

PARALLEL PROGRAMMING USING MPI – SPEEDUP AND MEMORY

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BEFORE WE BEGIN

□ A FEW THINGS ...

- *This is more of an introductory workshop on MPI*
- *No prior background on MPI is needed*
- *Some basic background on sequential programming would be assumed.*
- *Examples will be shown in FORTRAN. The concepts are equally valid for C.*
- *The codes for the examples are written by the speaker himself. Please be 'aggressive' to point out any 'shabby' coding habits that you come across.*
- *The remarks and conclusions made hereafter are solely the speaker's personal opinions. The speaker does not represent any of the official implementers of MPI.*



OUTLINE

- ❖ **PARALLEL PROGRAMMING**
- ❖ **GETTING STARTED WITH MPI**
- ❖ **SPEEDUP**
- ❖ **MPI SHARED MEMORY**
- ❖ **SUMMARY**



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WHY PARALLEL PROGRAMMING?

❑ THE BIG PICTURE

Growth of processor clock-rate is slowing down – the main reasons being :

- size limits of the processor components
- higher power consumption at higher clock rates.

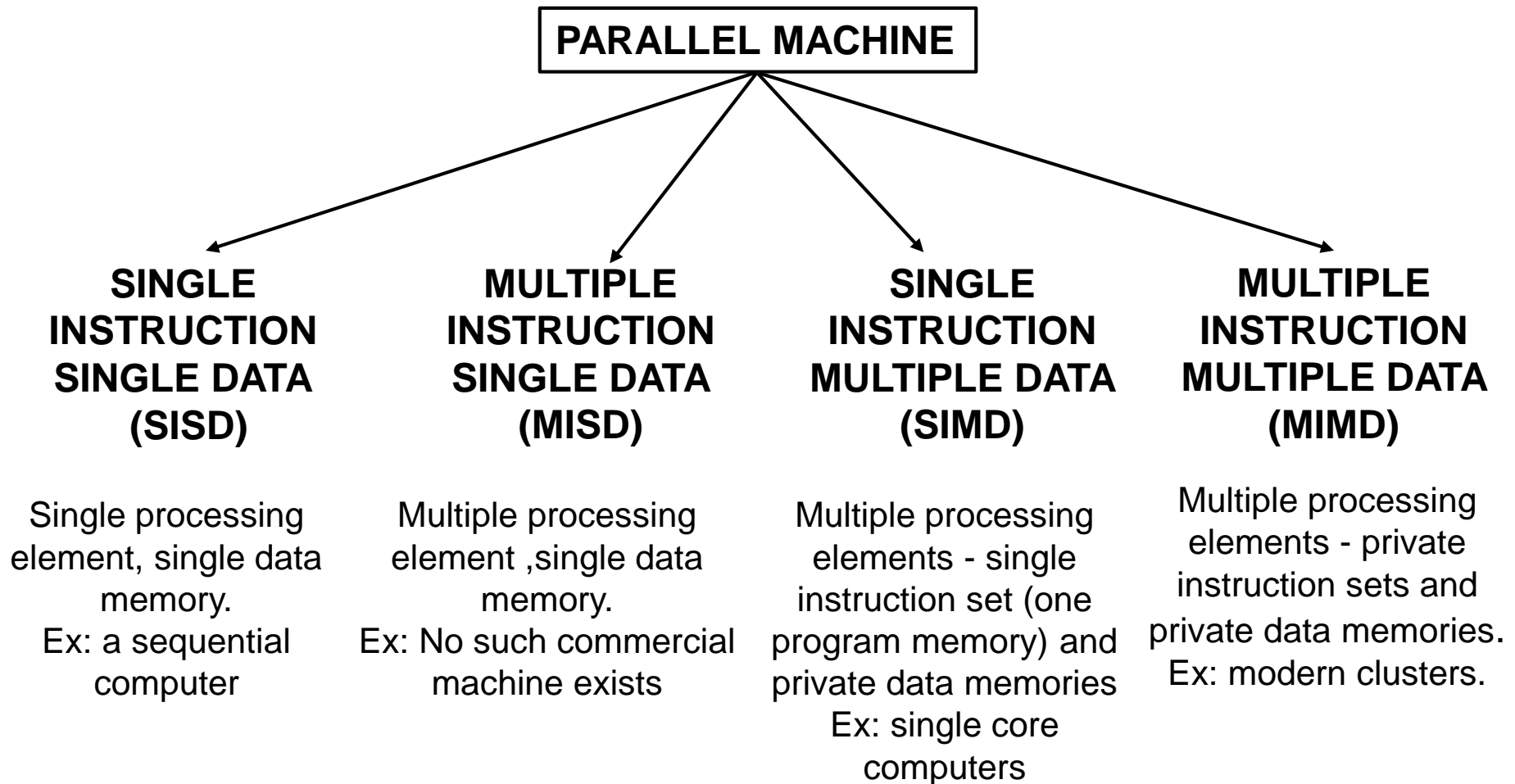
What does that mean to us?

- **Slow execution of codes and more time to reach solution**
- **Limit on available memory**

But that's limited by processor manufacturing. What do we programmers do?

