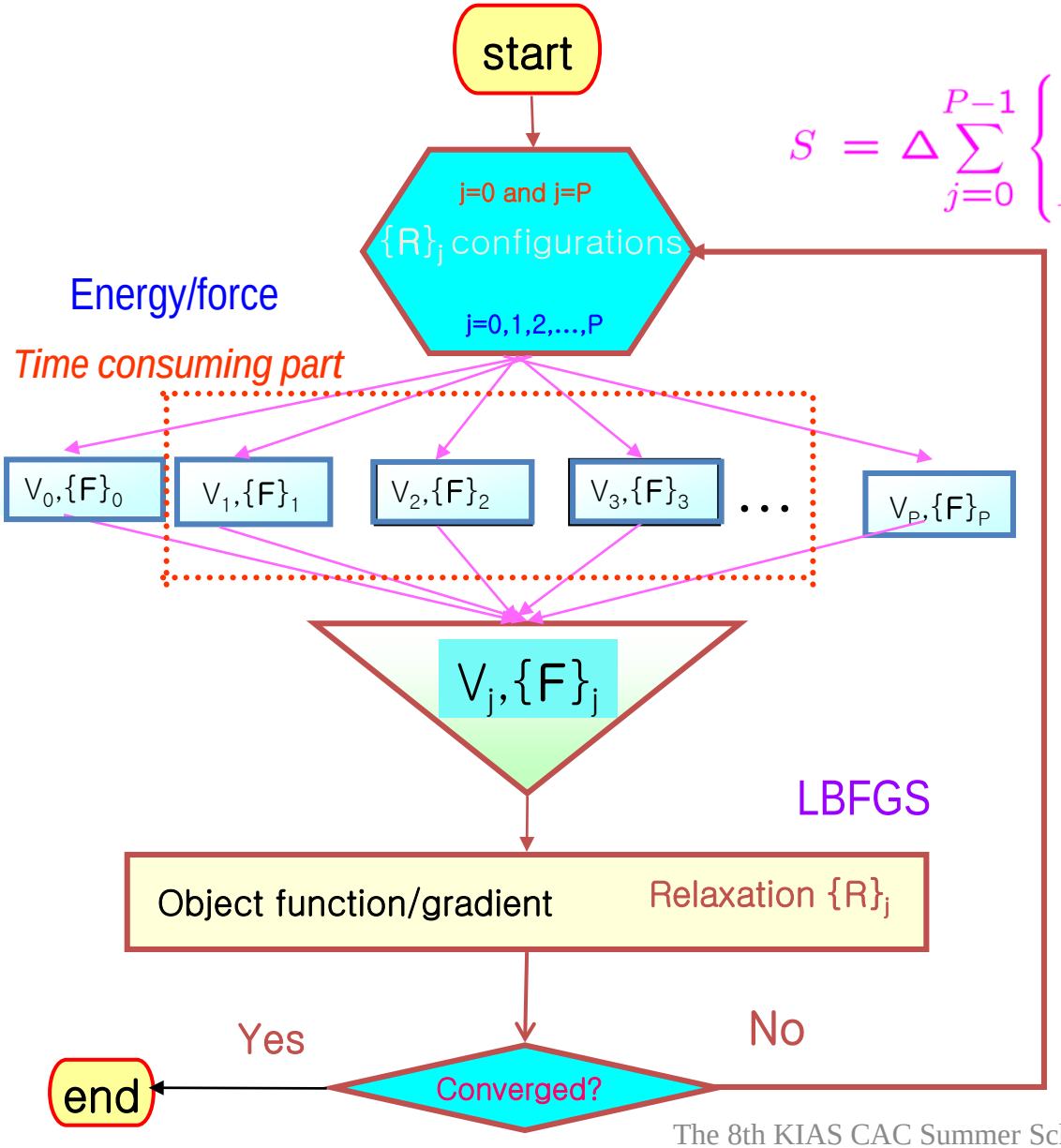
real a(25), rbuf(MAX) integer displs(NX), rcounts(NX), nsize
do i= 1, nsize
displs(i) = (i-1) * stride
rcounts(i) = 25
enddo
call mpi_gatherv(a, 25, MPI_REAL, rbuf, rcounts, displs, & MPI_REAL, root, comm, ierr)



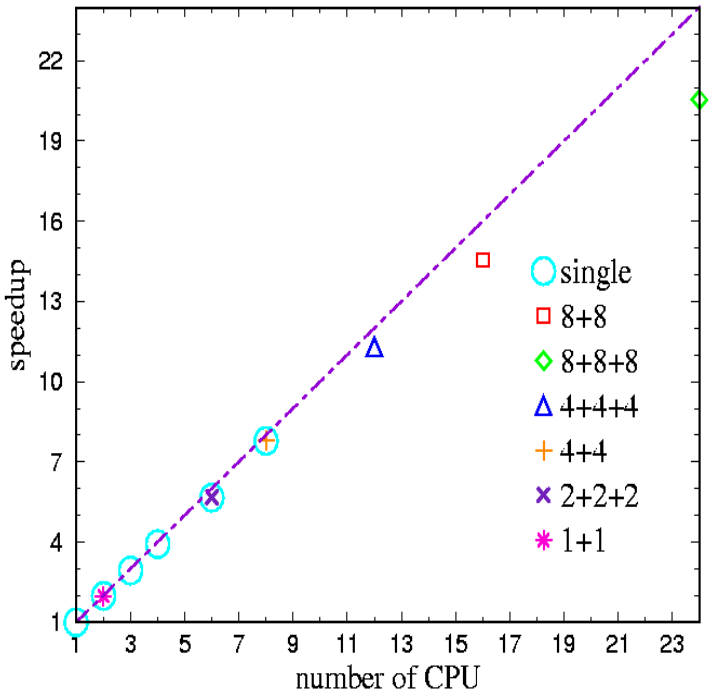
real a(25), sbuf(MAX) integer displs(NX), scounts(NX), nsize
do i= 1, nsize
displs(i) = (i-1) * stride
scounts(i) = 25
enddo
call mpi_scatterv(sbuf, scounts, displs, MPI_REAL, a, 25, & MPI_REAL, root, comm, ierr)

http://www.cac.cornell.edu/Ranger/MPIcc/gathervscatterv.aspx

Parallel ADMD



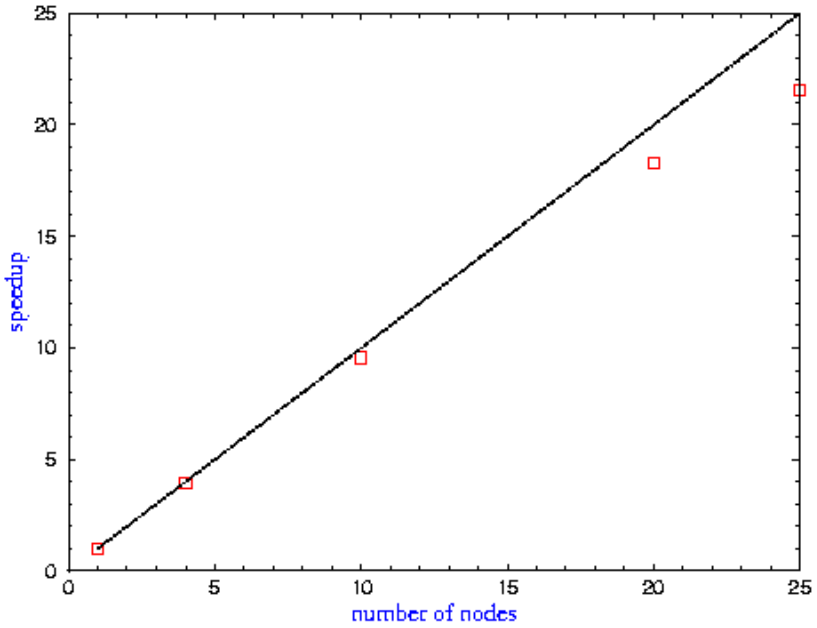
$$S = \Delta \sum_{j=0}^{P-1} \left\{ \sum_{I=1}^{N} \frac{M_I}{2} \left(\frac{\vec{R}_I^{\,j} - \vec{R}_I^{\,j+1}}{\Delta} \right)^2 + V(\{\vec{R}_I^{\,j}\}) \right\}$$

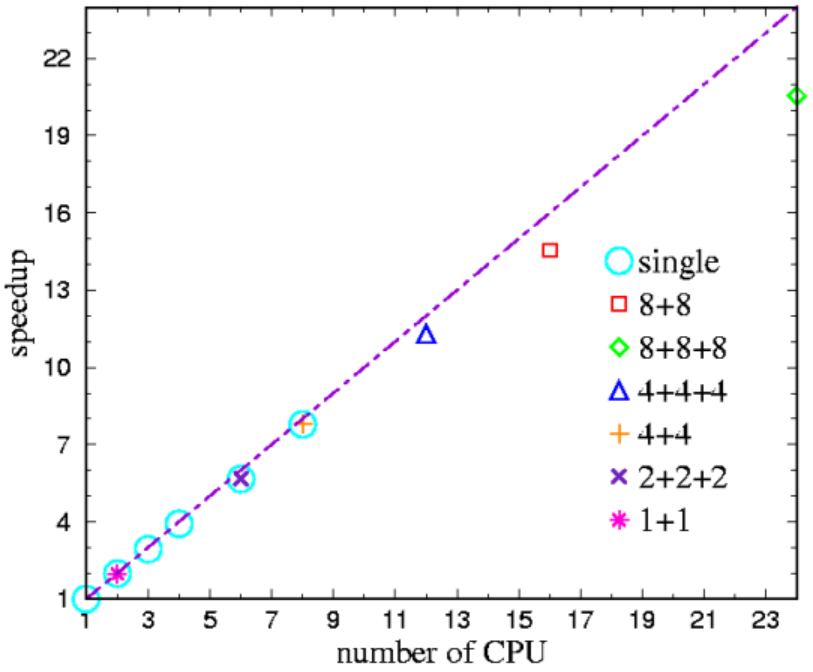


{Communication}/{CPU} ratio

Distributed computing

Observed speedup





top 각 노드에서 직접 확인

GLOBUS; MPICH_G2

```
      program main
      include 'mpif.h'
      integer ierr
      call MPI_INIT(ierr)
      print*, 'hello world'
      call MPI_FINALIZE(ierr)
      end
```

```
mpif77 hello_world_parallel_1.f
mpiexec –n 2 ./a.out
mpiexec –np 2 ./a.out
```

ASCII vs. binary

> 10 speedup

Format	C	FORTRAN
ASCII	`fprintf()`	open(6,file='test',form='formatted') write(6,*)
Binary	`fwrite()`	open(6,file='test',form='unformatted') write(6)

포트란 direct access 기법이 MPI 환경하에서 유용한 입출력 방식으로 사용되는 한 예를 소개합니다.

