INTRODUCTION TO MPI

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Parallel Computing Paradigms

- Parallel Computing Paradigms
  - Message Passing (MPI, …)
    - Distributed or shared memory
  - Directives (OpenMP, …)
    - Shared memory only
  - Multi-Level Parallel programming (MPI + OpenMP)
    - Shared (and distributed) memory

MPI Topics to Cover

- Fundamentals
- Basic MPI Functions
- Point-to-point Communications
- Compilations and Executions
- Collective Communications
- Dynamic Memory Allocations
- MPI Timer
- Cartesian Topology

What is MPI ?

- MPI stands for Message Passing Interface.
- It is a library of subroutines/functions, not a computer language.
- Programmer writes fortran/C code, insert appropriate MPI subroutine/function calls, compile and finally link with MPI message passing library.
- In general, MPI codes run on shared-memory multi-processors, distributed-memory multi-computers, cluster of workstations, or heterogeneous clusters of the above.
- MPI-2 enhancements
  - One-sided communication, parallel I/O, external interfaces
- MPI-3 enhancements
  - Nonblocking collective ops., new one-sided comm., new fortran bindings

Why MPI ?

- To provide efficient communication (message passing) among networks/clusters of nodes
- To enable more analyses in a prescribed amount of time.
- To reduce time required for one analysis.
- To increase fidelity of physical modeling.
- To have access to more memory.
- To enhance code portability; works for both shared- and distributed-memory.
- For “embarrassingly parallel” problems, such as many Monte-Carlo applications, parallelizing with MPI can be trivial with near-linear (or superlinear) speedup.

MPI Preliminaries

- MPI’s pre-defined constants, function prototypes, etc., are included in a header file. This file must be included in your code wherever MPI function calls appear (in “main” and in user subroutines/functions) :
  - #include “mpi.h” for C codes
  - #include “mpi++.h” * for C++ codes
  - include “mpif.h” for f77 and f9x codes
- MPI_Init must be the first MPI function called.
- Terminates MPI by calling MPI_Finalize.
- These two functions must only be called once in user code.

* More on this later …

MPI Preliminaries (continued)

- C is case-sensitive language. MPI function names always begin with “MPI_”, followed by specific name with leading character capitalized, *e.g.*, MPI_Comm_rank. MPI pre-defined constant variables are expressed in upper case characters, *e.g.*, MPI_COMM_WORLD.
- Fortran is not case-sensitive. No specific case rules apply.
- MPI fortran routines return error status as last argument of subroutine call, *e.g.*,

  call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
- Error status is returned as “int” function value for C MPI functions, *e.g.*,

  int ierr = MPI_Comm_rank(MPI_COMM_WORLD, rank);

What is A Message ?

- Collection of data (array) of MPI data types
    - Basic data types such as int /integer, float/real
    - Derived data types
- Message “envelope” – source, destination, tag, communicator

Modes of Communication

- Point-to-point communication
  - Blocking – returns from call when task completes
    - Several send modes; one receive mode
  - Nonblocking – returns from call without waiting for task to complete
    - Several send modes; one receive mode
- Collective communication

MPI Data Types vs C Data Types

- MPI types -- C types
  - MPI_INT – signed int
  - MPI_UNSIGNED – unsigned int
  - MPI_FLOAT – float
  - MPI_DOUBLE – double
  - MPI_CHAR – char
  - . . .

MPI vs Fortran Data Types

- MPI_INTEGER – INTEGER
- MPI_REAL – REAL
- MPI_DOUBLE_PRECISION – DOUBLE PRECISION
- MPI_CHARACTER – CHARACTER(1)
- MPI_COMPLEX – COMPLEX
- MPI_LOGICAL – LOGICAL
- . . .

MPI Data Types

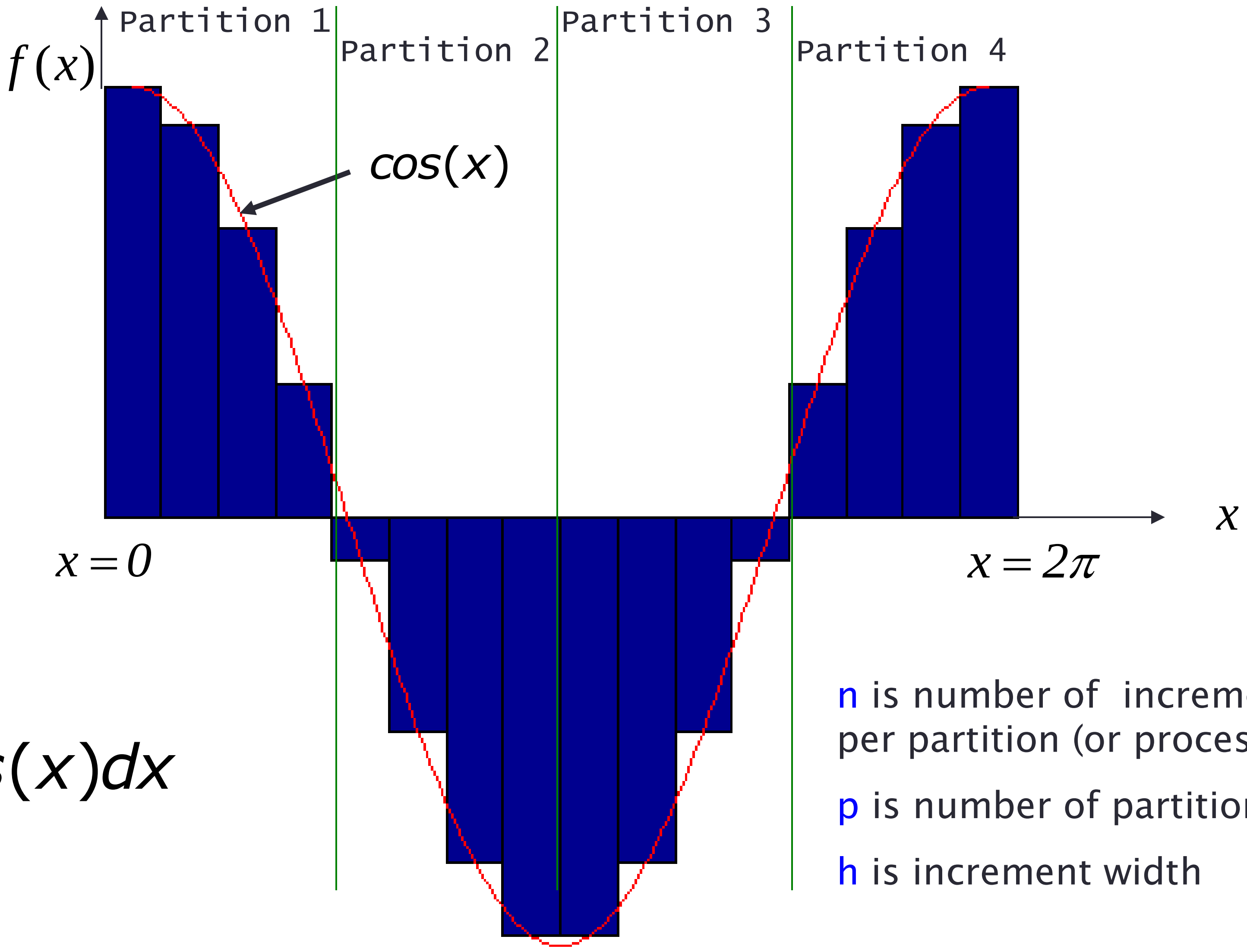
- MPI_PACKED
- MPI_BYTE
- User-derived types

Some MPI Implementations

There are a number of implementations :

- MPICH (ANL)
- LAM (UND/OSC)
- CHIMP (EPCC)
- OpenMPI (installed on Katana)
- Vendor implementations (SGI, IBM, …)
- Codes developed under one implementation should work on another without problems.
- Job execution procedures of implementations may differ.