- **Simple, use multiple processors**

□ FLYNN'S TAXONOMY





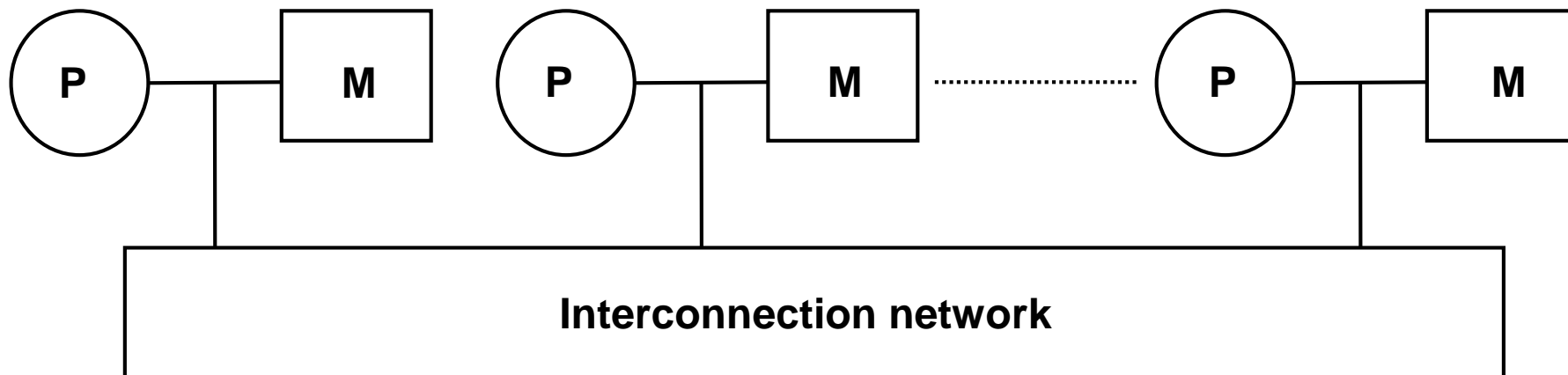
OUTLINE

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- ❖ MPI SHARED MEMORY
- ❖ SUMMARY

WHAT IS MPI?

W.P. Petersen and P. Arbenz, Introduction to Parallel Programming
Oxford University Press, 2004

❑ An MIMD system



- Message Passing Interface (MPI) establishes data access between nodes
- MPI is a standard message passing system on both shared and distributed systems
- A communicator group of processes perform a certain task
- Arbitrary master-slave relation

❑ MPI IMPLEMENTATIONS

MPICH (<http://www.mpich.org/>), Argonne National Laboratory

MVAPICH (<http://mvapich.cse.ohio-state.edu/>), Ohio State University

OpenMPI (<https://www.open-mpi.org/>), U of Tennessee, Los Alamos National Laboratory, Indiana University, and U of Stuttgart

INTEL MPI (<https://software.intel.com/en-us/intel-mpi-library>), Intel

❑ MPI ON CCR AT UB

module avail intel-mpi
module avail mvapich2
module avail openmpi



Different modules available under each of these.
Try to use the latest ones to get new features.

- Some implementations might have hardware interconnect specific modules.
Load the one appropriate for you.

FIRST PROGRAM

□ HELLO WORLD WITH MPI

We want each proc to print its id

```
|-----|
PROGRAM hello_world
|-----|
USE mpi
|
IMPLICIT NONE
|
INTEGER      :: id, ierr, p
|
CALL mpi_init(ierr)
CALL mpi_comm_rank (MPI_COMM_WORLD, id, ierr)
CALL mpi_comm_size (MPI_COMM_WORLD, p, ierr)
|
PRINT '(" Total number of procs", i3, " and my id is ", i3)',p, id
|
CALL mpi_finalize(ierr)
|
END PROGRAM hello_world
```

Initializes the MPI environment, ierr is almost ubiquitous in MPI FORTRAN, denotes the error code incase of an error

Gives id of a proc

Gives number of procs

Kills MPI

Global Communicator, a predefined constant

BUILDING YOUR CODE WITH MPI

BUILD



```
#!/bin/bash

module load intel/15.0
module load intel-mpi/5.0.2
which mpiifort
export MPIF90=mpiifort
$MPIF90 -traceback -g hello_world.f90 -o hello.x
```

LAUNCH



```
# count the number of processors
np=`srun hostname -s | wc -l`
export I_MPI_PMI_LIBRARY=/usr/lib64/libpmi.so
srun -n $np hello.x
```

Integrates Intel-MPI to SLURM

OUTPUT



```
Total number of procs 8 and my id is 0
Total number of procs 8 and my id is 1
Total number of procs 8 and my id is 2
Total number of procs 8 and my id is 3
Total number of procs 8 and my id is 4
Total number of procs 8 and my id is 5
Total number of procs 8 and my id is 6
Total number of procs 8 and my id is 7
```

BASIC MPI COMMANDS

We will only discuss a partial list of commands that are commonly used.