포트란 문법에서 파일을 다룰 때, 디폴트는 순차적 (" sequential ") 접근을 의미한다.
읽을 때, 적을 때 마찬가지이다.
아래와 같은 경우, 통상 디폴트 옵션에 따라서 access='sequential' 는 생략하는 경우가 대부분이다.

```
open(1,file='fort.1',form='formatted',access='sequential')
```

```
open(2,file='fort.2',access='direct', recl=8*nnn)
```

위와 같이 할 경우, 즉 명시적으로 direct 접근을 활용한다고 선언하면, 레코드 길이를 정한 상태에서 데이터에 직접 접근할 수 있다. 즉, 읽고 적을 수 있다. 데이터 부분, 부분별로 적고 읽을 수 있다.
프로그램 실행 중에 데이터를 읽고 적을 수 있다. 데이터는 부분으로 나누어져 있어서 전부일 필요가 없다.

데이터 용량이 클 때, 유용하게 사용할 수 있는 기법이다.
사실상 하나의 배열처럼 프로그램에서 불러서 사용할 수 있다.

이 편리한 방법은 MPI 환경에서도 여전히 유용하다. 노드간 통신을 수행한 다음 0 번 노드가 파일 적기를 담당할 수 있다. 데이터 용량이 클 경우 노드가 클 수 있다. 하지만, 각 노드에서 적절히 배당된 레코드에 각자 적어 버리면, 나중에 이 단일 파일에 접근할 수 있다. 노드간 통신 없이 파일에 적을 수 있다.

노드별로 서로 다른 레코드에 직접 접근해서 각자 데이터를 적고 읽을 수 있다.


```
!234567890
program d_access
implicit none
include 'mpif.h'
integer myid, nproc, ierr, iroot, kount
real*8 time_start,time_end
integer nsites
real*8, allocatable :: spin_lattice(:),tspin_lattice(:)
real*8 before,after
integer kdum,kk
call MPI_INIT( ierr )
call MPI_COMM_RANK( MPI_COMM_WORLD, myid, ierr )
call MPI_COMM_SIZE( MPI_COMM_WORLD, nproc, ierr )
if(myid == 0 .and. nproc > 1) print *, nproc," processes are alive"
if(myid == 0 .and. nproc ==1) print *, nproc," process is alive"
time_start=MPI_WTIME()

nsites=100
allocate(spin_lattice(nsites))
allocate(tspin_lattice(nsites))
spin_lattice=0.d0
tspin_lattice=0.d0
before=float(myid)
print*, before, myid,' node,in the memory'
open(97,file='fort.97',access='direct',recl=8*(nsites+1))
write(97,rec=myid+1) before,(spin_lattice(kdum),kdum=1,nsites)
close(97)
```

포트란 프로그램 실행 중(on the fly) 특정 파일 지우기는 아래와 같이 실행하면 된다.

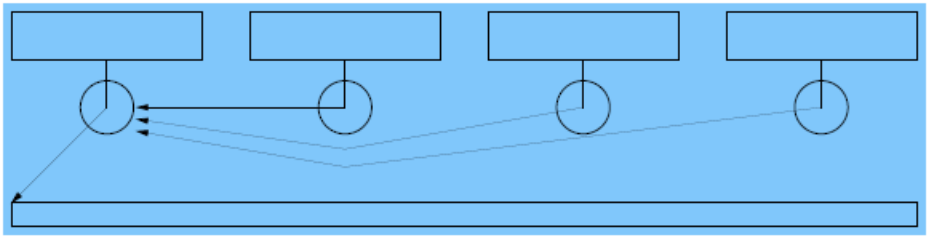
```
OPEN(11,FILE='del')
CLOSE(11,STATUS='DELETE') ! 파일 지우기를 실행함.
```

MPI 인 경우 0 번 노드에서만 지워야한다. 모든 노드가 다 지울 수 없다.

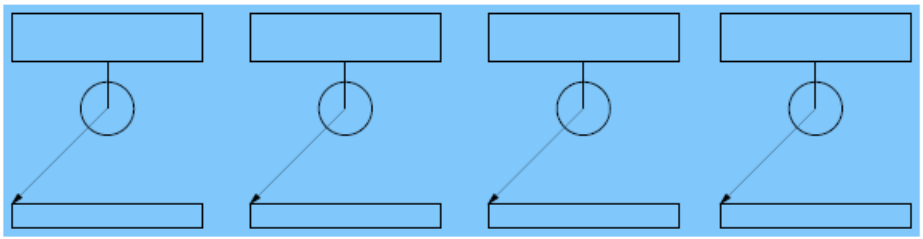
```
call MPI_BARRIER( MPI_COMM_WORLD, ierr )
if(myid == 0)then ! -----[ process id = 0
open(97,file='fort.97',access='direct',recl=8*(nsites+1))
before=2.d222
do kk=1,nproc
read(97,rec=kk) after,(tspin_lattice(kdum),kdum=1,nsites)
print*, after, kk-1,' node,in the file'
! if(before > after)then
! before=after
! spin_lattice=tspin_lattice
! endif
enddo
close(97)
! print*, before,' before'
endif ! --------=== } process id =0

deallocate(spin_lattice)
deallocate(tspin_lattice)
time_end=MPI_WTIME()
if(myid == 0) then ! --------=== { process id =0
write(6,'(4(f14.5,1x,a))') (time_end-time_start),'s', (time_end-time_start)/60.d0,'m', (time_end-time_start)/3600.d0,'h',
(time_end-time_start)/3600.d0/24.d0,'d'
endif ! --------=== } process id =0
call MPI_FINALIZE(ierr)
stop
end program d_access
```

I/O → Parallel I/O

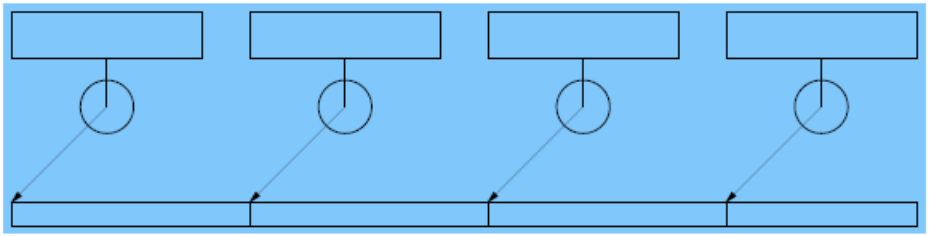
- Non-parallel I/O



- I/O to separate files



- Parallel I/O



Non-parallel I/O from an MPI program

```
#include "mpi.h"
#include <stdio.h>
#define BUFSIZE 100
int main(int argc, char *argv[])
{
int i, myrank, numprocs, buf[BUFSIZE];
MPI_Status status;
FILE *myfile;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
for (i=0; i<BUFSIZE; i++)
buf[i] = myrank * BUFSIZE + i;
if (myrank != 0)
MPI_Send(buf, BUFSIZE, MPI_INT, 0, 123, MPI_COMM_WORLD);
else {
myfile = fopen("testfile", "w");
fwrite(buf, sizeof(int), BUFSIZE, myfile);
for (i=1; i<numprocs; i++) {
MPI_Recv(buf, BUFSIZE, MPI_INT, i, 123, MPI_COMM_WORLD, &status);
fwrite(buf, sizeof(int), BUFSIZE, myfile);
}
fclose(myfile);
}
MPI_Finalize();
return 0;
}
```

Non-MPI I/O to separate files

```
#include "mpi.h"
#include <stdio.h>
#define BUFSIZE 100
int main(int argc, char *argv[])
{
int i, myrank, buf[BUFSIZE];
char filename[128];
FILE *myfile;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
for (i=0; i<BUFSIZE; i++)
buf[i] = myrank * BUFSIZE + i;
sprintf(filename, "testfile.%d", myrank);
myfile = fopen(filename, "w");
fwrite(buf, sizeof(int), BUFSIZE, myfile);
fclose(myfile);
MPI_Finalize();
return 0;
}
```

MPI I/O to separate files

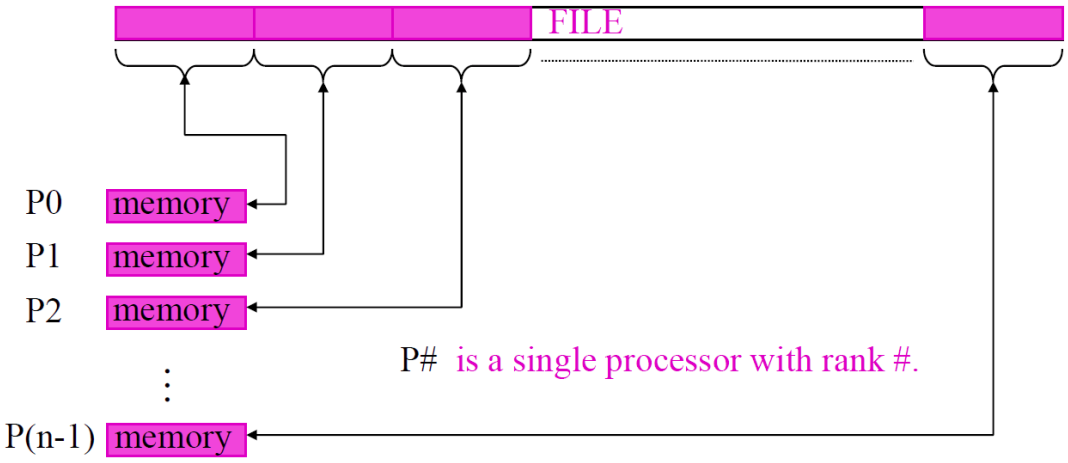
```
#include "mpi.h"
#include <stdio.h>
#define BUFSIZE 100
int main(int argc, char *argv[])
{
int i, myrank, buf[BUFSIZE];
char filename[128];
MPI_File myfile;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
for (i=0; i<BUFSIZE; i++)
buf[i] = myrank * BUFSIZE + i;
sprintf(filename, "testfile.%d", myrank);
MPI_File_open(MPI_COMM_SELF, filename, MPI_MODE_WRONLY | MPI_MODE_CREATE, MPI_INFO_NULL, &myfile);
MPI_File_write(myfile, buf, BUFSIZE, MPI_INT, MPI_STATUS_IGNORE);
MPI_File_close(&myfile);
MPI_Finalize();
return 0;
}
```