Integrate cos(x) by Mid-point Rule



$$\int_0^{2\pi} cos(x)dx$$

n is number of increments per partition (or processor)

p is number of partitions

h is increment width

Example 1 (Integration)

We will introduce some fundamental MPI function calls through the computation of a simple integral by the Mid-point rule.

$$\int_a^b \cos(x)dx = \sum_{i=0}^{p-1}\sum_{j=0}^{n-1}\int_{a_i+j*h}^{a_i+(j+1)*h} \cos(x)dx$$

$$\approx \sum_{i=0}^{p-1}\left[\sum_{j=0}^{n-1}\cos(a_{ij})*h\right]; \qquad h = (b-a)/p/n;$$

$$ai = a + i*n*h; \qquad a_{ij} = ai + (j+0.5)*h$$

p is number of partitions and n is increments per partition

Example 1 - Serial fortran code

```
Program Example1
implicit none
integer n, p, i, j
real h, integral_sum, a, b, integral, pi, ai
pi = acos(-1.0)  !  = 3.14159...
a = 0.0          ! lower limit of integration
b = pi/2.        ! upper limit of integration
p = 4            ! number of partitions (processes)
n = 500          ! number of increments in each partition
h = (b-a)/p/n    ! length of increment
ai = a + i*n*h
integral_sum = 0.0      ! Initialize solution to the integral
do i=0,p-1       ! Integral sum over all partitions
   integral_sum = integral_sum + integral(ai,h,n)
enddo
print *,'The Integral =', integral_sum
stop
end
```

. . Serial fortran code (cont'd)

example1.f continues . . .

```
      real function integral(ai, h, n)
! This function computes the integral of the ith partition
      implicit none
      integer n, i, j      ! i is partition index; j is increment index
      real h, h2, aij, ai

      integral = 0.0              ! initialize integral
      h2 = h/2.
      do j=0,n-1                  ! sum over all "j" integrals
        aij = ai+ (j+0.5)*h       ! lower limit of integration of "j"
        integral = integral + cos(aij)*h    ! contribution due "j"
      enddo

      return
      end
```

Example 1 - Serial C code

```
#include <math.h>
#include <stdio.h>
float integral(float a, int i, float h, int n);
void main() {
    int n, p, i, j, ierr;
    float h, integral_sum, a, b, pi, ai;
    pi = acos(-1.0);  /* = 3.14159... *
    a = 0.;           /* lower limit of integration */
    b = pi/2.;        /* upper limit of integration */
    p = 4;            /* # of partitions */
    n = 500;          /* increments in each process */
    h = (b-a)/n/p;    /* length of increment */
    integral_sum = 0.0;
    for (i=0; i<p; i++) { /* integral sum over partitions */
      ai = a + i*n*h;    /* lower limit of int. for partition i */
      integral_sum += integral(ai,h,n); }
    printf("The Integral =%f\n", integral_sum);
}
```

. . Serial C code (cont'd)

example1.c continues . . .

```
float integral(float ai, float h, int n) {
  int j;
  float aij, integ;
  integ = 0.0;                  /* initialize integral */
  for (j=0; j<n; j++) {         /* sum over integrals in partition i*/
    aij = ai + (j+0.5)*h;       /* lower limit of integration of j*/
    integ += cos(aij)*h;        /* contribution due j */
  }
  return integ;
}
```

Example 1_1 - Parallel C code

Two main styles of programming: SPMD, MPMD. The following demonstrates SPMD, which is more frequently used than MPMD,

MPI functions used in this example:

- MPI_Init, MPI_Comm_rank, MPI_Comm_size
- MPI_Send, MPI_Recv, MPI_Finalize

```
#include <mpi.h>
float integral(float ai, float h, int n);   // prototyping
void main(int argc, char* argv[])
{
    int n, p, myid, tag, proc, ierr;
    float h, integral_sum, a, b, ai, pi, my_int;
    int master = 0;  /* processor performing total sum */
    MPI_Comm comm;
    MPI_Status status;
```

. . . Parallel C code (cont'd)

```
comm = MPI_COMM_WORLD;
ierr = MPI_Init(&argc,&argv);        // starts MPI
MPI_Comm_rank(comm, &myid);          // get current process id
MPI_Comm_size(comm, &p);             // get number of processes

pi = acos(-1.0);     // = 3.14159...
a = 0.;              // lower limit of integration
b = pi*1./2.;        // upper limit of integration
n = 500;             // number of increment within each process
tag = 123;           // set the tag to identify this particular job
h = (b-a)/n/p;       // length of increment
ai = a + myid*n*h;  // lower limit of integration for partition myid
my_int = integral(ai, h, n)    // compute local sum due myid
```

… Parallel C code (cont'd)

```
 printf("Process %d has the partial integral of %f\n", myid,my_int);
 MPI_Send(&my_int, 1, MPI_FLOAT,
                  master,       // message destination
                  tag,          // message tag
                  comm);
  if(myid == master) {  // Receives serialized
     integral_sum = 0.0;
     for (proc=0;proc<p;proc++) { //loop on all procs to collect local sum (serial !)
        MPI_Recv(&my_int, 1, MPI_FLOAT,   // triplet …
                        proc,        // message source
                        tag,         // message tag
                        comm, &status);   // not safe
        integral_sum += my_int; }
     printf("The Integral =%f\n",integral_sum); // sum of my_int
  }
  MPI_Finalize();          // let MPI finish up
}
```

Example 1_1 - Parallel f77 code

Two main styles of programming: SPMD, MPMD. The following demonstrates SPMD, which is more frequently used than MPMD,

MPI functions used in this example:

- MPI_Init, MPI_Comm_rank, MPI_Comm_size
- MPI_Send, MPI_Recv, MPI_Finalize

```
PROGRAM Example1_1
 implicit none
 integer n, p, i, j, ierr, master, myid
 real h, integral_sum, a, b, integral, pi, ai
 include "mpif.h"   ! pre-defined MPI constants, ...
 integer source, tag, status(MPI_STATUS_SIZE)
 real my_int

 data master/0/    ! 0 is the master processor  responsible
                   ! for collecting integral sums ...
```

. . . Parallel fortran code (cont'd)

```
! Starts MPI processes ...
    call MPI_Init(ierr)
! Get current process id
    call MPI_Comm_rank(MPI_COMM_WORLD, myid, ierr)
! Get number of processes from command line
    call MPI_Comm_size(MPI_COMM_WORLD, p, ierr)

! executable statements before MPI_Init is not
! advisable; side effect implementation-dependent   (historical)

   pi = acos(-1.0)      ! = 3.14159...
   a = 0.0              ! lower limit of integration
   b = pi/2.            ! upper limit of integration
   n = 500              ! number of increments in each process
   h = (b - a)/ p / n   ! (uniform) increment size
   tag = 123            ! set tag for job
   ai = a + myid*n*h    ! Lower limit of integration for partition myid
```

... Parallel fortran code (cont'd)

```
  my_int = integral(ai, h, n)    ! compute local sum due myid
  write(*,"('Process ',i2,' has the partial integral of',
&        f10.6)")myid,my_int
  call MPI_Send(my_int, 1, MPI_REAL, master, tag,
&       MPI_COMM_WORLD, ierr)    ! send my_int to master

  if(myid .eq. master) then
    do source=0,p-1    ! loop on all  procs to collect local sum (serial !)
      call MPI_Recv(my_int, 1, MPI_REAL, source, tag,
&             MPI_COMM_WORLD, status, ierr)   ! not safe
      integral_sum = integral_sum + my_int
    enddo
    print *,'The Integral =', integral_sum
 endif
 call MPI_Finalize(ierr)                   ! let MPI finish up
end
```