❑ ENVIRONMENT MANAGEMENT

4 such routines are used and explained in the hello_world program (slide 10)

❑ POINT-TO-POINT COMMUNICATIONS

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

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

- **buf** is the data sent (received).
- **count** is the length of the data (like number of elements in an array)
- **dest (source)** is which proc id the data is going to (coming from)
- **tag** is an unique identification to a message. send tag = receive tag
(wild card MPI_ANY_TAG will receive any message)

Petersen and Arbenz, IPP, Oxford University Press, 2004

BASIC MPI COMMANDS

□ EXAMPLE – send and receive

We want to send the proc ids of each proc to all other procs by point-to-point communication

```

DO iproc = 1, np
!
src = iproc - 1
!
DO jproc = 1, np
!
dest = jproc - 1
!
IF (p_id .EQ. src .AND. .NOT. (dest.EQ.src) ) &
CALL MPI_SEND (p_id, 1, MPI_INTEGER, dest , 10, MPI_COMM_WORLD, ierr)
!
IF (p_id .EQ. dest .AND. .NOT. (dest.EQ.src) ) THEN
CALL MPI_RECV (p_id_, 1, MPI_INTEGER, src , 10, MPI_COMM_WORLD, MPI_STATUS_IGNORE, ierr)
PRINT '( " I am proc", i3, " and my buddy is proc", i3 )', p_id, p_id_
ENDIF
!
CALL MPI_BARRIER(MPI_COMM_WORLD, ierr)
!
ENDDO
!
ENDDO
  
```

src sends its p_id to dest
p_id is the id of the current proc

dest receives it
note both tags are equal
p_id_ is the id of the sending proc

Will come to this in next slide

Total number of procs is 2

OUTPUT ➡

```

I am proc 0 and my buddy is proc 1
I am proc 1 and my buddy is proc 0
  
```

BASIC MPI COMMANDS

❑ COLLECTIVE COMMUNICATIONS – *broadcast, barrier, and reduction*

MPI_BARRIER (comm, ierr)

Petersen and Arbenz, IPP, Oxford University Press, 2004

- Each proc in **comm** waits until all of them reach at this step

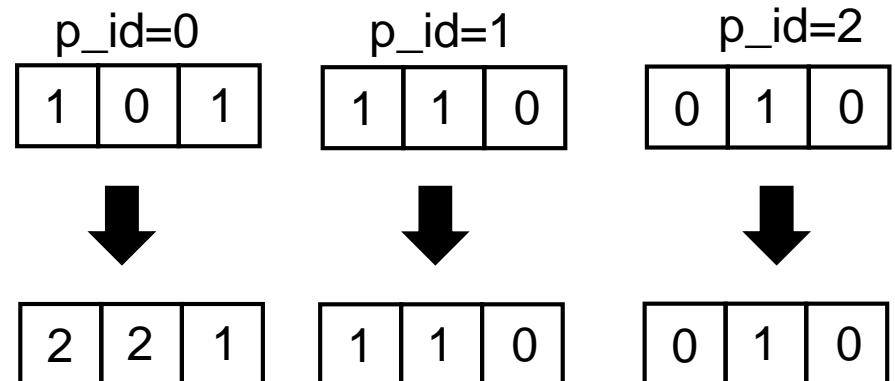
MPI_BCAST (data, count, datatype, root, comm, ierr)

- Proc **root** spreads **data** of length **count** to all other procs in **comm**.

MPI_REDUCE (segment, result, count, datatype, operator, root, comm, ierr)

- Proc dependent **segments** are merged as **result** in **root**. The merging is defined by **operator**.

MPI_REDUCE
(with operator = MPI_SUM and root=0)



BASIC MPI COMMANDS

□ EXAMPLE – broadcast and barrier

We want one proc to read input and broadcast among others

```
! ----- Read input arguments -----
! --- Only one proc reads and then bcasts to others -----
!
```

```
IF (p_id.EQ.master) THEN
```



Only p_id = master does the i/o job

```
DO iiarg = 1, iargc()
```

```
!
```

```
CALL getarg( iiarg, inp_string(iiarg) )
```

```
!
```

```
ENDDO
```

```
READ ( inp_string(1), *) flag
```

```
READ ( inp_string(2), *) m
```

```
READ ( inp_string(3), *) n
```

```
!
```

```
ENDIF
```

```
!
```

```
CALL mpi_barrier (MPI_COMM_WORLD, ierr)
```

```
CALL mpi_bcast(m,1,MPI_INTEGER,master,MPI_COMM_WORLD,ierr)
```

```
CALL mpi_bcast(n,1,MPI_INTEGER,master,MPI_COMM_WORLD,ierr)
```

```
CALL mpi_bcast(flag,10,MPI_CHARACTER,master,MPI_COMM_WORLD,ierr)
```

Other procs wait until master is done



Input data is broadcasted to other procs

BASIC MPI COMMANDS

□ EXAMPLE – reduction

We want to compute $\{c\}_{n \times 1} = [A]_{n \times m} \{b\}_{m \times 1}$

```

! ----- Split sample among procs -----
!
n_per_proc = n / np
rest = MOD ( n , np)
IF (p_id .LE. (rest - 1)) n_per_proc = n_per_proc + 1
!
lower_bound = n_per_proc * p_id + 1
IF (p_id .GE. rest) lower_bound = (n_per_proc + 1) * rest + n_per_proc * (p_id - rest) + 1
upper_bound = lower_bound + n_per_proc - 1
.....
.....

! ----- Compute the proc wise split parts and then reduce to a single proc -----
!
DO i = lower_bound, upper_bound
!
  DO j = 1, m
    c(i) = c(i) + A(i,j)*b(j)
  !
!
  ENDDO
!
ENDDO
!
CALL mpi_barrier (MPI_COMM_WORLD, ierr)
CALL mpi_reduce (c,c_tot,n,MPI_FLOAT,MPI_SUM,master,MPI_COMM_WORLD,ierr)