Parallel MPI I/O to a single file

```
#include "mpi.h"
#include <stdio.h>
#define BUFSIZE 100
int main(int argc, char *argv[])
{
int i, myrank, buf[BUFSIZE];
MPI_File thefile;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
for (i=0; i<BUFSIZE; i++)
buf[i] = myrank * BUFSIZE + i;
MPI_File_open(MPI_COMM_WORLD, "testfile", MPI_MODE_CREATE | MPI_MODE_WRONLY, MPI_INFO_NULL, &thefile);
MPI_File_set_view(thefile, myrank*BUFSIZE*sizeof(int), MPI_INT, MPI_INT, "native", MPI_INFO_NULL);
MPI_File_write(thefile, buf, BUFSIZE, MPI_INT, MPI_STATUS_IGNORE);
MPI_File_close(&thefile);
MPI_Finalize();
return 0;
}
```

| : C

\+ : Fortran



Reading a file (1/3)

```
#include "mpi.h"
#include <stdio.h>
int main(int argc, char *argv[])
{
int myrank, numprocs, bufsize, *buf, count;
MPI_File thefile;
MPI_Status status;
MPI_Offset filesize;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
MPI_File_open(MPI_COMM_WORLD, "testfile", MPI_MODE_RDONLY, MPI_INFO_NULL, &thefile);
MPI_File_get_size(thefile, &filesize);              /* in bytes */
filesize = filesize / sizeof(int);                  /* in number of ints */
bufsize = filesize / numprocs + 1;                  /* local number to read */
buf = (int *) malloc (bufsize*sizeof(int));
MPI_File_set_view(thefile, myrank*bufsize*sizeof(int), MPI_INT, MPI_INT, "native", MPI_INFO_NULL);
MPI_File_read(thefile, buf, bufsize, MPI_INT, &status);
MPI_Get_count(&status, MPI_INT, &count);
printf("process %d read %d ints₩n", myrank, count);
MPI_File_close(&thefile);
MPI_Finalize();
return 0;
}
```

Reading a file (2/3)

```
#include<stdio.h>
#include "mpi.h"
#define FILESIZE 80
int main(int argc, char **argv){
int rank, size, bufsize, nints;
MPI_File fh;
MPI_Status status;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);
bufsize = FILESIZE/size;
nints = bufsize/sizeof(int);
int buf[nints];
MPI_File_open(MPI_COMM_WORLD,"dfile",MPI_MODE_RDONLY,MPI_INFO_NULL,&fh);
MPI_File_seek(fh, rank * bufsize, MPI_SEEK_SET);
MPI_File_read(fh, buf, nints, MPI_INT, &status);
printf("\nrank: %d, buf[%d]: %d", rank, rank*bufsize, buf[0]);
MPI_File_close(&fh);
MPI_Finalize();
return 0;
}
```

Declaring a File Pointer

Calculating Buffer Size

After opening the file, read data from files by using either MPI_File_seek & MPI_File_read or MPI_File_read_at

Reading a file (3/3)

```
#include<stdio.h>
#include "mpi.h"
#define FILESIZE 80
int main(int argc, char **argv){
int rank, size, bufsize, nints;
MPI_File fh;
MPI_Status status;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);
bufsize = FILESIZE/size;
nints = bufsize/sizeof(int);
int buf[nints];
MPI_File_open(MPI_COMM_WORLD,"dfile",MPI_MODE_RDONLY,MPI_INFO_NULL,&fh);
MPI_File_read_at(fh, rank*bufsize, buf, nints, MPI_INT, &status);
printf("\nrank: %d, buf[%d]: %d", rank, rank*bufsize, buf[0]);
MPI_File_close(&fh);
MPI_Finalize();
return 0;
}
```

After opening the file, read data from files by using either MPI_File_seek & MPI_File_read or MPI_File_read_at

Writing a file (1/2)

```
#include<stdio.h>
#include "mpi.h"
int main(int argc, char **argv){
int i, rank, size, offset, nints, N=16 ;
MPI_File fhw;
MPI_Status status;
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);
int buf[N];
for ( i=0;i<N;i++){
buf[i] = i ;
 }
 offset = rank*(N/size)*sizeof(int);
MPI_File_open(MPI_COMM_WORLD, "datafile", MPI_MODE_CREATE|MPI_MODE_WRONLY, MPI_INFO_NULL, &fhw);
printf("\nRank: %d, Offset: %d\n", rank, offset);
MPI_File_write_at(fhw, offset, buf, (N/size), MPI_INT, &status);
MPI_File_close(&fhw);
MPI_Finalize();
return 0;
}
```

For writing, use either **MPI_File_set_view** & **MPI_File_write** or **MPI_File_write_at**

Writing a file (2/2)

```
#include<stdio.h>
#include "mpi.h"
int main(int argc, char **argv){
 int i, rank, size, offset, nints, N=16;
 MPI_File fhw;
 MPI_Status status;
 MPI_Init(&argc, &argv);
 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
 MPI_Comm_size(MPI_COMM_WORLD, &size);
 int buf[N];
 for ( i=0;i<N;i++){
 buf[i] = i ;
 }
 offset = rank*(N/size)*sizeof(int);
MPI_File_open(MPI_COMM_WORLD, "datafile3", MPI_MODE_CREATE|MPI_MODE_WRONLY, MPI_INFO_NULL, &fhw);
 printf("\nRank: %d, Offset: %d\n", rank, offset);
 MPI_File_set_view(fhw, offset, MPI_INT, MPI_INT, "native", MPI_INFO_NULL);
 MPI_File_write(fhw, buf, (N/size), MPI_INT, &status);
 MPI_File_close(&fhw);
 MPI_Finalize();
 return 0;
}
```

For writing, use either **MPI_File_set_view** & **MPI_File_write** or **MPI_File_write_at**

Reading a file (FORTRAN)

```
integer istatus(MPI_STATUS_SIZE)
Integer (kind=MPI_OFFSET_KIND) ioffset
Call MPI_FILE_OPEN(MPI_COMM_WORLD,'/pfs/datafile', MPI_MODE_RDONLY, MPI_INFO_NULL,&
fh, ierr)
nints = FILESIZE / (nprocs*INTSIZE)
ioffset =rank*nints*INTSIZE
call MPI_FILE_READ_AT(fh, ioffset, buf, nints, MPI_INTEGER, istatus, ierr)
call MPI_GET_COUNT(istatus, MPI_INTEGER, count, ierr)
print *, 'process ', rank, 'read ', count,'integers'
call MPI_FILE_CLOSE(fh, ierr)
```

MPI_File_open flags:

- **MPI_MODE_RDONLY** (read only)
- **MPI_MODE_WRONLY** (write only)
- **MPI_MODE_RDWR** (read and write)
- **MPI_MODE_CREATE** (create file if it doesn't exist)
- Use bitwise-or '|' in C, or addition '+" in Fortran, to combine multiple flags

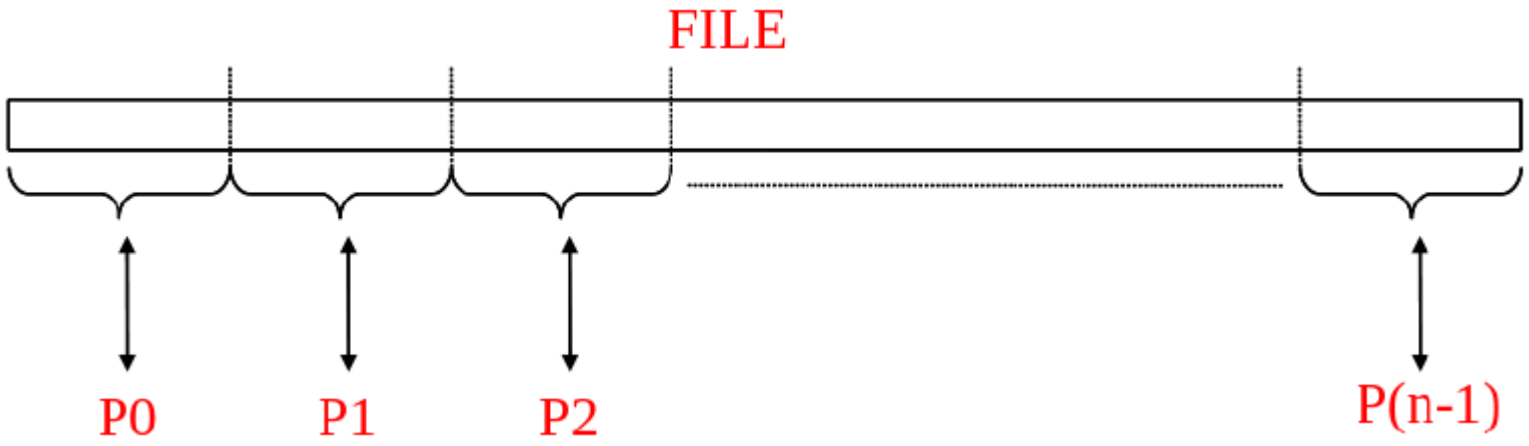
To write into a file, use MPI_File_write or MPI_File_write_at, or…

Writing to a file (FORTRAN)

```
PROGRAM main
use mpi
integer ierr, i, myrank, BUFSIZE, thefile
parameter (BUFSIZE=100)
integer buf(BUFSIZE)
integer(kind=MPI_OFFSET_KIND) disp
call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
do i = 0, BUFSIZE
buf(i) = myrank * BUFSIZE + i
enddo

call MPI_FILE_OPEN(MPI_COMM_WORLD, 'testfile', MPI_MODE_WRONLY + MPI_MODE_CREATE, &
MPI_INFO_NULL, thefile, ierr)
call MPI_TYPE_SIZE(MPI_INTEGER, intsize, ierr)
disp = myrank * BUFSIZE * intsize
call MPI_FILE_SET_VIEW(thefile, disp, MPI_INTEGER, MPI_INTEGER, 'native', MPI_INFO_NULL, ierr)
call MPI_FILE_WRITE(thefile, buf, BUFSIZE, MPI_INTEGER,MPI_STATUS_IGNORE, ierr)
call MPI_FILE_CLOSE(thefile, ierr)
call MPI_FINALIZE(ierr)
END PROGRAM main
```