Message Passing to Self

- It is valid to send/recv message to/from itself
- On IBM pSeries, env variable MP_EAGER_LIMIT may be used to control buffer memory size.
- Above example hangs if MP_EAGER_LIMIT set to 0
- Good trick to use to see if code is “safe”
- Not available with MPICH

Example 1_2 - Parallel C code

```
#include <mpi.h>
#include <math.h>
#include <stdio.h>
float  integral(float a, int i, float h, int n); /* prototype */
void main(int argc, char *argv[]) {
   int n, p, i;
   float h, result, a, b, pi, my_int, ai;
   int myid, source, master, tag;
   MPI_Status status;                          /* MPI data type */
   MPI_Init(&argc, &argv);                     /* start MPI processes */
   MPI_Comm_rank(MPI_COMM_WORLD, &myid); /* current proc. id */
   MPI_Comm_size(MPI_COMM_WORLD, &p);       /* # of processes */
```

… Parallel C code (continued)

```
  pi = acos(-1.0);     /* = 3.14159... */
  a = 0.;              /* lower limit of integration */
  b = pi/2.;           /* upper limit of integration */
  n = 500;             /* number of increment within each process */
  master = 0;
/* define the process that computes the final result */
  tag = 123;           /* set the tag to identify this particular job */
  h = (b-a)/n/p;       /* length of increment */
  ai = a + myid*n*h;  /* lower limit of int. for partition myid */
  my_int = integral(ai,h,n);   /* local sum due process myid */
  printf("Process %d has the partial integral of %f\n", myid,my_int);
```

… Parallel C code (continued)

```
  if(myid == 0) {
     integral_sum = my_int;
     for (source=1;source<p;i++) {
          MPI_Recv(&my_int, 1, MPI_FLOAT, source, tag,
               MPI_COMM_WORLD, &status);  /* safe */
        integral_sum += my_int;
     }
     printf("The Integral =%f\n", integral_sum);
  } else {
    MPI_Send(&my_int, 1, MPI_FLOAT, master, tag,
            MPI_COMM_WORLD);  /* send my_int to "master" */
  }
    MPI_Finalize();      /* let MPI finish up ... */
}
```

Essentials of Communication

- Sender must specify valid destination.
- Sender and receiver data type, tag, communicator must match.
- Receiver can receive from non-specific (but valid) source.
- Receiver returns extra (status) parameter to report info regarding message received.
- Sender specifies size of sendbuf; receiver specifies *upper bound* of recvbuf.

Compilation & Execution

In the following slides, the compilation and job running procedures will be outlined for the computer systems maintained by RCS's Shared Computing Cluster (SCC)

How To Compile On the SCC

On the SCC:

- scc1 % mpif77 example.f (F77)
- scc1 % mpif90 example.f (F90)
- scc1 % mpicc example.c (C)
- scc1 % mpiCC example.C (C++)

• The above scripts should be used for MPI code compilation as they automatically include appropriate include files (–I) and library files (–L) for successful compilations.
• Above script names are generic. Compilers available are: Gnu and Portland Group.
• Two MPI implementations are available: MPICH and OpenMPI.
•See http://www.bu.edu/tech/support/research/software-and-programming/programming/multiprocessor/

How To Run Jobs On the SCC

Interactive jobs:

- `scc1 % mpirun -np 4 a.out`

Batch jobs (via Open GridEngine):

- `scc1 % qsub myscript`

See http://www.bu.edu/tech/support/research/system-usage/running-jobs/parallel-batch/

Output of Example1_1

```
Scc1 % mpirun -np 4 example1_1
Process 1 has the partial result of  0.324423
Process 2 has the partial result of  0.216773
Process 0 has the partial result of  0.382683
Process 3 has the partial result of  0.076120
  The Integral =    1.000000
```

Processing out of order !

Example1_3 – Parallel Integration

MPI functions used for this example:

- MPI_Init, MPI_Comm_rank, MPI_Comm_size, MPI_Finalize
- MPI_Recv, MPI_Isend, MPI_Wait
- MPI_ANY_SOURCE, MPI_ANY_TAG

```
PROGRAM Example1_3
    implicit none
    integer n, p, i, j, proc, ierr, master, myid, tag, request
    real h, a, b, integral, pi, ai, my_int, integral_sum
    include "mpif.h"    ! This brings in pre-defined MPI constants, ...
    integer status(MPI_STATUS_SIZE)
    data master/0/
```

Example1_3 (continued)

```
c**Starts MPI processes ...
     call MPI_Init(ierr)
     call MPI_Comm_rank(MPI_COMM_WORLD, myid, ierr)
     call MPI_Comm_size(MPI_COMM_WORLD, p, ierr)

     pi = acos(-1.0)      !  = 3.14159...
     a = 0.0              ! lower limit of integration
     b = pi/2.            ! upper limit of integration
     n = 500              ! number of increment within each process
     dest = master        ! define process that computes the final result
     tag = 123            ! set the tag to identify this particular job
     h = (b-a)/n/p        ! length of increment

     ai = a + myid*n*h;   ! starting location of partition "myid"
     my_int = integral(ai,h,n)     ! Integral of process myid
     write(*,*)'myid=',myid,',  my_int=',my_int
```

Example1_3 (continued)

```
   if(myid .eq. master) then                               ! the following serialized
     integral_sum = my_int
     do k=1,p-1
       call MPI_Recv(my_int, 1, MPI_REAL,
  &        MPI_ANY_SOURCE, MPI_ANY_TAG,  ! more efficient and
  &        MPI_COMM_WORLD, status, ierr)        ! less prone to deadlock
       integral_sum = integral_sum + my_int       ! sum of local integrals
     enddo
   else
     call MPI_Isend(my_int, 1, MPI_REAL, dest, tag,
  &      MPI_COMM_WORLD, req, ierr)    ! send my_int to "dest"
C**more computation here . . .
     call MPI_Wait(req, status, ierr)        ! wait for nonblock send ...
   endif
c**results from all procs have been collected and summed ...
   if(myid .eq. 0) write(*,*)'The Integral =',integral_sum
   call MPI_Finalize(ierr)                           ! let MPI finish up ...
   stop
   end
```

Practice Session

1. Write a C or FORTRAN program to print the statement
   "Hello, I am process X of Y processes“
   where X is the current process while Y is the number of processes for job.

2. Write a C or FORTRAN program to do the following:
   1. On process 0, send a message
      "Hello, I am process 0" to other processes.
   2. On all other processes, print the process's ID, the message it receives and where the message came from.