```

n is split among np . Each proc gets n_per_proc

when $\text{mod}(n, np) \neq 0$

index bounds on each proc

Each proc computes its own share

Total $\{c\}_{n \times 1}$ reduced to master

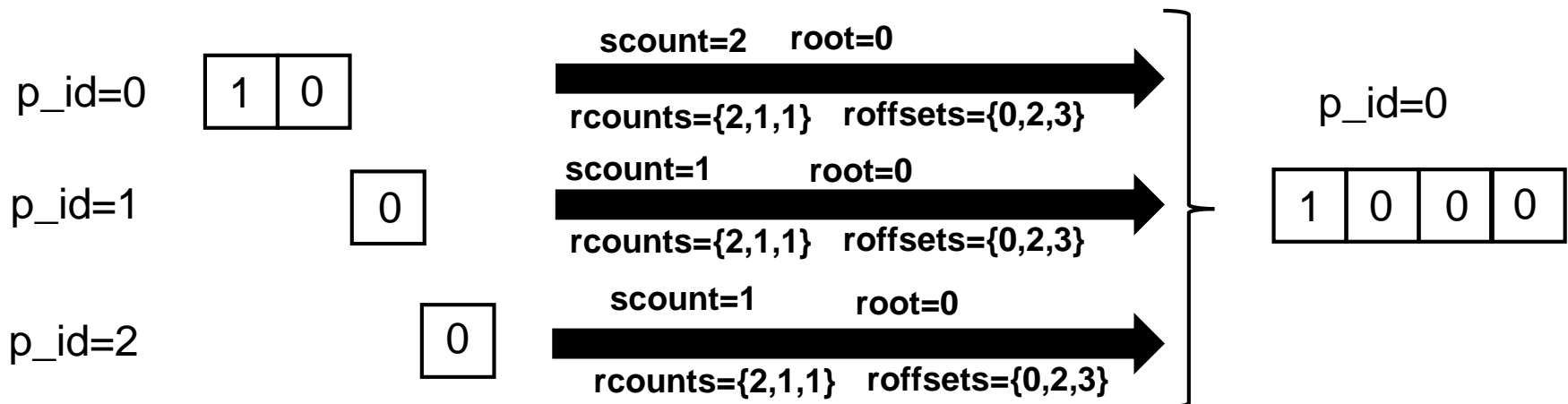
BASIC MPI COMMANDS

❑ COLLECTIVE COMMUNICATIONS – *scatter(v) and gather(v)*

- **MPI_SCATTER (MPI_GATHER)** – distribute (assemble) data segments
- **MPI_SCATTERV (MPI_GATHERV)** – additional features to non-uniformly distribute (assemble) data segments.
- We discuss the latter ones as that would clarify the former ones too.

Petersen and Arbenz, IPP, Oxford University Press, 2004

**MPI_GATHERV (segment, scount, stype,
result, rcounts, roffsets, rtype, root, comm, ierr)**



BASIC MPI COMMANDS

□ EXAMPLE – *gatherv*

Again we want to compute $\{c\}_{n \times 1} = [A]_{n \times m} \{b\}_{m \times 1}$

```

DO i = 1, n_per_proc
  !
  DO j = 1, m
    !
    c(i) = c(i) + A(i,j)*b(j)
    !
  ENDDO
  !
ENDDO
  !

```

Each proc computes its share.

However, note that the size of the vector c in each proc is n_per_proc unlike the reduction case where it was n . Similar argument is valid for the matrix A

```

.....
counts(:) = 0
offsets(:) = 0
counts(p_id+1) = n_per_proc
offsets(p_id+1) = lower_bnd - 1
.....

```

Each proc gets its own send counts and offsets

counts and offsets are merged in arrays using
allreduce (all procs get the merged result)

```

CALL mpi_barrier(MPI_COMM_WORLD, ierr)
CALL mpi_allreduce(counts, all_counts, np, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD, ierr)
CALL mpi_allreduce(offsets, all_offsets, np, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD, ierr)
!
CALL mpi_gather(c, n_per_proc, MPI_FLOAT, c_tot, all_counts, all_offsets, MPI_FLOAT, master, &
               MPI_COMM_WORLD, ierr)

```

Segments of c are gathered in c_tot

MPI DATATYPES

□ COMMONLY USED ELEMENTARY MPI FORTRAN DATATYPES

MPI TYPE	FORTRAN TYPE
MPI_INTEGER	INTEGER(KIND=4)
MPI_INTEGER8	INTEGER(KIND=8)
MPI_FLOAT	REAL (KIND=4)
MPI_DOUBLE	REAL (KIND=8)
MPI_COMPLEX	COMPLEX
MPI_LOGICAL	LOGICAL
MPI_CHARACTER	CHARACTER(LEN=1)

MPI 3.0 Standard <http://mpi-forum.org/docs/mpi-3.0/mpi30-report.pdf>



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RULE OF THE GAME

T. Rauber and G. Runger, Parallel Programming, Springer 2013

□ AMDAHL'S LAW

$$S_p(n) = \frac{1}{f + \frac{1-f}{p}}$$

- $S_p(n)$ is the limit in actual speedup of the entire code of a given size n
- p is the speed up of the code that benefits from the increase in resources.
- f is the fraction of the total execution time taken by the sequential part of the code

Take home message – *Overall speedup is limited by the percentage of the sequential part of the code*

SPEEDUP – EXAMPLE

❑ **Goal** – Improve scalability/speedup through optimizing code.

❑ **Task** – Compute the value of π stochastically.