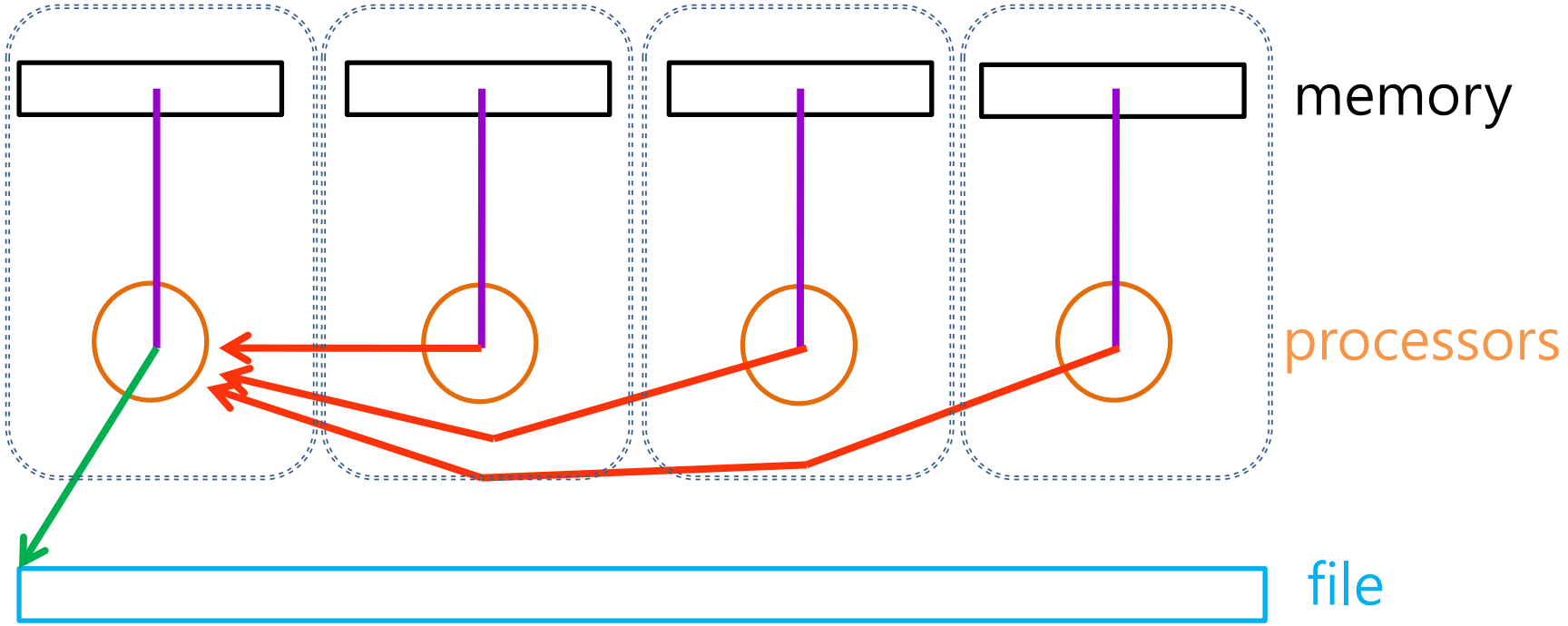
- What is Parallel I/O?

Multiple processes of a parallel program accessing data (reading or writing) from a common file.



Parallel I/O (1/3)

Sequential I/O from an parallel program

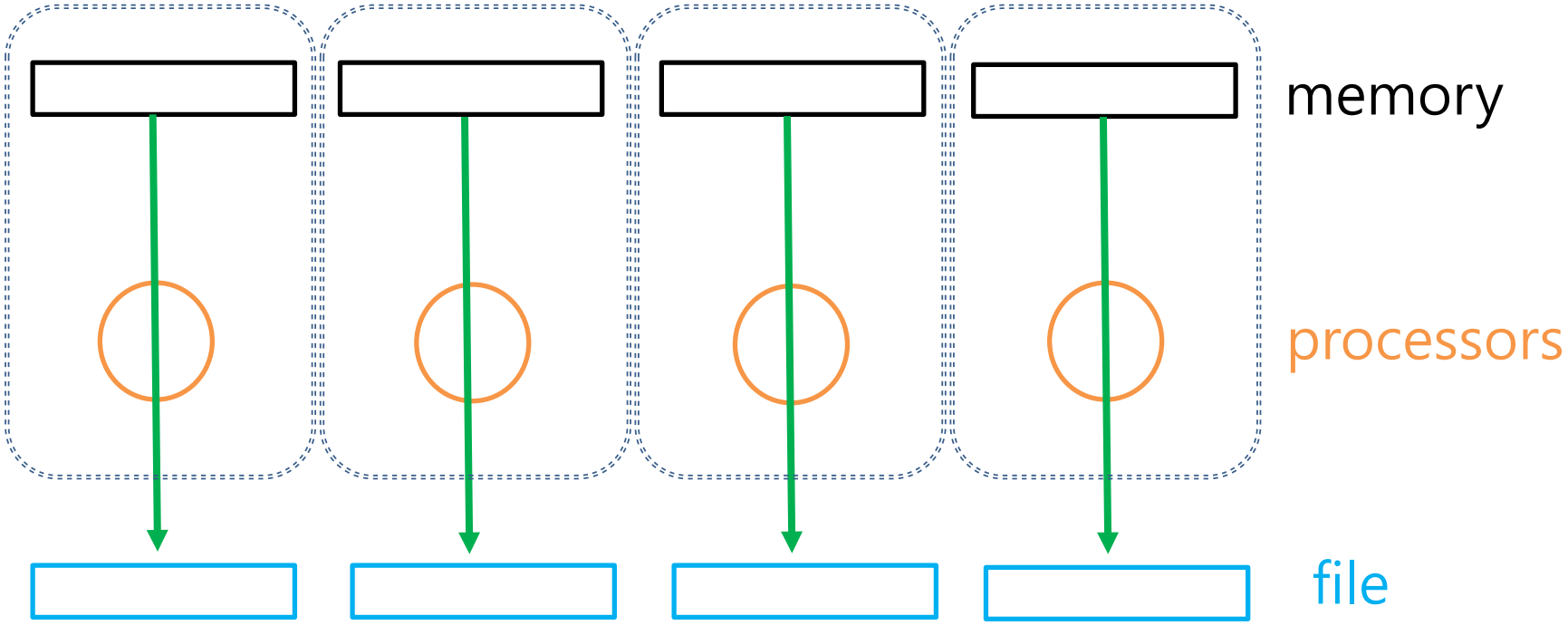


Send : write

Recv : read

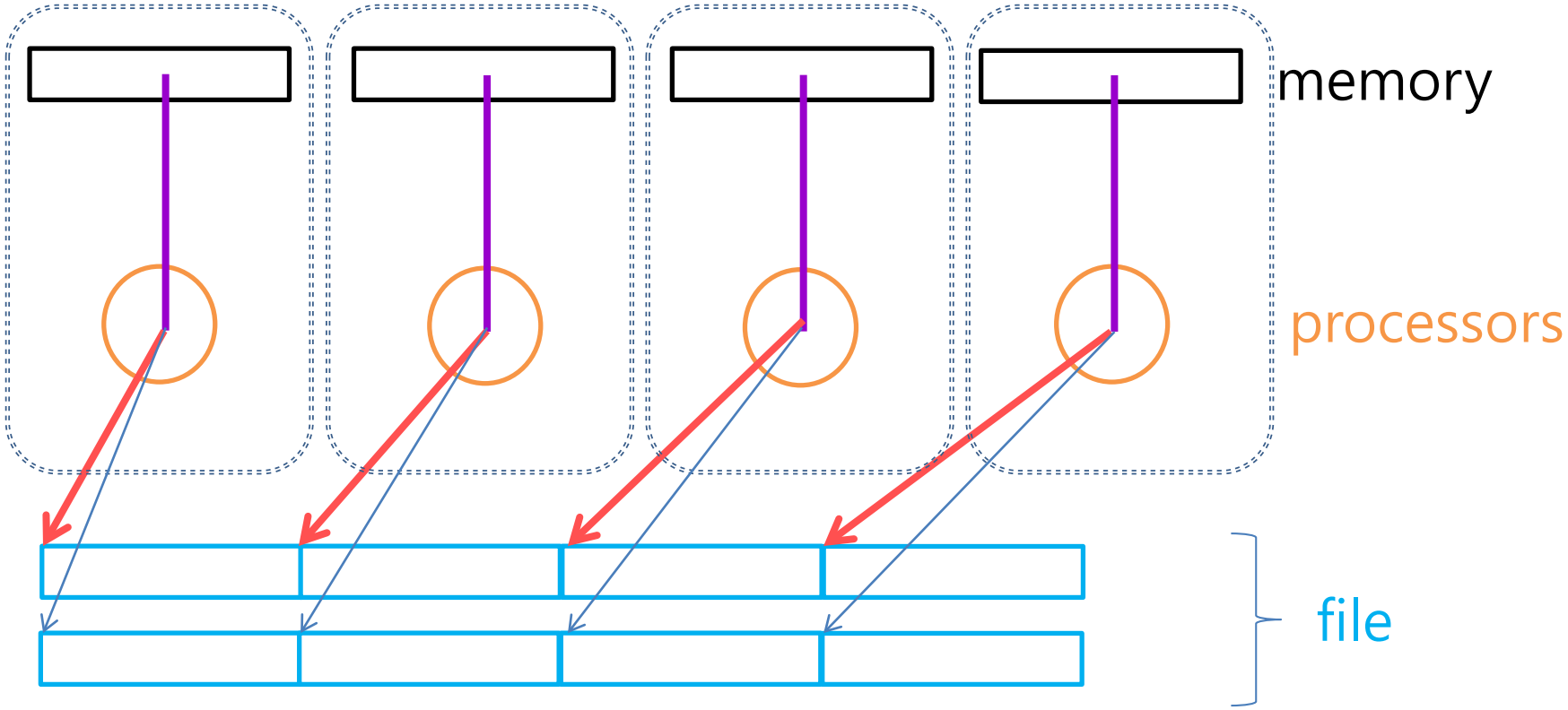
Parallel I/O (2/3)

Parallel I/O to multiple files



Parallel I/O (3/3)