Makefile and programs are in /scratch/kadin/MPI

Example1_4 Parallel Integration

MPI functions and constants used for this example:

- MPI_Init, MPI_Comm_rank, MPI_Comm_size, MPI_Finalize
- MPI_Bcast, MPI_Reduce, MPI_SUM

```
PROGRAM Example1_4
implicit none
integer n, p, i, j, ierr, master
real h, integral_sum, a, b, integral, pi, ai

include "mpif.h"      ! This brings in pre-defined MPI constants, ...
integer myid, source, dest, tag, status(MPI_STATUS_SIZE)
real my_int

data master/0/
```

Example1_4 (continued)

```
c**Starts MPI processes ...
      call MPI_Init(ierr)
      call MPI_Comm_rank(MPI_COMM_WORLD, myid, ierr)
      call MPI_Comm_size(MPI_COMM_WORLD, p, ierr)

      pi = acos(-1.0)   !  = 3.14159...
      a = 0.0           ! lower limit of integration
      b = pi/2.         ! upper limit of integration
      h = (b-a)/n/p     ! length of increment
      dest = 0          ! define the process that computes the final result
      tag = 123         ! set the tag to identify this particular job
      if(myid .eq. master) then
         print *,'The requested number of processors =',p
         print *,'enter number of increments within each process'
         read(*,*)n
      endif
```

Example1_4 (continued)

```
c**Broadcast "n" to all processes
      call MPI_Bcast(n, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, ierr)
      ai = a + myid*h*n
      my_int = integral(ai,h,n)
      write(*,"('Process ',i2,' has the partial sum of',f10.6)")
     &          myid, my_int

      call MPI_Reduce(my_int, integral_sum, 1, MPI_REAL, MPI_SUM,
     &            dest, MPI_COMM_WORLD, ierr)   ! Compute integral sum

      if(myid .eq. master) then
        print *,'The Integral Sum =', integral_sum
      endif

      call MPI_Finalize(ierr)                      ! let MPI finish up ...
      stop
      end
```

Example1_5 Parallel Integration

New MPI functions and constants used for this example:

- MPI_Init, MPI_Comm_rank, MPI_Comm_size, MPI_Finalize
- MPI_Pack, MPI_Unpack
- MPI_FLOAT_INT, MPI_MINLOC, MPI_MAXLOC, MPI_PACKED

```
#include <mpi.h>
#include <math.h>
#include <stdio.h>
float fct(float x) { return cos(x); }
/* Prototype */
float integral(float ai, float h, int n);
int main(int argc, char* argv[])
{
```

Example1_5 (cont'd)

```
int n, p;
float h,integral_sum, a, b, pi, ai;
int myid, dest, m, index, minid, maxid, Nbytes=1000, master=0;
char line[10], scratch[Nbytes];
struct {
        float val;
        int   loc; } local_sum, min_sum, max_sum;

MPI_Init(&argc,&argv);                        /* starts MPI */
MPI_Comm_rank(MPI_COMM_WORLD, &myid);  /* process id */
MPI_Comm_size(MPI_COMM_WORLD, &p);      /* num of procs*/
pi = acos(-1.0);  /* = 3.14159... */
dest = 0;         /* define the process to compute final result */
comm = MPI_COMM_WORLD;
```

Example1_5 (cont'd)

```
if(myid == master) {
        printf("The requested number of processors = %d\n",p);
        printf("enter number of increments within each process\n");
        (void) fgets(line, sizeof(line), stdin);
        (void) sscanf(line, "%d", &n);
        printf("enter a & m\n");
        printf(" a = lower limit of integration\n");
        printf(" b = upper limit of integration\n");
        printf("   = m * pi/2\n");
        (void) fgets(line, sizeof(line), stdin);
        (void) sscanf(line, "%d %d", &a, &m);
        b = m * pi / 2.;
}
```

Example1_5 (cont'd)

```
 If (myid == master) {
/* to be efficient, pack all things into a buffer for broadcast */
      index = 0;
      MPI_Pack(&n, 1, MPI_INT,   scratch, Nbytes, &index, comm);
      MPI_Pack(&a, 1, MPI_FLOAT, scratch, Nbytes, &index, comm);
      MPI_Pack(&b, 1, MPI_FLOAT, scratch, Nbytes, &index, comm);
      MPI_Bcast(scratch, Nbytes, MPI_PACKED, master, comm);
  } else {
      MPI_Bcast(scratch, Nbytes, MPI_PACKED, master, comm);
/* things received have been packed, unpack into expected locations */
      index = 0;
      MPI_Unpack(scratch, Nbytes, &index, &n, 1, MPI_INT,   comm);
      MPI_Unpack(scratch, Nbytes, &index, &a, 1, MPI_FLOAT, comm);
      MPI_Unpack(scratch, Nbytes, &index, &b, 1, MPI_FLOAT, comm);
   }
```

Example1_5 (cont'd)

```
    h = (b-a)/n/p;     /* length of increment */
    ai = a + myid*h*n;
    local_sum.val = integral(ai,h,n);
    local_sum.loc = myid;
 printf("Process %d has the partial sum of %f\n", myid, local_sum.val);

/* data reduction with MPI_SUM */
    MPI_Reduce(&local_sum.val, &integral_sum, 1, MPI_FLOAT,
MPI_SUM, dest, comm);

/* data reduction with MPI_MINLOC */
    MPI_Reduce(&local_sum, &min_sum, 1, MPI_FLOAT_INT,
MPI_MINLOC, dest, comm);

/* data reduction with MPI_MAXLOC */
    MPI_Reduce(&local_sum, &max_sum, 1, MPI_FLOAT_INT,
MPI_MAXLOC, dest, comm);
```

Example1_5 (cont'd)

```
 if(myid == master) {
        printf("The Integral = %f\n", integral_sum);
        maxid = max_sum.loc;
        printf("Proc %d has largest integrated value of %f\n",maxid,
max_sum.val);
        minid = min_sum.loc;
        printf("Proc %d has smallest integrated value of %f\n", minid,
min_sum.val);
      }

      MPI_Finalize();                          /* let MPI finish up ... */
}
```

C++ example

```
#include <mpi.h>
#include <iostream>
using namespace std;
int main(int argc, char *argv[]) {
  int rank, size;
  MPI::Init(argc, argv);
  rank = MPI::COMM_WORLD.Get_rank();
  size = MPI::COMM_WORLD.Get_size();
  cout << "Hello world! I am " << rank <<
          "of " << size << endl;
  MPI::Finalize();
  return 0; }

Twister % mpCC -DHAVE_MPI_CXX -o hello hello.C
Twister % hello -procs 4
```