❑ **Method** –

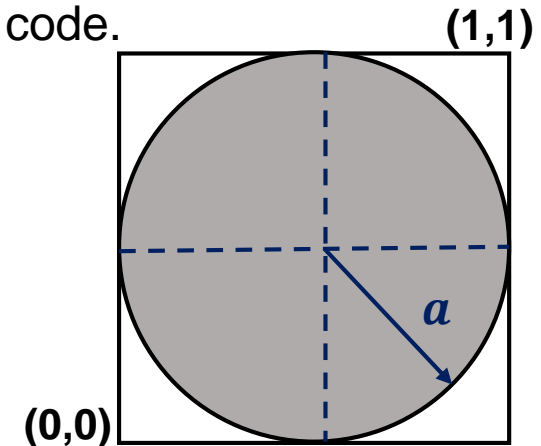
➤ Generate random points (x, y) inside an unit square.

➤ Count the fraction of them falling inside an unit circle.

➤ $\pi = 4 \times \frac{\text{Points inside unit circle}}{\text{Total number of points}}$

➤ This is referred to as the dartboard algorithm [Message Passing Interface, B. Barney, LLNL]

✓ ***We would compute this in parallel using MPI in different ways and compare the speedup and accuracy of the calculation.***



Square area = $4a^2$

Circle area = πa^2

SPEEDUP – EXAMPLE

□ SEQUENTIAL VERSION

```

c_ser = 0
DO i = 1,n
    !
    CALL RANDOM_NUMBER(r1)
    CALL RANDOM_NUMBER(r2)
    !
    a = (r1*r1 + r2*r2)
    IF(a.LT.(1.0)) c_ser = c_ser + 1
    !
END DO
!
PRINT'("Serially calculated Pi  = ",f16.10)',4.0D0*float(c_ser)/float(n)

```

In-built pseudo random number generator (RNG)
with a period of $2^{1024} - 1$ (<https://gcc.gnu.org/>)
Based on XORshift logic.

Output 3.1400

✓ A higher value of the sample size (n) will produce more accurate result

SPEEDUP – EXAMPLE

□ PARALLEL VERSION 1

```
DO i = 1, n_per_proc
  !
  CALL RANDOM_NUMBER(r1)
  CALL RANDOM_NUMBER(r2)
  !
  a = r1*r1 + r2*r2
  IF(a.LT.(1.0)) c_par = c_par + 1
  !
END DO
!
CALL mpi_barrier (MPI_COMM_WORLD, ierr)
CALL mpi_allreduce (c_par,c_par_tot,1,MPI_INTEGER,MPI_SUM,MPI_COMM_WORLD,ierr)
```

Same program run on split samples and reduced at the end

Each proc gets n_per_proc number of samples

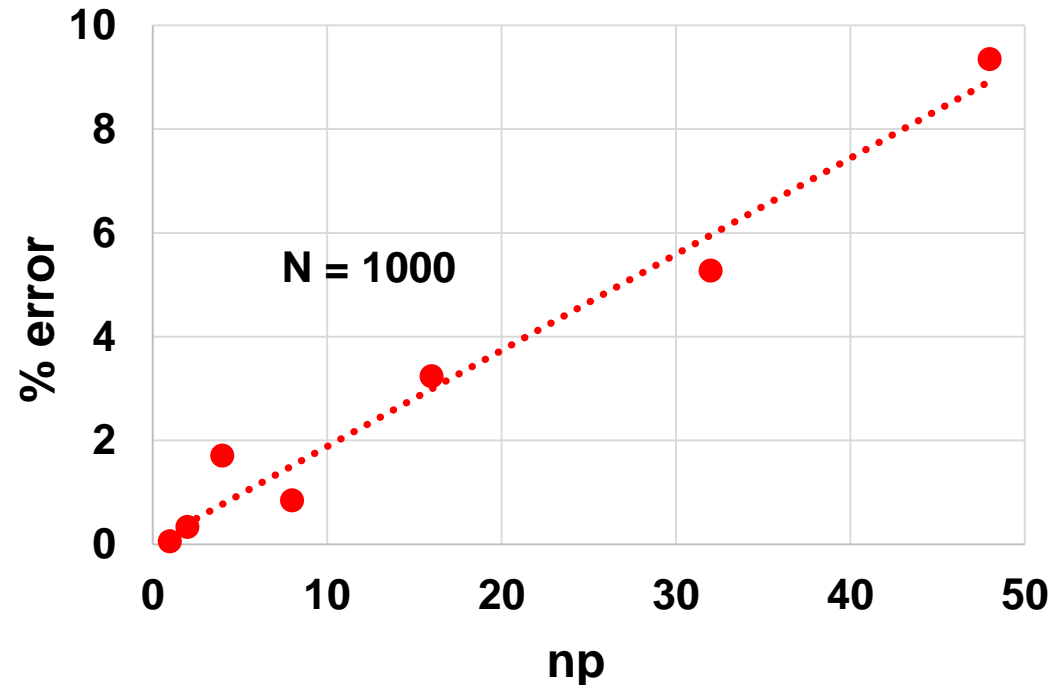
all_reduce merges the results

**Output NOT ACCURATE and
ACCURACY DROPS WITH INCREASING NUMBER OF PROCS !**

SPEEDUP – EXAMPLE

□ PARALLEL VERSION 1

- Aliasing among the RNGs in different procs.
- Effective sample size drops
- Poor statistics.
- For very large number of procs result becomes unreliable.
- For this particular problem you can get away with any significant error simply choosing a very high N
- But think about large problem sizes where you cannot afford to have a high N.