Parallel I/O to a single file

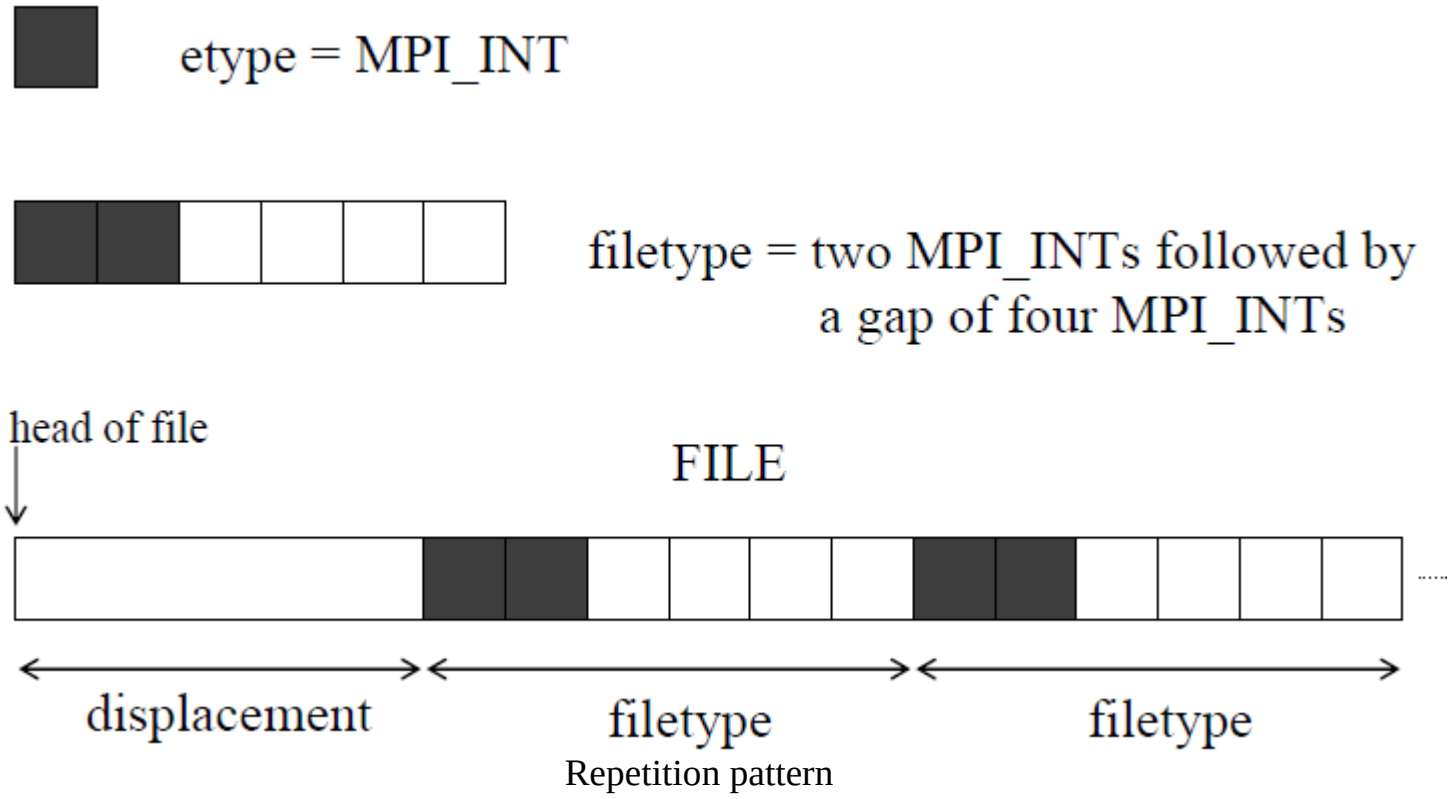


parallel MPI write into multiple files

```
!  ! example of parallel MPI write into multiple files
PROGRAM main
    ! Fortran 90 users can (and should) use
    !     use mpi
    ! instead of include 'mpif.h' if their MPI implementation provides a
    ! mpi module.
    include 'mpif.h'

    integer ierr, i, myrank, BUFSIZE, thefile
    parameter (BUFSIZE=100)
    integer buf(BUFSIZE)
    character*12 ofname

    call MPI_INIT(ierr)
    call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)

    do i = 1, BUFSIZE
        buf(i) = myrank * BUFSIZE + i
    enddo
    write(ofname,'(a8,i4.4)') 'testfile',myrank
    open(unit=11,file=ofname,form='unformatted')
    write(11) buf

    call MPI_FINALIZE(ierr)
END PROGRAM main
```

From Dr. Jongsoo Kim (KASI), The 1st KIAS CAC Summer School on Parallel Computing

Specified by a triplet (*displacement*, *etype*, and *filetype*) passed to **MPI_File_set_view**



MPI_MODE_RDWR
MPI_MODE_RDONLY
MPI_MODE_WRONLY
MPI_MODE_CREATE

```
! example of parallel MPI write into a single file, in Fortran
    PROGRAM main
    ! Fortran 90 users can (and should) use
    !     use mpi
    ! instead of include 'mpif.h' if their MPI implementation provides a
    ! mpi module.
    include 'mpif.h'

    integer ierr, i, myrank, BUFSIZE, thefile
    parameter (BUFSIZE=100)
    integer buf(BUFSIZE)
    integer(kind=MPI_OFFSET_KIND) disp

    call MPI_INIT(ierr)
    call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)

    do i = 0, BUFSIZE
       buf(i) = myrank * BUFSIZE + i
    enddo
    call MPI_FILE_OPEN(MPI_COMM_WORLD, 'testfile', MPI_MODE_WRONLY +   MPI_MODE_CREATE,   MPI_INFO_NULL, thefile, ierr)
    ! assume 4-byte integers
    disp = myrank * BUFSIZE * 4
    call MPI_FILE_SET_VIEW(thefile, disp, MPI_INTEGER,  MPI_INTEGER, 'native', MPI_INFO_NULL, ierr)
    call MPI_FILE_WRITE(thefile, buf, BUFSIZE, MPI_INTEGER, MPI_STATUS_IGNORE, ierr)
    call MPI_FILE_CLOSE(thefile, ierr)
    call MPI_FINALIZE(ierr)

END PROGRAM main
```

| : C

\+ : Fortran

For writing, use either **MPI_File_set_view** & **MPI_File_write** or **MPI_File_write_at**

MPI_MODE_CREATE | MPI_MODE_WRONLY
MPI_MODE_WRONLY + MPI_MODE_CREATE

http://www.mcs.anl.gov/research/projects/mpi/usingmpi2/examples/starting/io3f_f90.htm

```
program write_individual_pointer
use mpi
implicit none
integer ier,nproc,myid,ifile,intsize
integer mode,info,ietype,ifiletype
integer istatus(MPI_STATUS_SIZE)
integer (kind=MPI_OFFSET_KIND) :: idisp
integer, parameter :: kount=100
integer ibuf(kount)
integer i
real*8 aa1,aa2

call MPI_INIT(ier)
call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ier)
call MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ier)
mode=ior(MPI_MODE_CREATE,MPI_MODE_WRONLY)
info=0
call MPI_TYPE_EXTENT(MPI_INTEGER,intsize,ier)
aa1=MPI_WTIME()
do i=1,kount
ibuf(i)=myid*kount+i
enddo
CALL MPI_FILE_OPEN(MPI_COMM_WORLD, 'test',mode, info, ifile, ier)
idisp=myid* kount* intsize
ietype=MPI_INTEGER
ifiletype=MPI_INTEGER
CALL MPI_FILE_SET_VIEW(ifile,idisp,ietype,ifiletype,'native',info, ier)
CALL MPI_FILE_WRITE(ifile,myid,1,MPI_INTEGER,istatus, ier)

write(6,*) 'hello form myid',myid,'i wrote:', myid,'.'
CALL MPI_FILE_CLOSE(ifile,ier)
aa2=MPI_WTIME()
call MPI_FINALIZE(ier)
end program write_individual_pointer
```

```
program write_individual_pointer
use mpi
implicit none
integer ier,nproc,myid,ifile,intsize
integer mode,info,ietype,ifiletype
integer istatus(MPI_STATUS_SIZE)
integer (kind=MPI_OFFSET_KIND) :: idisp
integer, parameter :: kount=100
integer ibuf(kount)
integer i,itest
real*8 aa1,aa2

call MPI_INIT(ier)
call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ier)
call MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ier)
mode=MPI_MODE_RDONLY
info=0
call MPI_TYPE_EXTENT(MPI_INTEGER,intsize,ier)
aa1=MPI_WTIME()
do i=1,kount
ibuf(i)=myid*kount+i
enddo
CALL MPI_FILE_OPEN(MPI_COMM_WORLD, 'test',mode, info, ifile, ier)
idisp=myid* kount* intsize
ietype=MPI_INTEGER
ifiletype=MPI_INTEGER
CALL MPI_FILE_SET_VIEW(ifile,idisp,ietype,ifiletype,'native',info, ier)
CALL MPI_FILE_READ(ifile,itest,1,MPI_INTEGER,istatus, ier)
write(6,*) 'hello form myid',myid,'i read:', itest,'.'
CALL MPI_FILE_CLOSE(ifile,ier)

aa2=MPI_WTIME()
call MPI_FINALIZE(ier)
end program write_individual_pointer
```

```
integer isize
character*9 string,fname



isize=4
call xnumeral( myid, string, isize)
fname='conf1'//trim(string)                !   confi10000, confi10001, confi10002
open(29,file=fname,form='formatted')
write(29,*) nparticle,mm
write(29,*) tau,beta,ss_lowest
do ia=1,nparticle
do j=0,mm
write(29,*) (qqq(jcomp,j,ia),jcomp=1,idims)
enddo
enddo
do ia=1,nparticle
write(29,*) iiq(ia)
enddo
close(29)
```

```
PROGRAM env
INCLUDE ’mpif.h’
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
PRINT *,’nprocs =’,nprocs,’myrank =’,myrank
CALL MPI_FINALIZE(ierr)
END
```

```
$ mpxlf env.f
** env === End of Compilation 1 ===
1501-510 Compilation successful for file env.f.
$ export MP_STDOUTMODE=ordered
$ export MP_LABELIO=yes
$ a.out -procs 3
0: nprocs = 3 myrank = 0
1: nprocs = 3 myrank = 1
2: nprocs = 3 myrank = 2
```

From Dr. Jongsoo Kim (KASI), The 1st CAC Summer School on Parallel Computing

```
PROGRAM bcast
INCLUDE ’mpif.h’
INTEGER imsg(4)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
IF (myrank==0) THEN
DO i=1,4
imsg(i) = i
ENDDO
                    ELSE
DO i=1,4
imsg(i) = 0
ENDDO
                    ENDIF
 PRINT *,’Before:’,imsg
 CALL MP_FLUSH(1)
 CALL MPI_BCAST(imsg, 4, MPI_INTEGER,  0, MPI_COMM_WORLD, ierr)
 PRINT *,’After :’,imsg
 CALL MPI_FINALIZE(ierr)
 END
```

```
$ a.out -procs 3
0: Before: 1 2 3 4
1: Before: 0 0 0 0
2: Before: 0 0 0 0
0: After : 1 2 3 4
1: After : 1 2 3 4
2: After : 1 2 3 4
```