Speedup Ratio and Parallel Efficiency

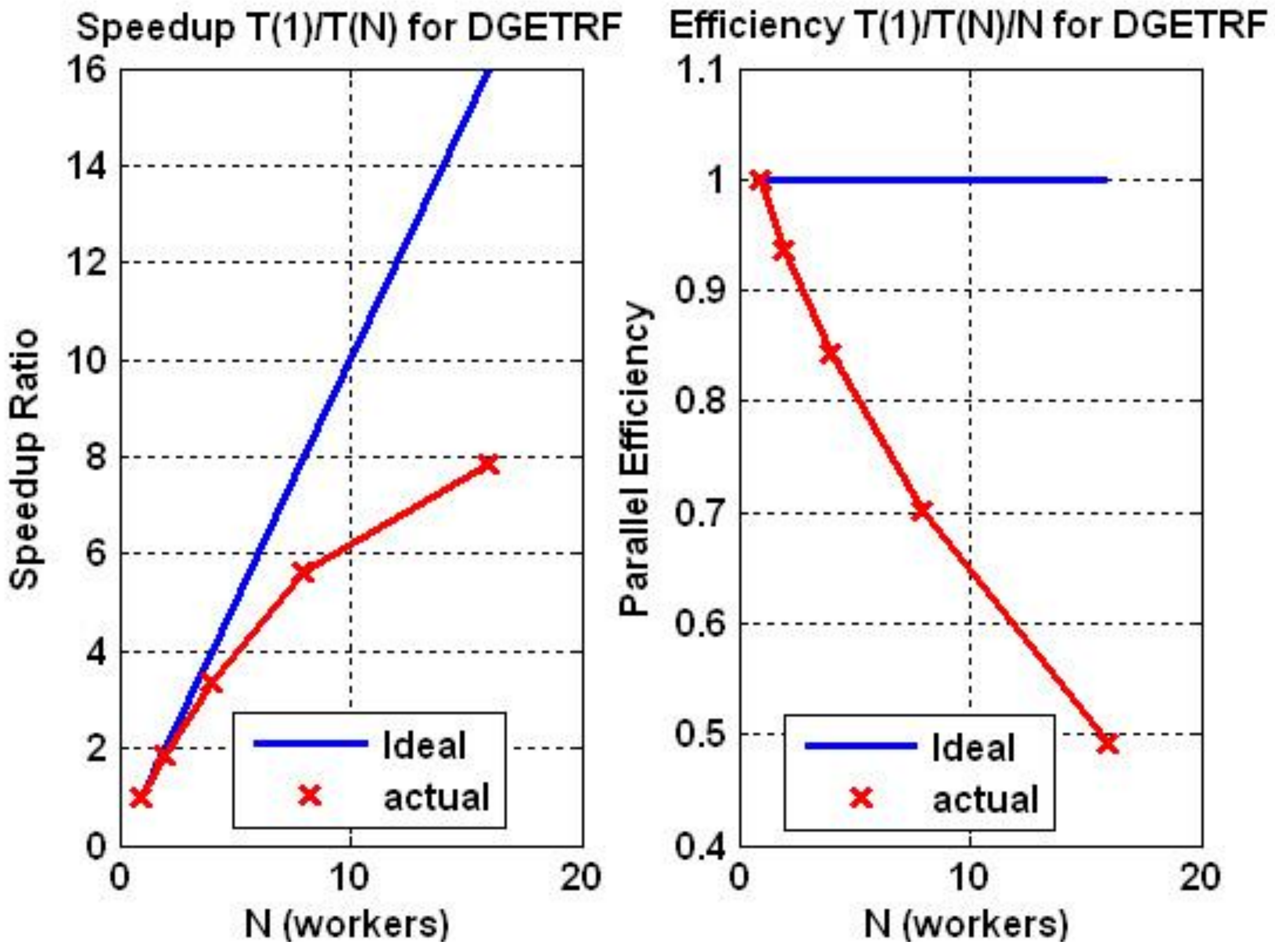
S is ratio of T_1 over T_N, *elapsed times of 1 and N* workers.
f is fraction of T_1 due sections of code not parallelizable.

$$S = \frac{T_1}{T_N} \langle \frac{T_1}{(f + \frac{1-f}{N})T_1} \langle \frac{1}{f} \quad as \quad N \rightarrow \infty$$

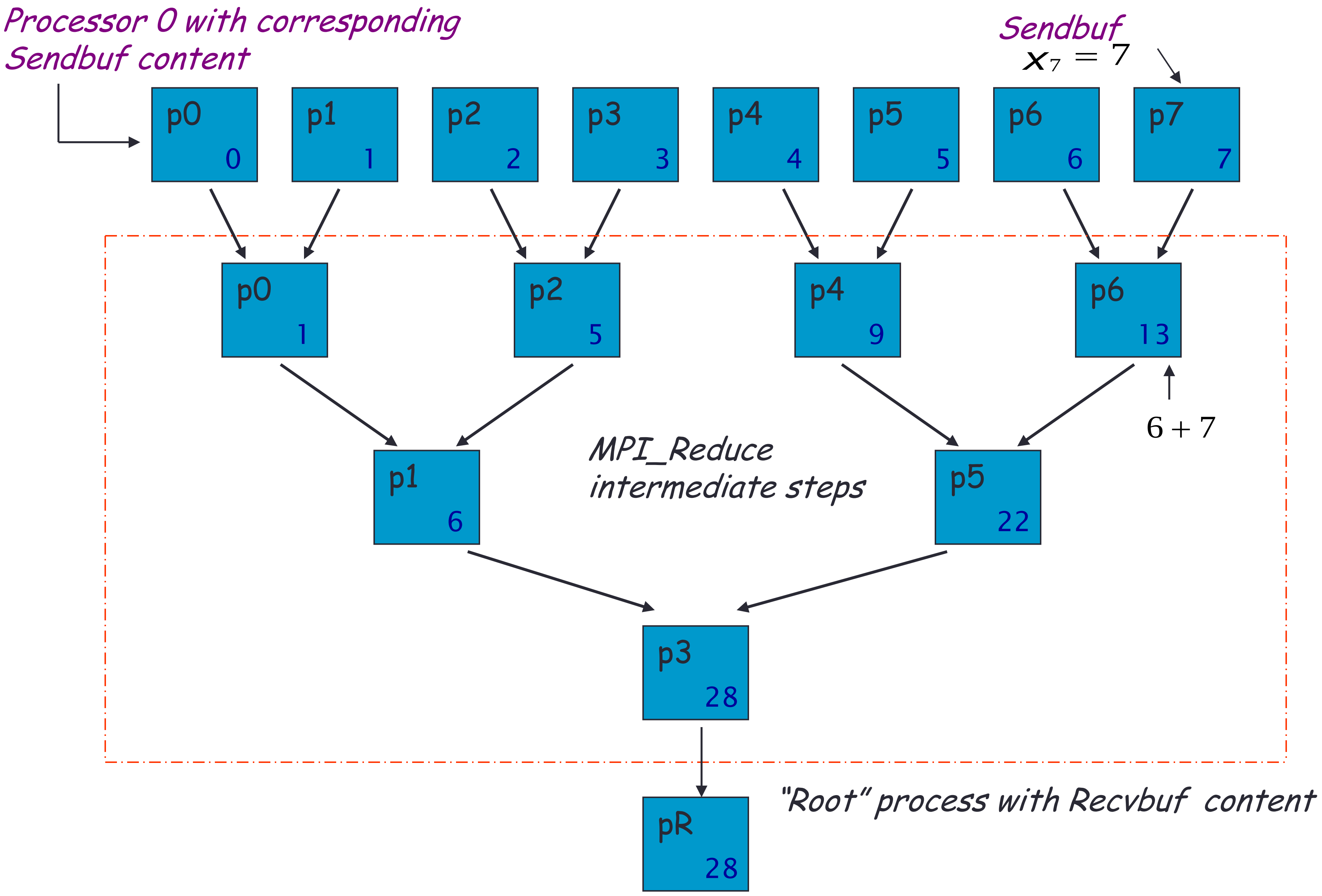
Amdahl's Law above states that a code with its parallelizable component comprising 90% of total computation time can at best achieve a 10X speedup with lots of workers. A code that is 50% parallelizable speeds up two-fold with lots of workers.

The parallel efficiency is $E = S / N$
Program that scales linearly ($S = N$) has parallel efficiency *1.*
A task-parallel program is usually more efficient than a data-parallel program. Data-parallel codes can sometimes achieve super-linear behavior due to efficient cache usage per worker.

Speedup Ratio & Parallel Efficiency



How MPI_Reduce Works On $x = \sum_{i=0}^{7} i$


Processor 0 with corresponding Sendbuf content
Sendbuf
$x_7 = 7$
p0 0
p1 1
p2 2
p3 3
p4 4
p5 5
p6 6
p7 7
p0 1
p2 5
p4 9
p6 13
$6 + 7$
MPI_Reduce intermediate steps
p1 6
p5 22
p3 28
pR 28
"Root" process with Recvbuf content

Collective Communications

Pass data among a group of processors.