SPEEDUP – EXAMPLE

□ PARALLEL VERSION 2

```
IF (ip.EQ.master) THEN
```

```
.....
```

```
DO i = 1, n
```

```
!
```

```
CALL RANDOM_NUMBER(x)
```

```
r1_all(i) = x
```

```
CALL RANDOM_NUMBER(x)
```

```
r2_all(i) = x
```

```
!
```

```
ENDDO
```

```
!
```

```
ENDIF
```

```
!
```

```
CALL mpi_barrier (MPI_COMM_WORLD, ierr)
```

```
.....
```

```
CALL mpi_scatterv ( r1_all, all_counts, all_offsets, MPI_DOUBLE, &  
                  r1, n per proc, MPI_DOUBLE, master, MPI_COMM_WORLD, ierr)
```

```
.....
```

```
DO i = 1, n_per_proc
```

```
!
```

```
a = (r1(i)*r1(i) + r2(i)*r2(i))
```

```
IF(a.LT.(1.0)) c_par = c_par + 1
```

```
!
```

```
END DO
```

```
!
```

```
CALL mpi_barrier (MPI_COMM_WORLD, ierr)
```

```
CALL mpi_allreduce (c_par,c_par_tot,1,MPI_INTEGER,MPI_SUM,MPI_COMM_WORLD,ierr)
```

RNG is called by only one proc to generate all the random numbers to avoid aliasing.

Random numbers are scattered across procs

‘area’ calculation in parallel

Output

Good accuracy 😊

Poor (no) speedup ☹️

Amdahl's law in action !

SPEEDUP – EXAMPLE

□ PARALLEL VERSION 3

```
CALL RANDOM_SEED(PUT=arr)
!
DO i = 1, n_per_proc
!
CALL RANDOM_NUMBER(r1)
CALL RANDOM_NUMBER(r2)
!
a = r1*r1 + r2*r2
IF(a.LT.(1.0)) c_par = c_par + 1
!
END DO
!
CALL mpi_barrier (MPI_COMM_WORLD, ierr)
CALL mpi_allreduce (c_par,c_par_tot,1,MPI_INTEGER,MPI_SUM,MPI_COMM_WORLD,ierr)
```

arr is dependent on the proc_id

Each proc gets its distinct own seed to start the RNG.

This ensures each proc gets a distinct number stream although they run in parallel

Avoids aliasing. Choose the initial seed carefully to minimize correlation among streams

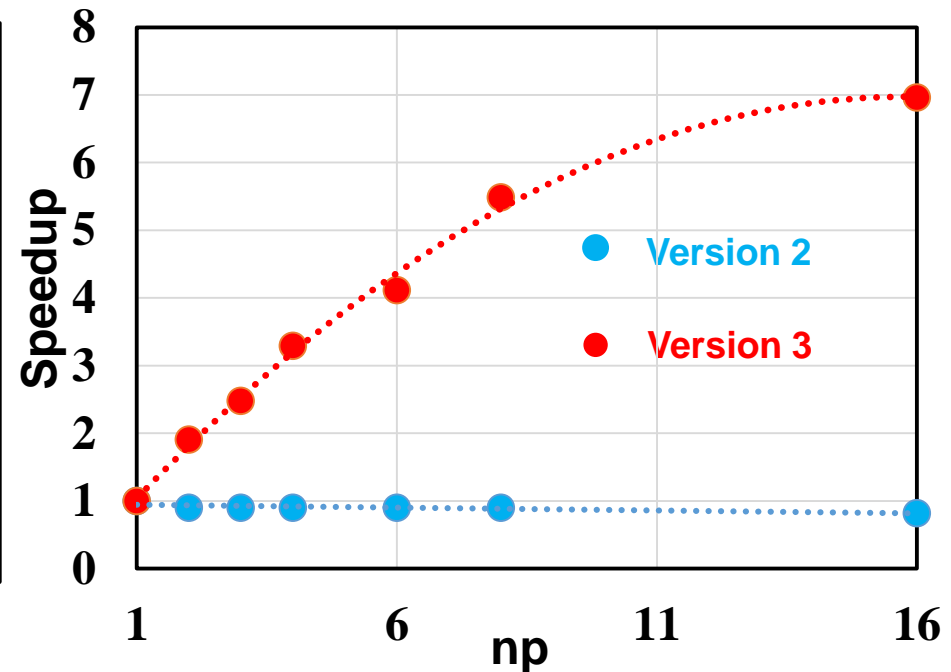
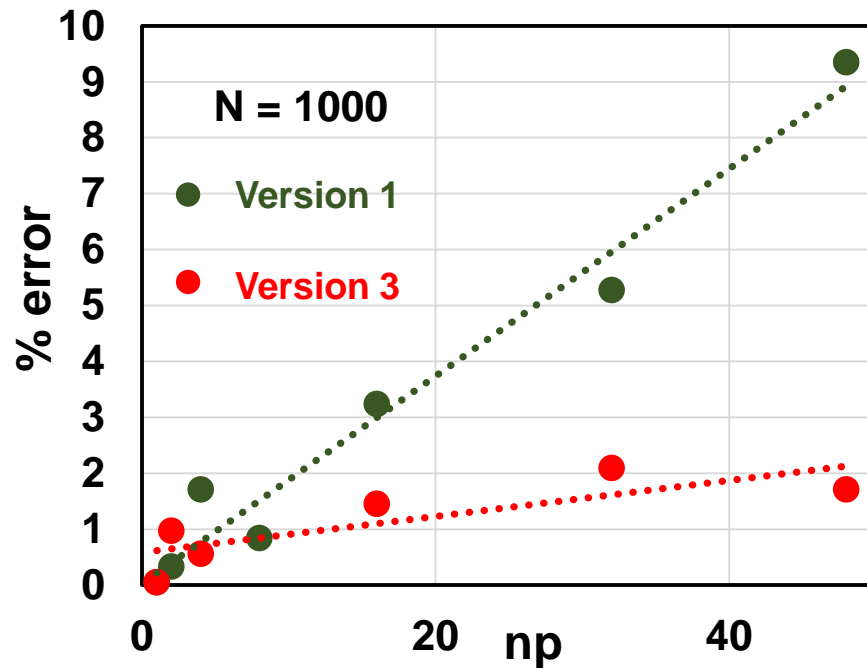
Output