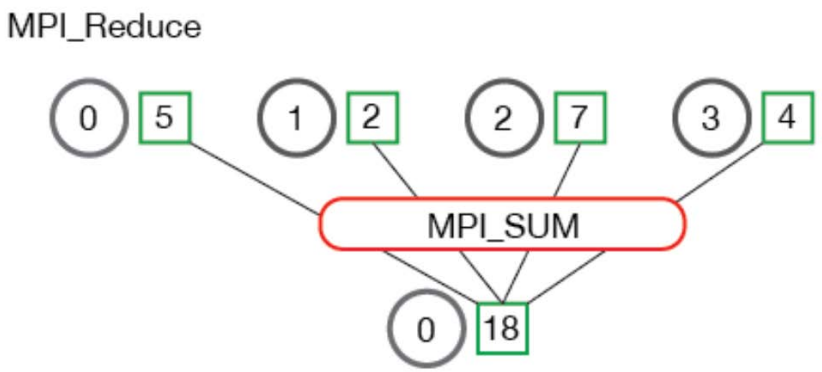
```
PROGRAM gather
INCLUDE ’mpif.h’
INTEGER irecv(3)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
isend = myrank + 1
CALL MPI_GATHER(isend, 1, MPI_INTEGER, irecv, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, ierr)
IF (myrank==0) THEN
PRINT *,’irecv =’,irecv
                    ENDIF
CALL MPI_FINALIZE(ierr)
END
```

mpirun –np 3 ./a.out

```
$ a.out -procs 3
0: irecv = 1 2 3
```

```
/*gather*/

#include <mpi.h>
#include <stdio.h>

void main (int argc, char *argv[]){

  int i, nprocs, myrank ;
  int isend, irecv[3];

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

  isend = myrank + 1;
  MPI_Gather(&isend,1,MPI_INT,irecv,1,MPI_INT,0, MPI_COMM_WORLD);
  if(myrank == 0) {
     printf(“ irecv = ”);
     for(i=0; i<3; i++)
        printf(“ %d”, irecv[i]); printf(“\n”);
  }
  MPI_Finalize();
}
```

```
 PROGRAM reduce
 INCLUDE ’mpif.h’
 REAL a(9)
 CALL MPI_INIT(ierr)
 CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
 CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
 ista = myrank * 3 + 1
 iend = ista + 2
 DO i=ista,iend
 a(i) = i
ENDDO
sum = 0.0
DO i=ista,iend
sum = sum + a(i)
ENDDO
CALL MPI_REDUCE(sum, tmp, 1, MPI_REAL, MPI_SUM, 0,MPI_COMM_WORLD, ierr)
sum = tmp
IF (myrank==0) THEN
PRINT *,’sum =’,sum
                    ENDIF
CALL MPI_FINALIZE(ierr)
END
```




```
$ a.out -procs 3
0: sum = 45.00000000
```

```
PROGRAM maxloc_p
INCLUDE ’mpif.h’
INTEGER n(9)
INTEGER isend(2), irecv(2)
DATA n /12, 15, 2, 20, 8, 3, 7, 24, 52/
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
 ista = myrank * 3 + 1
 iend = ista + 2
 imax = -999
 DO i = ista, iend
 IF (n(i) > imax) THEN
 imax = n(i)
 iloc = i
                        ENDIF
 ENDDO
 isend(1) = imax
 isend(2) = iloc
  CALL MPI_REDUCE(isend, irecv, 1, MPI_2INTEGER, MPI_MAXLOC, 0, MPI_COMM_WORLD, ierr)
  IF (myrank == 0) THEN
  PRINT *, ’Max =’, irecv(1), ’Location =’, irecv(2)
                          ENDIF
  CALL MPI_FINALIZE(ierr)
  END
```

```
$ a.out -procs 3
0: Max = 52 Location = 9
```

```
      SUBROUTINE para_range(n1, n2, nprocs, irank, ista, iend)
      iwork = (n2 - n1) / nprocs + 1
      ista = MIN(irank * iwork + n1, n2 + 1)
      iend = MIN(ista + iwork - 1, n2)
      END

PROGRAM main
PARAMETER (n = 1000)
DIMENSION a(n)
DO i = 1, n
a(i) = i
ENDDO
sum = 0.0
DO i = 1, n
sum = sum + a(i)
ENDDO
PRINT *,'sum =',sum
END
```

```
PROGRAM main
INCLUDE ’mpif.h’
PARAMETER (n = 1000)
DIMENSION a(n)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
CALL para_range(1, n, nprocs, myrank, ista, iend)
DO i = ista, iend
a(i) = i
ENDDO
sum = 0.0
DO i = ista, iend
sum = sum + a(i)
ENDDO
CALL MPI_REDUCE(sum, ssum, 1, MPI_REAL, MPI_SUM, 0, MPI_COMM_WORLD, ierr)
sum = ssum
IF (myrank == 0) PRINT *,’sum =’,sum
CALL MPI_FINALIZE(ierr)
END
```

```
DO i = n1, n2
computation
ENDDO

DO i = n1 + myrank, n2, nprocs
computation
ENDDO
```

```
PROGRAM main
INCLUDE ’mpif.h’
PARAMETER (n = 1000)
DIMENSION a(n)
CALL MPI_INIT(ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
DO i = 1 + myrank, n, nprocs
 a(i) = i
ENDDO
sum = 0.0
DO i = 1 + myrank, n, nprocs
sum = sum + a(i)
ENDDO
CALL MPI_REDUCE(sum, ssum, 1, MPI_REAL, MPI_SUM, 0, MPI_COMM_WORLD, ierr)
sum = ssum
PRINT *,’sum =’,sum
CALL MPI_FINALIZE(ierr)
END
```

```
DO i = n1, n2
computation
ENDDO
```

```
DO ii = n1 + myrank * iblock, n2, nprocs * iblock
DO i = ii, MIN(ii + iblock - 1, n2)
computation
ENDDO
ENDDO
```

shrink

FORTRAN 90

```
PROGRAM main
 INCLUDE ’mpif.h’
 PARAMETER (n1 = 1, n2 = 1000)
 REAL, ALLOCATABLE :: a(:)
 CALL MPI_INIT(ierr)
 CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
 CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
 CALL para_range(n1, n2, nprocs, myrank, ista, iend)
 ALLOCATE (a(ista:iend))
 DO i = ista, iend
 a(i) = i
 ENDDO
 sum = 0.0
 DO i = ista, iend
 sum = sum + a(i)
ENDDO
 DEALLOCATE (a)
CALL MPI_REDUCE(sum, ssum, 1, MPI_REAL,MPI_SUM, 0, MPI_COMM_WORLD, ierr)
sum = ssum
PRINT *,’sum =’,sum
CALL MPI_FINALIZE(ierr)
END
```

shrink

FORTRAN 90

```
      PROGRAM main
      implicit none
      real sum1,ssum
      integer i,ista,iend
      integer ierr,n1,n2,nprocs,myrank
      INCLUDE 'mpif.h'
      PARAMETER (n1 = 1, n2 = 1000)
      REAL, ALLOCATABLE :: a(:)

      CALL MPI_INIT(ierr)
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
      CALL para_range(n1, n2, nprocs, myrank, ista, iend)
      ALLOCATE (a(ista:iend))
      DO i = ista, iend
      a(i) = i
      ENDDO
!     sum1 = 0.0
!     DO i = ista, iend
!     sum1 = sum1 + a(i)
!    ENDDO
     sum1=sum(a)
      DEALLOCATE (a)
     CALL MPI_REDUCE(sum1, ssum, 1, MPI_REAL,MPI_SUM, 0, MPI_COMM_WORLD, ierr)
     sum1 = ssum
     PRINT *,'sum1 =',sum1, myrank
     CALL MPI_FINALIZE(ierr)
     END
```

```
      subroutine equal_load(n1,n2,nproc,myid,istart,ifinish)
!     Written by In-Ho Lee, KRISS, September (2006)
      implicit none
      integer nproc,myid,istart,ifinish,n1,n2
      integer iw1,iw2
      iw1=(n2-n1+1)/nproc ; iw2=mod(n2-n1+1,nproc)
      istart=myid*iw1+n1+min(myid,iw2)
      ifinish=istart+iw1-1 ; if(iw2 > myid) ifinish=ifinish+1
!     print*, n1,n2,myid,nproc,istart,ifinish
      if(n2 < istart) ifinish=istart-1
      return
      end
```

```
!234567890
implicit none
include 'mpif.h'
integer, allocatable :: isend(:), irecv(:)
integer, allocatable :: ircnt(:), idisp(:)
integer ierr,nproc,myid
integer i,iscnt
integer ndsize

call MPI_INIT(ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD,nproc,ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD,myid,ierr)
ndsize=10
allocate(isend(ndsize),irecv(nproc*ndsize))
allocate(ircnt(0:nproc-1),idisp(0:nproc-1))
ircnt=ndsize
idisp(0)=0
do i=1,nproc-1
idisp(i)=idisp(i-1)+ircnt(i)
enddo
do i=1,ndsize          ! node specific data with a data-size ndsize
isend(i)=myid+1
enddo
iscnt=ndsize
call MPI_GATHERV(isend, iscnt, MPI_INTEGER, irecv, ircnt, idisp, MPI_INTEGER,0, MPI_COMM_WORLD, ierr)
if(myid == 0)then
print*, 'irecv= ',irecv
endif
deallocate(ircnt,idisp)
deallocate(isend,irecv)
call MPI_FINALIZE(ierr)
stop
end
```

```
irecv= 1 1 1 1 1
1 1 1 1 1 2
2 2 2 2 2 2
2 2 2 3 3 3
3 3 3 3 3 3
3 4 4 4 4 4
4 4 4 4 4
```

```
!234567890
      program integration
      implicit none
      include 'mpif.h'
      integer i,n
      integer myid,nproc,ierr,kount,iroot
      real*8 ff,xx,xsum,pi,hh,xpi
      character*8 fnnd ; character*10 fnnt
      integer itemp,itemq,irate
      ff(xx)= 4.0d0/(1.0d0+xx*xx)
      call MPI_init(ierr)
      call MPI_comm_size(MPI_COMM_WORLD,nproc,ierr)
      call MPI_comm_rank(MPI_COMM_WORLD,myid,ierr)
      if(myid == 0 .and. nproc > 1) print *,  nproc," processes are alive"
      if(myid == 0 .and. nproc ==1) print *,  nproc," process is alive"
      if(myid == 0)then   ! -----[   process id = 0
      call date_and_time(date=fnnd,time=fnnt)
      write(6,'(a10,2x,a8,2x,a10)') 'date,time ', fnnd,fnnt
                endif  ! -----]   process id = 0
      if( myid == 0) then
      write(6,*) 'number of intervals?'
      read(5,*) n
      write(6,*) 'number of intervals:',n
      end if
      iroot=0
      call MPI_bcast(n,1,MPI_INTEGER, iroot, MPI_COMM_WORLD, ierr)
      hh=1.d0/float(n)
      xsum=0.0d0
      do i=myid +1, n, nproc
         xx=(float(i)-0.5d0)*hh
         xsum=xsum+ff(xx)
      end do
      xpi=hh*xsum
      call MPI_reduce(xpi,pi, 1, MPI_DOUBLE_PRECISION, MPI_SUM, 0, MPI_COMM_WORLD,ierr)
      if( myid == 0 )then
      write(6,'(a,f18.8)')  'estimated pi value', pi
      end if
      call MPI_finalize(ierr)
      end program integration
```

```
      program main
      include "mpif.h"
      double precision  PI25DT
      parameter       (PI25DT = 3.14159265358979323846264338327950288419716939937510d0)
      double precision  mypi, pi, h, sum, x, f, a
      double precision starttime, endtime
      integer n, myid, numprocs, i, ierr
c                             function to integrate
      f(a) = 4.d0 / (1.d0 + a*a)

      call MPI_INIT(ierr)
      call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
      call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

10    if ( myid .eq. 0 ) then
        print *, 'Enter the number of intervals: (0 quits) '
        read(*,*) n
      endif
c                             broadcast n
      starttime = MPI_WTIME()
      call MPI_BCAST(n,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierr)
c                             check for quit signal
      if ( n .le. 0 ) goto 30
c                             calculate the interval size
      h = 1.0d0/n
      sum  = 0.0d0
      do 20 i = myid+1, n, numprocs
        x = h * (dble(i) - 0.5d0)
        sum = sum + f(x)
20    continue
      mypi = h * sum
c                             collect all the partial sums
      call MPI_REDUCE(mypi,pi,1,MPI_DOUBLE_PRECISION,MPI_SUM,0,
     &                MPI_COMM_WORLD,ierr)
c                             node 0 prints the answer.
      endtime = MPI_WTIME()
      if (myid .eq. 0) then
        print *, 'pi is ', pi, ' Error is', abs(pi - PI25DT)
        print *, 'time is ', endtime-starttime, ' seconds'
      endif
      goto 10
30    call MPI_FINALIZE(ierr)
      stop
      end
```