Collective Functions

Process 0	Process 1*	Process 2	Process 3	Operation	Process 0	Process 1*	Process 2	Process 3
	b			MPI_Bcast	b	b	b	b
a	b	c	d	MPI_Gather		a,b,c,d		
a	b	c	d	MPI_Allgather	a,b,c,d	a,b,c,d	a,b,c,d	a,b,c,d
	a,b,c,d			MPI_Scatter	a	b	c	d
a,b,c,d	e,f,g,h	i,j,k,l	m,n,o,p	MPI_Alltoall	a,e,i,m	b,f,j,n	c,g,k,o	d,h,l,p
SendBuff	**SendBuff**	**SendBuff**	**SendBuff**	⇨	**ReceiveBuff**	**ReceiveBuff**	**ReceiveBuff**	**ReceiveBuff**

- ***This example uses 4 processes***
- ***Rank 1 is, arbitrarily, designated data gather/scatter process***
- ***a, b, c, d are scalars or arrays of any data type***
- ***Data are gathered/scattered according to rank order***

Collectives Example Code

```
      program collectives_example
      implicit none
      integer p, ierr, i, myid, root
      include "mpif.h"        ! This brings in pre-defined MPI constants, ...
      character*1 x(0:3), y(0:3), alphabets(0:15)
      data alphabets/'a','b','c','d','e','f','g','h','i','j','k','l',
     &               'm','n','o','p'/
      data root/1/            ! process 1 is the data sender/receiver
c**Starts MPI processes ...
      call MPI_Init(ierr)     ! starts MPI
      call MPI_Comm_rank(MPI_COMM_WORLD, myid, ierr) ! current pid
      call MPI_Comm_size(MPI_COMM_WORLD, p, ierr)    ! # of procs
```

Collectives Example (cont'd)

```
  if (myid .eq. 0) then
     write(*,*)
     write(*,*)'* This program demonstrates the use of collective',
&                    ' MPI functions'
     write(*,*)'* Four processors are to be used for the demo'
     write(*,*)'* Process 1 (of 0,1,2,3) is the designated root'
     write(*,*)
     write(*,*)
     write(*,*)' Function Proc Sendbuf Recvbuf'
     write(*,*)' -------- ---- ------- -------'
 endif
```

Gather Operation

```
alphabets(0) = 'a'
alphabets(1) = 'b'

  . . .

alphabets(14) = 'o'
alphabets(15) = 'p'
```

```
c**Performs a gather operation
      x(0) = alphabets(myid)
      do i=0,p-1
         y(i) = ' '
      enddo
      call MPI_Gather(x,1,MPI_CHARACTER,  ! Send-buf,count,type,
     &                y,1,MPI_CHARACTER,  ! Recv-buf,count?,type?,
     &                root,               ! Data destination
     &               MPI_COMM_WORLD,ierr)    ! Comm, flag
      write(*,"('MPI_Gather:',t20,i2,(3x,a1),t40,4(3x,a1))")myid,x(0),y
```

Recv-buf according to rank order

All-gather Operation

```
c**Performs an all-gather operation
      x(0) = alphabets(myid)
      do i=0,p-1
         y(i) = ' '
      enddo
      call MPI_Allgather(x,1,MPI_CHARACTER,       ! send buf,count,type
     &                   y,1,MPI_CHARACTER,       ! recv buf,count,type
     &                   MPI_COMM_WORLD,ierr)     ! comm,flag
      write(*,"('MPI_Allgather:',t20,i2,(3x,a1),t40,4(3x,a1))")myid,x(0),y
```

Scatter Operation

```
c**Perform a scatter operation
      if (myid .eq. root) then
        do i=0, p-1
           x(i) = alphabets(i)
           y(i) = ' '
        enddo
      else
         do i=0,p-1
             x(i) = ' '
             y(i) = ' '
          enddo
      endif
      call MPI_scatter(x,1,MPI_CHARACTER,          ! Send-buf,count,type
     &                 y,1,MPI_CHARACTER,          ! Recv-buf,count,type
     &                 root,                       ! data origin
     &                 MPI_COMM_WORLD,ierr)        ! comm,flag
      write(*,"('MPI_scatter:',t20,i2,4(3x,a1),t40,4(3x,a1))")myid,x,y
```

Alltoall Operation

```
c**Perform an all-to-all operation
      do i=0,p-1
          x(i) = alphabets(i+myid*p)
          y(i) = ' '
      enddo
      call MPI_Alltoall(x,1,MPI_CHARACTER,          ! send buf,count,type
     &                  y,1,MPI_CHARACTER,          ! recv buf,count,type
     &                  MPI_COMM_WORLD,ierr)        ! comm,flag
      write(*,"('MPI_Alltoall:',t20,i2,4(3x,a1),t40,4(3x,a1))")myid,x,y
```

Broadcast Operation

```
c**Performs a broadcast operation
      do i=0, p-1
         x(i) = ' '
         y(i) = ' '
      enddo
      if(myid .eq. root) then
         x(0) = 'b'
         y(0) = 'b'
      endif
      call MPI_Bcast(y,1,MPI_CHARACTER,                 ! buf,count,type
     &                   root,MPI_COMM_WORLD,ierr)  ! root,comm,flag
       write(*,"('MPI_Bcast:',t20,i2,4(3x,a1),t40,4(3x,a1))")myid,x,y

       call MPI_Finalize(ierr)     ! let MPI finish up ...
       end
```

Example 1.6 Integration (modified)

```
#include <mpi.h>
#include <math.h>
#include <stdio.h>
float fct(float x)
{
      return cos(x);
}
/* Prototype */
float integral(float a, int i, float h, int n);
int main(int argc, char* argv[])
{
int n, p, myid, i;
      float h, integral_sum, a, b, pi, my_int;
      float buf[50], tmp;
```

Example 1.6 (cont'd)

```
MPI_Init(&argc,&argv);                         /* starts MPI */
MPI_Comm_rank(MPI_COMM_WORLD, &myid);  /* current proc id */
MPI_Comm_size(MPI_COMM_WORLD, &p);         /* num of procs */

pi = acos(-1.0);  /* = 3.14159... */
a = 0.;                /* lower limit of integration */
b = pi*1./2.;       /* upper limit of integration */
n = 500;             /* number of increment within each process */
h = (b-a)/n/p;     /* length of increment */

my_int = integral(a,myid,h,n);

printf("Process %d has the partial sum of %f\n", myid,my_int);

MPI_Gather(&my_int, 1, MPI_FLOAT, buf, 1, MPI_FLOAT, 0,
MPI_COMM_WORLD);
```

Example 1.6 (cont'd)

```
  MPI_Scatter(buf, 1, MPI_FLOAT, &tmp, 1, MPI_FLOAT, 0,
MPI_COMM_WORLD);
     printf("Result sent back from buf = %f\n", tmp);

     if(myid == 0) {
       integral_sum = 0.0;
       for (i=0; i<p; i++) {
         integral_sum += buf[i];
       }
       printf("The Integral =%f\n", integral_sum);
     }

     MPI_Finalize();                      /* let MPI finish up ... */
}
```

MPI_Probe, MPI_Wtime (f90)

This example demonstrates dynamic memory allocation and parallel timer.

```
Program dma_example
implicit none
include "mpif.h"
integer, parameter :: real_kind = selected_real_kind(8,30)
real(real_kind), dimension(55) :: sdata
real(real_kind), dimension(:), allocatable :: rdata
real(real_kind) :: start_time, end_time
integer :: p, i, count, myid, n, status(MPI_STATUS_SIZE), ierr

!* Starts MPI processes ...
call MPI_Init(ierr)                               !* starts MPI
call MPI_Comm_rank(MPI_COMM_WORLD, myid, ierr)  ! myid
call MPI_Comm_size(MPI_COMM_WORLD, p, ierr)   ! Num. proc
```