Good accuracy 😊

Good speedup 😊

SPEEDUP – EXAMPLE

□ PERFORMANCE COMPARISON



- The sample size, N , for speedup comparison is taken to be much higher so that the problem size becomes reasonable to compare the speedup.
- I use INTEL MKL (<https://software.intel.com/en-us/intel-mkl>) RNGs where separate generators can be used for each proc.



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WHY SHARED MEMORY (SHM)?

❑ PROBLEM WITH DISTRIBUTED MEMORY (PURE MPI)

- Each proc has its own copy of all the variables.
- This becomes a problem as array sizes grow and is redundant for SHM procs
- Total memory requirement exceeds the given node's memory capacity.
- Plus, unnecessary MPI calls among the SHM procs.

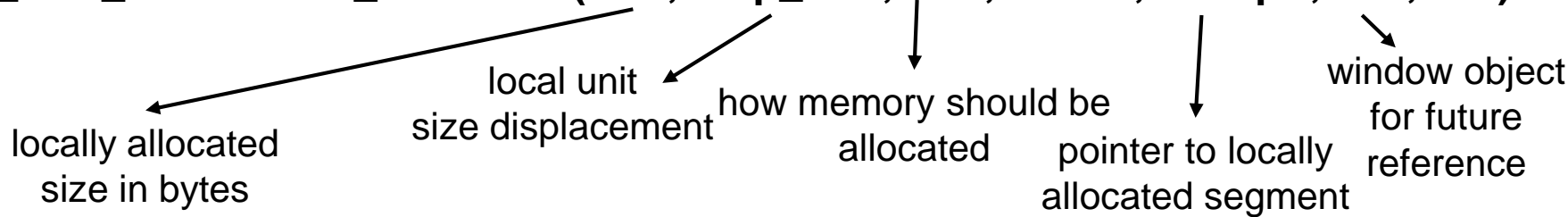
❑ SHARING THE MEMORY AMONG PROCS (HYBRID)

- Allocate a shared memory window in each proc that is accessible to all procs
- Split the variable among procs, one proc can access other's share.
- This hybrid approach drastically cuts down the memory requirement
- Different ways – MPI+OpenMP, MPI+MPI-3, etc.

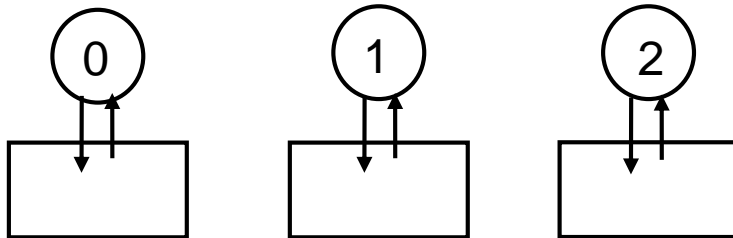
Let's see how this can be done using MPI. You need to use MPI-3 for SHM

SHM ALLOCATION

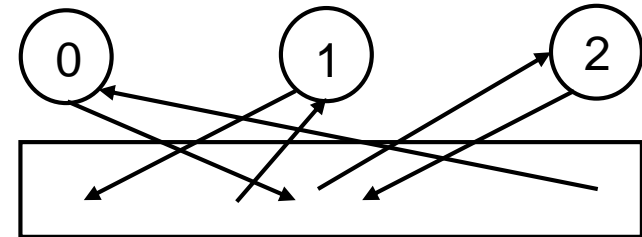
MPI_WIN_ALLOCATE_SHARED (size, disp_unit, info, comm, baseptr, win, ierr)



Normal allocation



Shared allocation

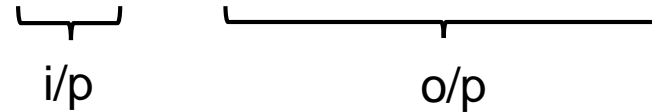


- Programmer's responsibility to make sure that all procs under comm can have a shared memory segment. Will see how.
- info = MPI_INFO_NULL allocates contiguous memory; segments are next to each other. Use ALLOC_SHARED_NONCONTIG for non-contiguous memory.

MPI 3.0 Standard <http://mpi-forum.org/docs/mpi-3.0/mpi30-report.pdf>

SHM ACCESS

MPI_WIN_SHARED_QUERY (win, rank, size, disp_unit, baseptr)



- Rank should be the local rank of the target proc
- baseptr points to the local segment in the target proc
- Often the storing and loading of data from remote target procs are referred to as *Remote Memory Access (RMA)*
- FORTRAN only

USE, INTRINSIC :: ISO_C_BINDING

CALL C_F_POINTER(baseptr, a, shape)



Or use Cray pointers. Some compilers may need separate option for Cray pointers during compilation.