$$\int_0^1 \frac{4}{1+x^2} dx = \pi$$

```
SUBROUTINE PAR_BLAS2(m, n, a, b, c, comm)
REAL a(m), b(m,n) ! local slice of array
REAL c(n) !result
REAL sum(n)
INTEGER n, comm, i, j, ierr

! local sum
DO j= 1, n
sum(j) = 0.0
DO i = 1, m
sum(j) = sum(j) + a(i)*b(i,j)
END DO
END DO

! global sum
CALL MPI_ALLREDUCE(sum, c, n, MPI_REAL, MPI_SUM, comm, ierr)

! return result at all nodes
RETURN
END
```

dot_product: compute a scalar product

```
      subroutine dot_product(global,x,y,n)
      implicit none
      include "mpif.h"
      integer n,i,ierr
      double precision global,x(n),y(n)
      double precision tmp,local
      local = 0.0d0
      global = 0.0d0
     do i=1,n
     local = local + x(i)*y(i)
    enddo
    call MPI_ALLREDUCE(local,tmp,1,MPI_DOUBLE_PRECISION,
   >  MPI_SUM, MPI_COMM_WORLD, ierr)
    global = tmp
    return
    end
```

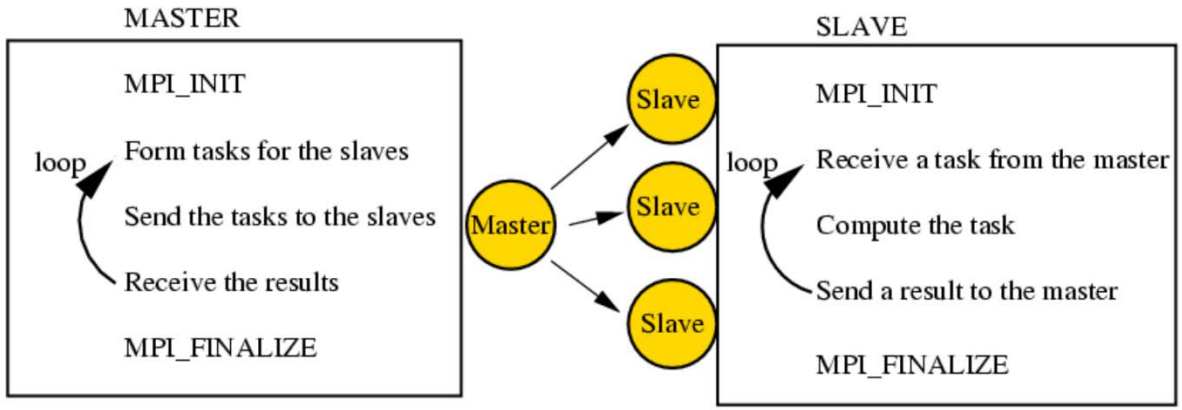
```
SUBROUTINE PAR_BLAS2(m, n, a, b, c, comm)
REAL a(m), b(m,n) ! local slice of array
REAL c(n) ! result
REAL sum(n)
INTEGER n, comm, i, j, ierr

! local sum
DO j= 1, n
sum(j) = 0.0
DO i = 1, m
sum(j) = sum(j) + a(i)*b(i,j)
END DO
END DO

! global sum
CALL MPI_REDUCE(sum, c, n, MPI_REAL, MPI_SUM,0, comm, ierr)

! return result at node zero (and garbage at the other nodes)
RETURN
END
```

```
!234567890
      program equal_load_sum
      implicit none
      include 'mpif.h'
      integer nn
      real*8, allocatable :: aa(:)
      integer nproc,myid,ierr,istart,ifinish
      integer i
      real*8 xsum,xxsum

      nn=10000

      call MPI_INIT(ierr)
      call MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ierr)
      call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)

      call equal_load(1,nn,nproc,myid,istart,ifinish)

      allocate(aa(istart:ifinish)) ! 단순한 인덱스의 분할 뿐만아니라 메모리의 분할이 이루어지고 있다. 노드별로

      do i=istart,ifinish
      aa(i)=float(i)
      enddo

      xsum=0.0d0
      do i=istart,ifinish
      xsum=xsum+aa(i)
      enddo

     call MPI_REDUCE(xsum,xxsum,1,MPI_DOUBLE_PRECISION,MPI_SUM,0,MPI_COMM_WORLD,ierr)
     xsum=xxsum

     if(myid == 0)then
     write(6,*) xsum,' xsum'
     endif

    deallocate(aa)
     call MPI_FINALIZE(ierr)
     end program equal_load_sum
```

수행해야 할 일들을 나누고 결과물을 받아오는 방식.

```
      allocate(exqq(natom_ac,3,0:np_ac), exforce(natom_ac,3,0:np_ac), exvofqj(0:np_ac))
      if(myid == 0)then    ! -----{ PROCESS ID = 0
      exqq=qq
                    endif   ! -----} PROCESS ID = 0
      iroot=0 ; kount=3*natom_ac*(np_ac+1)
      call MPI_BCAST(exqq, kount,MPI_REAL8, iroot,MPI_COMM_WORLD,ierr)
      n1=0 ; n2=np_ac
      call equal_load(n1,n2,nproc,myid,jstart,jfinish)
!
      exforce=0.0d0 ; exvofqj=0.0d0
      do j=jstart,jfinish
      call xtinker(exqq(1,1,j),exforce(1,1,j),exvofqj(j),natom_ac,isequence,isymbol,iattyp,ii12)
      enddo
      iroot=0 ; kount=3*natom_ac*(np_ac+1)
      call MPI_REDUCE(exforce,force_ac,kount,MPI_DOUBLE_PRECISION,MPI_SUM,iroot,MPI_COMM_WORLD,ierr)
      iroot=0 ; kount=(np_ac+1)
      call MPI_REDUCE(exvofqj,vofqj,kount,MPI_DOUBLE_PRECISION,MPI_SUM,iroot,MPI_COMM_WORLD,ierr)
!
      deallocate(exforce, exvofqj, exqq)
```

```
real*8 aa(n,n), bb(n,n)

 do j=1,n
 do i=1,n
 aa(i,j)=0.d0
 bb(i,j)=0.0d0
 enddo
 enddo

 do j=1,n
 do i=1+myid,n, nproc
 aa(i,j)=...
 enddo
 enddo

 call MPI_REDUCE(aa,bb,n*n, MPI_DOUBLE_PRECISION, MPI_SUM, 0, MPI_COMM_WORLD, ierr)
```



참조

http://incredible.egloos.com/3880690

MPI-IO: The "Big Six"

While there are a large number of MPI-IO calls, most basic I/O can be handled with just six routines:

- MPI_File_open() – associate a file with a file handle.
- MPI_File_seek() – move the current file position to a given location in the file.
- MPI_File_read() – read some fixed amount of data out of the file beginning at the current file position.
- MPI_File_write() – write some fixed amount of data into the file beginning at the current file position.
- MPI_File_sync() – flush any caches associated with the file handle.
- MPI_File_close() – close the file handle.

Most of the other MPI-IO routines are variations or optimizations on these basic calls.

MPI_File_open()

• C syntax:
int MPI_File_open(MPI_Comm comm, char *filename, int amode, MPI_Info info, MPI_File *fh);
• Fortran syntax:
subroutine MPI_File_open(icomm, filename, iamode, info, ifh, ierr)
character*(*) filename
integer icomm, iamode, info, ifh, ierr
• ifh is the file handle, which will be used by all other MPI-IO routines to refer to the file. In C, this must be passed as an address (i.e. &fh).
• filename is the name of the file to open. It may use a relative or absolute path. It may also contain a file system identifier prefix, e.g.:
– ufs: -- normal UNIX-style file system
– nfs: -- NFS file system
– pvfs: -- PVFS file system

MPI_File_open() (con't)

• amode is the access mode to open the file with. It should be a bitwise ORing (C) or sum (Fortran) of the following:
– MPI_MODE_RDONLY (read-only)
– MPI_MODE_RDWR (read/write)
– MPI_MODE_WRONLY (write-only)
– MPI_MODE_CREATE (create file if it doesn't exist)
– MPI_MODE_EXCL (error if file does already exist)
– MPI_MODE_DELETE_ON_CLOSE (delete file when closed)
– MPI_MODE_UNIQUE_OPEN (file cannot be opened by other processes)
– MPI_MODE_SEQUENTIAL (file can only be accessed sequentially)
– MPI_MODE_APPEND (set initial file position to the end of the file)
• info is a set of file hints, the creation of which will be discussed later.
When in doubt, use MPI_INFO_NULL.

MPI_File_open mode	Description
MPI_MODE_RDONLY	read only
MPI_MODE_WRONLY	write only
MPI_MODE_RDWR	read and write
MPI_MODE_CREATE	create file if it doesn't exist

MPI_File_seek()

• C syntax:

int MPI_File_seek(MPI_File fh, MPI_Offset offset, int whence);

• Fortran syntax:

subroutine MPI_File_seek(ifh, ioffset, iwhence, ierr)

integer ifh, ioffset, iwhence, ierr

• offset determines how far from the current file position to move the current file position; this can be negative, although seeking beyond the beginning of the file (or the current view if one is in use) is an error.

• whence determines to where the seek offset is relative:

– MPI_SEEK_SET (relative to the beginning of the file)

– MPI_SEEK_CUR (relative to the current file position)

– MPI_SEEK_END (relative to the end of the file)

• Seeks are done in terms of the current record type (MPI_BYTE by default, although this can be changed by setting a file view).

MPI_File_read()

• C syntax:

int MPI_File_read(MPI_File fh, void *buf, int count,MPI_Datatype type, MPI_Status *status);

• Fortran syntax:

subroutine MPI_File_read(ifh, buf, icount, itype,istatus, ierr)

<type> BUF(*)

integer ifh, icount, itype, istatus(MPI_STATUS_SIZE),ierr

• This reads count values of datatype type from the file into buf. buf must be at least as big as count*sizeof(type).

• istatus can be used to query for information such as how many bytes were actually read.