MPI_Probe, MPI_Wtime (f90 cont'd)

```
start_time = MPI_Wtime()      ! start timer, measured in seconds
if (myid == 0) then
  sdata(1:50)= (/ (i, i=1,50) /)
  call MPI_Send(sdata, 50, MPI_DOUBLE_PRECISION, 1, 123, &
              MPI_COMM_WORLD, ierr)
else
  call MPI_Probe(0, MPI_ANY_TAG, MPI_COMM_WORLD, status, 
ierr)
  call MPI_Get_count(status, MPI_DOUBLE_PRECISION, count, ierr)
  allocate( rdata(count) )
  call MPI_Recv(rdata, count, MPI_DOUBLE_PRECISION, 0, &
              MPI_ANY_TAG, MPI_COMM_WORLD, status, ierr)
  write(*,'(5f10.2)')rdata(1:count:10)
endif
end_time = MPI_Wtime()          ! stop timer
```

MPI_Probe, MPI_Wtime (f90 cont'd)

```
if (myid .eq. 1) then
  WRITE(*,"('   Total cpu time =',f10.5,' x ',i3)") end_time -
start_time,p
endif

call MPI_Finalize(ierr)                    !* let MPI finish up ...

end program dma_example
```

MPI_Probe, MPI_Wtime (C)

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

int main(int argc, char* argv[])
{
      double sdata[55], *rdata, start_time, end_time;
      int p, i, count, myid, n;
      MPI_Status status;

/* Starts MPI processes ... */
      MPI_Init(&argc, &argv);                    /* starts MPI */
      MPI_Comm_rank(MPI_COMM_WORLD, &myid);  /* get
current process id */
      MPI_Comm_size(MPI_COMM_WORLD, &p);     /* get number
of processes */
```

MPI_Probe, MPI_Wtime (C cont'd)

```
start_time = MPI_Wtime();   /* starts timer */
if (myid == 0) {
        for(i=0;i<50;++i) { sdata[i]=(double)i; }

MPI_Send(sdata,50,MPI_DOUBLE,1,123,MPI_COMM_WORLD);
} else {
        MPI_Probe(0,MPI_ANY_TAG,MPI_COMM_WORLD,&status);
        MPI_Get_count(&status,MPI_DOUBLE,&count);
        MPI_Type_size(MPI_DOUBLE,&n);   /* sizeof  */
        rdata= (double*) calloc(count,n);
        MPI_Recv(rdata,count,MPI_DOUBLE,0,MPI_ANY_TAG,
                        MPI_COMM_WORLD, &status);
        for(i=0;i<count;i+=10) {
          printf("rdata element %d is %f\n",i,rdata[i]);}
      }
end_time = MPI_Wtime();    /* ends timer */
```

MPI_Probe, MPI_Wtime (C cont'd)