MPI 3.0 Standard <http://mpi-forum.org/docs/mpi-3.0/mpi30-report.pdf>

SPLITTING THE COMMUNICATOR

❑ MAKING SURE PROCS HAVE A SHM SEGMENT

- First job in any SHM program is to split the communicator group into SHM communicator groups (shmcomm)
- This ensures all procs under shmcomm can have a shared memory segment.
- If we work on a single node (unusual for big codes), MPI_COMM_WORLD and shmcomm are same.

❑ EXAMPLE

```
! ***** Split global comm into SMP comms; the third argument 0 says that SMP ranks *****
! ***** should be consistent with global ranks *****
!
CALL MPI_COMM_SPLIT_TYPE (MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED, 0, MPI_INFO_NULL, shmcomm, ierr)
CALL mpi_comm_rank (shmcomm, my_rank, ierr)      Rank within shmcomm
CALL mpi_comm_size (shmcomm, my_size, ierr)      Size of shmcomm
```

SHM – EXAMPLE

❑ ALLOCATE SHARED MEMORY

We want to store a 2D array $A_{mk \times nk}$ inside a shared window

```

! ***** Allocate shared memory. Change MPI_INFO_NULL to ALLOC_SHARED_NONCONTIG if you *****
! ***** want noncontiguous memory segments. *****
!
shapel = (/loc_size, nk/)
size1 = DP_size * shapel(1) * shapel(2)
!
IF (p_id.LT.my_size) PRINT '( " My rank is ", i3, " and local size is ", i3)' , my_rank, loc_size
!
CALL MPI_WIN_ALLOCATE_SHARED (size1, 1 , MPI_INFO_NULL, shmcomm, p, smwin, ierr)
!
CALL C_F_POINTER(p, a, shapel) ! to assign C pointer target to FORTRAN pointer
!
.....
CALL DD(a)
CALL MPI_Win_fence (0, smwin, ierr)
CALL DD(a)
!
DO i = 1, loc_size
  DO j = 1, nk
    a(i, j) = FLOAT ( ( p_id + my_rank + 2 ) * ( i + j ) )
  ENDDO
ENDDO
!
CALL DD(a)
CALL MPI_Win_fence (0, smwin, ierr)
CALL DD(a)

```

loc_size is mk split over np
size1 is the actual size in bytes

fence. Different from MPI_BARRIER.
Ensures no wrong loading of data during the RMA operation.

Fortran only, DD is just an user defined empty routine to make sure register copies of a are written back to memory. See MPI 3.0 Standard (page 638) for more details

SHM – EXAMPLE

❑ SHARED QUERY

Next we want to remote access some elements of the array

```
DO iproc = 1, my_size - 1
!
  IF ( imk.GT.all_offsets(iproc) .AND. imk.LE.all_offsets(iproc+1) ) THEN
!
    ipool = iproc - 1
    ipos  = imk - all_offsets(iproc)
    PRINT '( (/1x), "proc address and local positions are ", 2i3, (/1x) )', ipool, ipos
    EXIT
!
  ELSEIF ( imk.GT.all_offsets(my_size)) THEN
!
    ipool = my_size - 1
    ipos  = imk - all_offsets(ipool)
    PRINT '( (/1x), "proc address and local positions are ", 2i3, (/1x))', ipool, ipos
    EXIT
!
  ENDIF
!
ENDDO
```

First find out which proc the asked element belongs to and what is its position inside that proc

Next access that element through shared query

```
! ***** Ask for remote proc attributes *****
!
CALL MPI_WIN_SHARED_QUERY (smwin, ipool, sizel, displ, p1, ierr)
rm_shape (2) = shapel(2)
rm_shape (1) = sizel / ( DP_size * rm_shape(2) )
!
CALL C_F_POINTER(p1, a1, rm_shape)
```

SHM – EXAMPLE

□ OUTPUT

```
My rank is 0 and local size is 14
My rank is 1 and local size is 13
My rank is 2 and local size is 13
```

Let's take $mk=40$, $nk=40$ with mk being split among 3 procs

Suppose one of the proc (say $p_id=0$) wants to access $A(21, :)$

32.0

36.0

40.0

44.0

48.0

.....

.....

176.0

180.0

184.0

188.0

Here we double-check the functionality of the code –

Definition of A : $A(i, j) = (p_id + my_rank + 2) * (i + j)$

Now $imk=21$ belongs to $p_id=1$ and $my_rank=1$

Local position of $imk=21$ in $p_id=3$ should be $ipos=(21-14) = 7$

Hence the array should be $A(21, j) = 4 * (7 + j) \forall j \in [1, 40]$

This is what we see at the output.



OUTLINE

- ❖ PARALLEL PROGRAMMING
- ❖ GETTING STARTED WITH MPI
- ❖ SPEEDUP
- ❖ MPI SHARED MEMORY
- ❖ **SUMMARY**

❑ SUMMARY

- Parallel programming becomes more important and powerful in scientific computing every passing year.
- MPI is an extremely useful and efficient standard to build parallel codes.
- Speedup in parallel codes is limited by the sequential percentage of the code.
- MPI shared memory provides excellent features to deal with large memory.

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THANK YOU ALL!

HAPPY PARALLEL PROGRAMMING!

... Enjoy responsibly ☺

Cheers,

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<https://sites.google.com/site/ghoshportal/>