MPI_File_write()

• C syntax:

int MPI_File_write(MPI_File fh, void *buf, int count, MPI_Datatype type, MPI_Status *status);

• Fortran syntax:

subroutine MPI_File_write(ifh, buf, icount, itype,istatus, ierr)

<type> BUF(*)

integer ifh, icount, itype, istatus(MPI_STATUS_SIZE), ierr

• This reads count values of datatype type from buf into the file. buf must be at least as big as count*sizeof(type).

• istatus can be used to query for information such as how many bytes were actually written.

MPI_File_sync()

• C syntax:

```
int MPI_File_sync(MPI_File fh);
```

• Fortran syntax:

```
subroutine MPI_File_sync(ifh, ierr)
integer ifh, ierr
```

• Forces any caches associated with a file handle to be flushed to disk; maybe be very expensive for large files on slow file systems.

• Provides a way to force written data to be committed to disk.

• Collective; must be called by all processes.

MPI_File_close()

• C syntax:

```
int MPI_File_close(MPI_File *fh);
```

• Fortran syntax:

```
subroutine MPI_File_close(ifh, ierr)
integer ifh, ierr
```

• This closes access to the file associated with the file handle ifh.

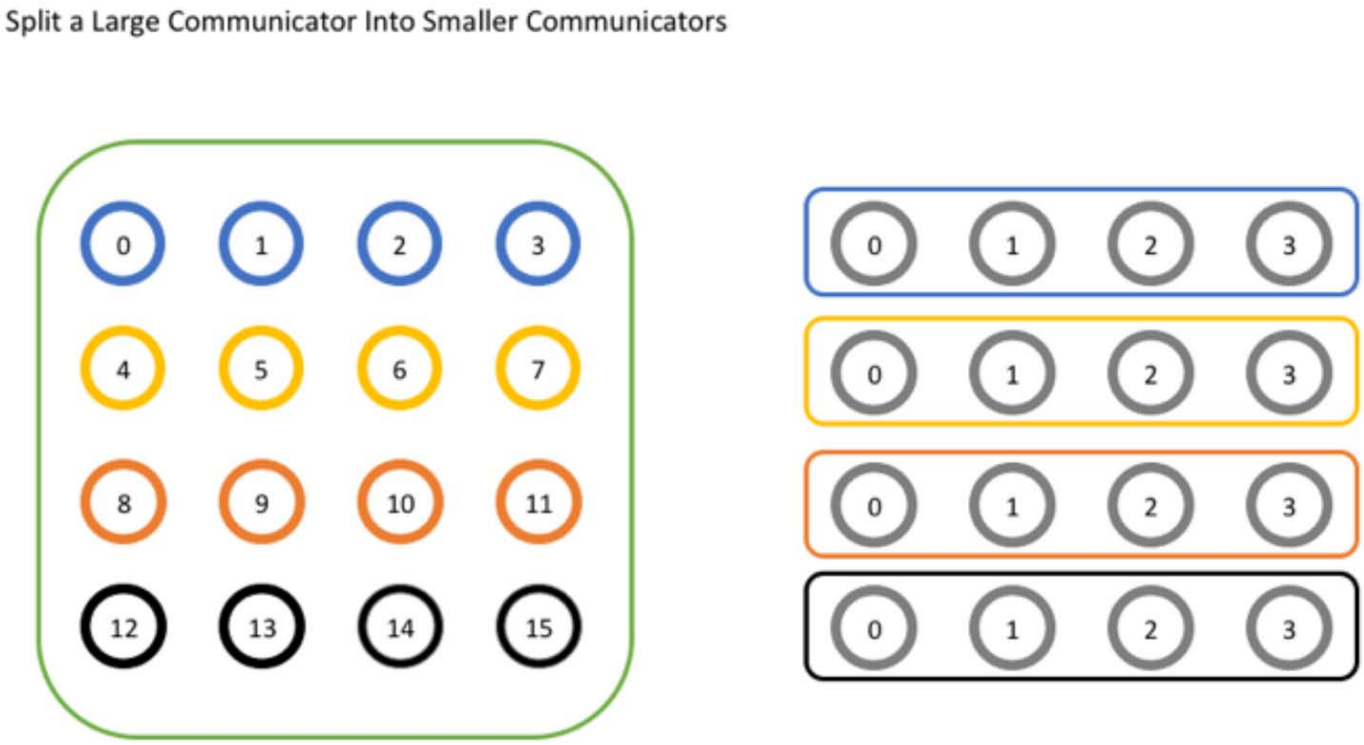
MPI I/O example

```
! Basic MPI-I/O
call MPI_BARRIER(MPI_COMM_WORLD,ierr)
tstart=MPI_WTIME()
call MPI_FILE_OPEN(MPI_COMM_WORLD,'u.dat',MPI_MODE_WRONLY,
MPI_INFO_NULL,outfile,ierr)
if (jstart.eq.2)  jstart=1
if (jend.eq.(jmax-1))   jend=jmax
call MPI_FILE_SEEK(outfile,(jstart-1)*imax*8,MPI_SEEK_SET,ierr)
do j=jstart,jend
call MPI_FILE_WRITE(outfile,u(1,j),imax,MPI_REAL8,istatus, ierr)
enddo
call MPI_FILE_SYNC(outfile,ierr)
call MPI_FILE_CLOSE(outfile,ierr)
call MPI_BARRIER(MPI_COMM_WORLD,ierr)
tend=MPI_WTIME()
if (rank.eq.0) then
write(*,*) 'Using basic MPI-I/O‘
write(*,*) 'Wrote ',8*imax*jmax,' bytes in ',tend-tstart, ' seconds.'
write(*,*) 'Transfer rate = ', (8*imax*jmax)/(tend-tstart)/(1024.**2), ' MB/s'
                endif
```

write into a single file, in Fortran

```
! example of parallel MPI write into a single file, in Fortran
        PROGRAM main
        include 'mpif.h'

        integer ierr, i, myrank, BUFSIZE, thefile
        parameter (BUFSIZE=100)
        integer buf(BUFSIZE)
        integer(kind=MPI_OFFSET_KIND) disp

        call MPI_INIT(ierr)
        call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)

       do i = 0, BUFSIZE
        buf(i) = myrank * BUFSIZE + i
      enddo
    call MPI_FILE_OPEN(MPI_COMM_WORLD, 'testfile', MPI_MODE_WRONLY + MPI_MODE_CREATE,  MPI_INFO_NULL, thefile, ierr)
  ! assume 4-byte integers
    disp = myrank * BUFSIZE * 4
    call MPI_FILE_SET_VIEW(thefile, disp, MPI_INTEGER, MPI_INTEGER, 'native', MPI_INFO_NULL, ierr)
    call MPI_FILE_WRITE(thefile, buf, BUFSIZE, MPI_INTEGER,  MPI_STATUS_IGNORE, ierr)
    call MPI_FILE_CLOSE(thefile, ierr)
    call MPI_FINALIZE(ierr)

    END PROGRAM main
```

Split a large communicator



Split a large communicator

```
                                        // Get the rank and size in the original communicator
int world_rank, world_size;
MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);
MPI_Comm_size(MPI_COMM_WORLD, &world_size);

int color = world_rank / 4;             // Determine color based on row

                                        // Split the communicator based on the color and use the
// original rank for ordering
MPI_Comm row_comm;
MPI_Comm_split(MPI_COMM_WORLD, color, world_rank, &row_comm);

int row_rank, row_size;
MPI_Comm_rank(row_comm, &row_rank);
MPI_Comm_size(row_comm, &row_size);

printf("WORLD RANK/SIZE: %d/%d \t ROW RANK/SIZE: %d/%d\n",world_rank, world_size, row_rank, row_size);

MPI_Comm_free(&row_comm);
```

Split a large communicator

```
                                                    // Get the rank and size in the original communicator
int world_rank, world_size;
MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);
MPI_Comm_size(MPI_COMM_WORLD, &world_size);
                                                    // Get the group of processes in MPI_COMM_WORLD
MPI_Group world_group;
MPI_Comm_group(MPI_COMM_WORLD, &world_group);

int n = 7;
const int ranks[7] = {1, 2, 3, 5, 7, 11, 13};
                                                  // Construct a group containing all of the prime ranks in world_group
MPI_Group prime_group;
MPI_Group_incl(world_group, 7, ranks, &prime_group);
                                                    // Create a new communicator based on the group
MPI_Comm prime_comm;
MPI_Comm_create_group(MPI_COMM_WORLD, prime_group, 0, &prime_comm);
int prime_rank = -1, prime_size = -1;
                                                    // If this rank isn't in the new communicator, it will be
                                                  // MPI_COMM_NULL. Using MPI_COMM_NULL for MPI_Comm_rank or
                                                  // MPI_Comm_size is erroneous
if (MPI_COMM_NULL != prime_comm) {
   MPI_Comm_rank(prime_comm, &prime_rank);
   MPI_Comm_size(prime_comm, &prime_size);
}
printf("WORLD RANK/SIZE: %d/%d \t PRIME RANK/SIZE: %d/%d\n",world_rank, world_size, prime_rank, prime_size);
MPI_Group_free(&world_group);
MPI_Group_free(&prime_group);
MPI_Comm_free(&prime_comm);
```

MPI Implementations

- Most parallel machine vendors have optimized versions
- Others:
  - http://www.mpi.nd.edu/MPI/Mpich
  - http://www-unix.mcs.anl.gov/mpi/mpich/
  - indexold.html
  - GLOBUS:
  - http://www.globus.org/mpi/
  - http://exodus.physics.ucla.edu/appleseed/

추가 참고 문헌

"parallel computing" on the search engine

https://computing.llnl.gov/tutorials/mpi/ http://condor.cc.ku.edu/~grobe/docs/intro-MPI.shtml

http://www-unix.mcs.anl.gov/mpi/

http://www.llnl.gov/computing/tutorials/workshops/workshop/parallel_comp/MAIN.html#Whatis

http://www.nas.nasa.gov/Groups/SciCon/Tutorials/MPIintro/toc.html

http://www-unix.mcs.anl.gov/mpi/tutorial/mpibasics/

http://www-unix.mcs.anl.gov/mpi/usingmpi/examples/main.htm

http://people.sc.fsu.edu/~jburkardt/f_src/f_src.html http://condor.cc.ku.edu/~grobe/docs/intro-MPI-C.shtml

http://people.sc.fsu.edu/~jburkardt/index.html

http://www.mcs.anl.gov/research/projects/mpi/tutorial/

http://www.bu.edu/tech/support/research/training-consulting/online-tutorials/mpi/

http://condor.cc.ku.edu/~grobe/docs/intro-MPI.shtml

Summary

- 새로운 패러다임 (병렬계산,성능/가격)
- 통신의 중요성 (latency + bandwidth)
- MPI 프로그램의 기본 이해 (SPMD)
- 실제문제 재설계 필요
- *점진적 병렬화 작업* (serial → parallel)
- 서로 다른 방식으로의 병렬화 모색
- 실질적 시간 절약 효과를 검증 해야 함