```
 if (myid == 1) {
        printf("Total time is %f x %d\n", end_time-start_time, p);
      }
      MPI_Finalize();                      /* let MPI finish up ... */
}
```

Cartesian Topology
As applied to a 2D Laplace Equation

Laplace Equation

Laplace Equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad (1)$$

Boundary Conditions:

$$\begin{aligned} u(x,0) &= \sin(\pi x) && 0 \le x \le 1 \\ u(x,1) &= \sin(\pi x)e^{-x} && 0 \le x \le 1 \\ u(0,y) = u(1,y) &= 0 && 0 \le y \le 1 \end{aligned} \qquad (2)$$

Analytical solution:

$$u(x,y) = \sin(\pi x)e^{-xy} \qquad 0 \le x \le 1;\ \ 0 \le y \le 1 \qquad (3)$$

Laplace Equation Discretized

Discretize Equation (1) by centered-difference yields:

$$u_{i,j}^{n+1} \cong \frac{u_{i+1,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n}}{4} \qquad i = 1,2,\ldots,m; \;\; j = 1,2,\ldots,m \qquad (4)$$

where *n* and *n+1* denote the current and the next time step, respectively, while

$$u_{i,j}^{n} = u^{n}(x_i, y_j) \qquad i = 0,1,2,\ldots,m+1; \;\; j = 0,1,2,\ldots,m+1 \qquad (5)$$

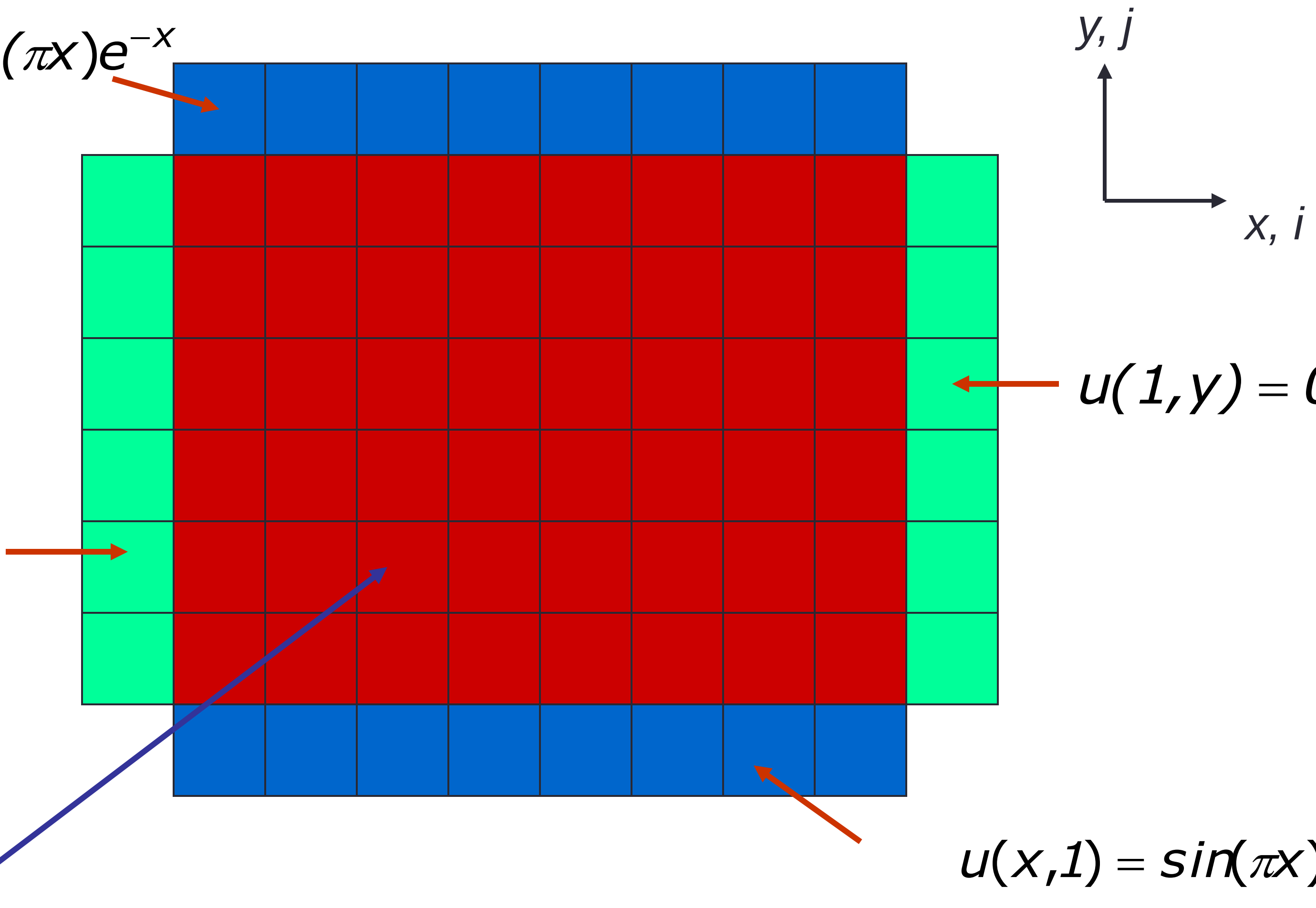
$$= u^{n}(i\Delta x, j\Delta y)$$

For simplicity, we take

$$\Delta x = \Delta y = \frac{1}{m+1}$$

Computational Domain

$u(x,1) = \sin(\pi x)e^{-x}$



$u(1,y) = 0$

$u(0,y) = 0$

$u(x,1) = \sin(\pi x)$

$$u_{i,j}^{n+1} \cong \frac{u_{i+1,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n}}{4}$$

$i = 1,2,\ldots,m; \quad j = 1,2,\ldots,m$

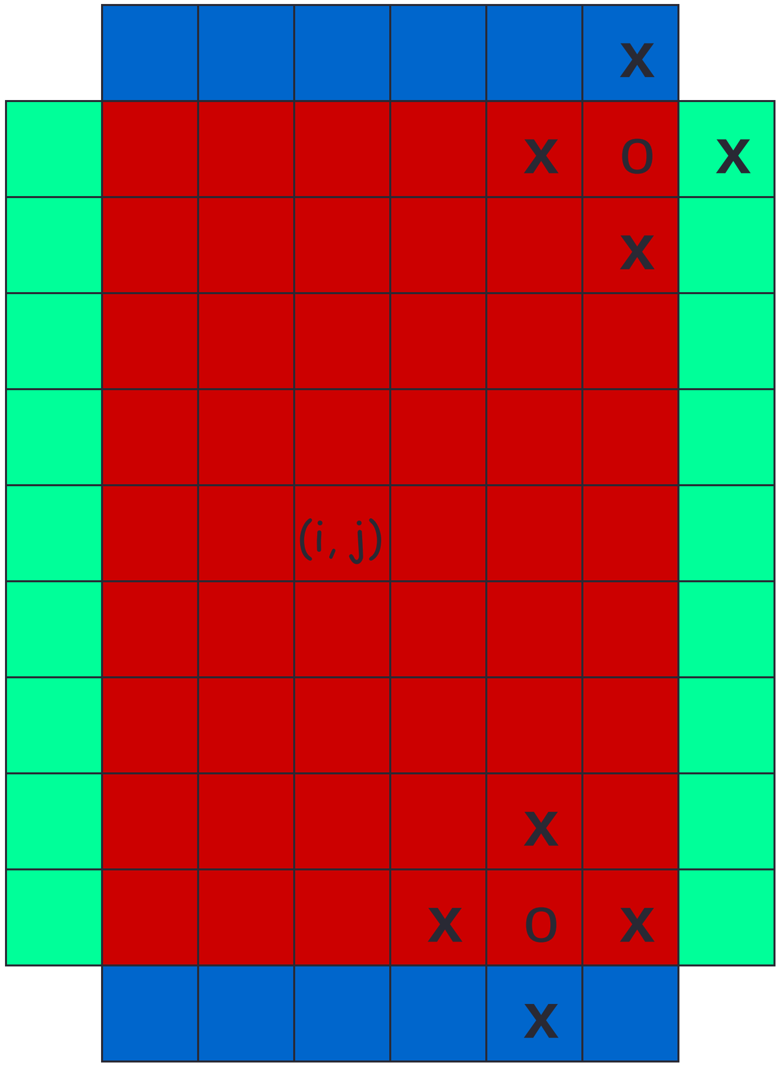
Five-point Finite-Difference Stencil

🟥 Interior (or solution) cells.

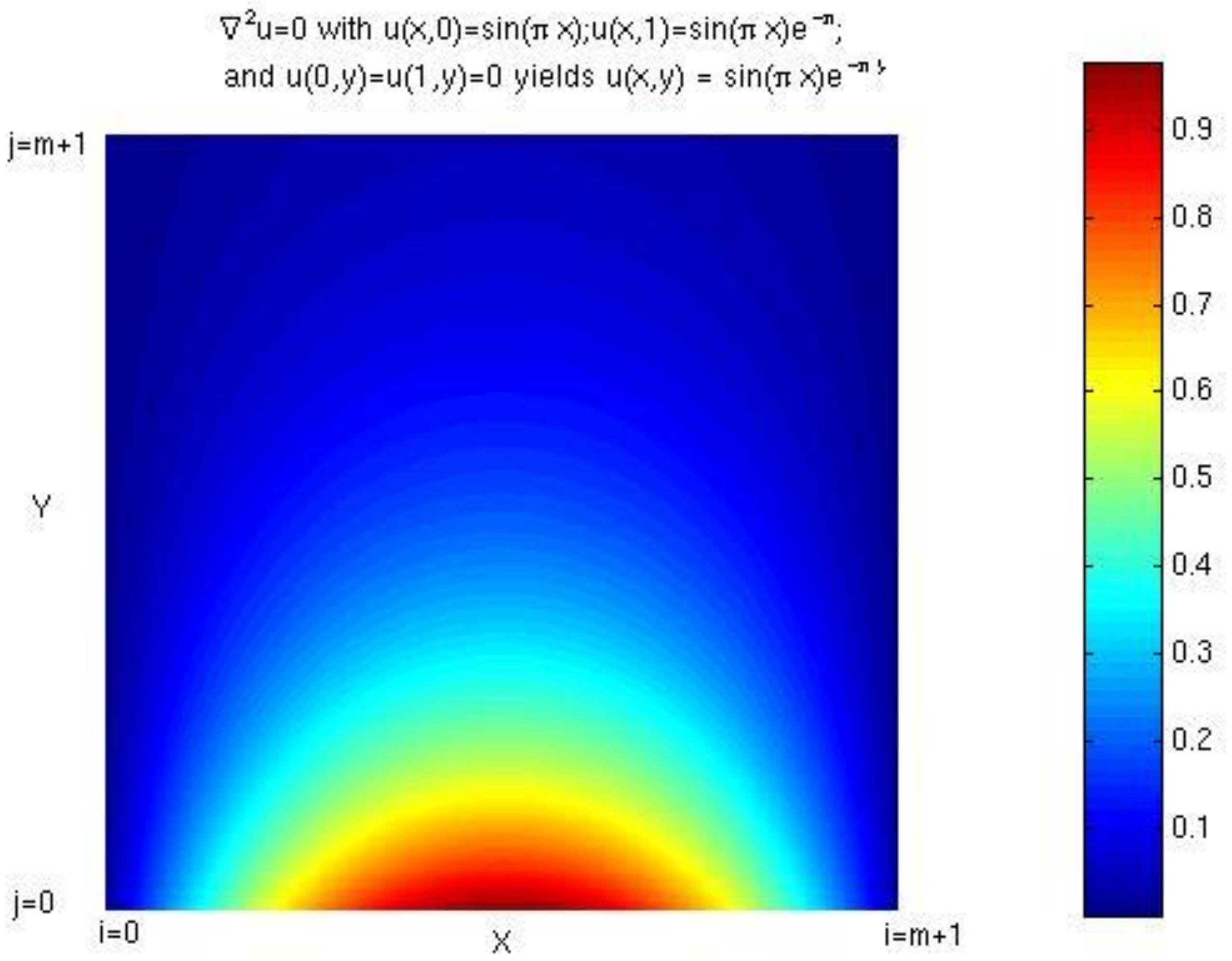
Where solution of the Laplace equation are sought.

🟦 🟩 Exterior (or boundary) cells.

Green cells denote cells where homo-geneous boundary conditions are imposed while non-homogeneous boundary conditions are colored in blue.

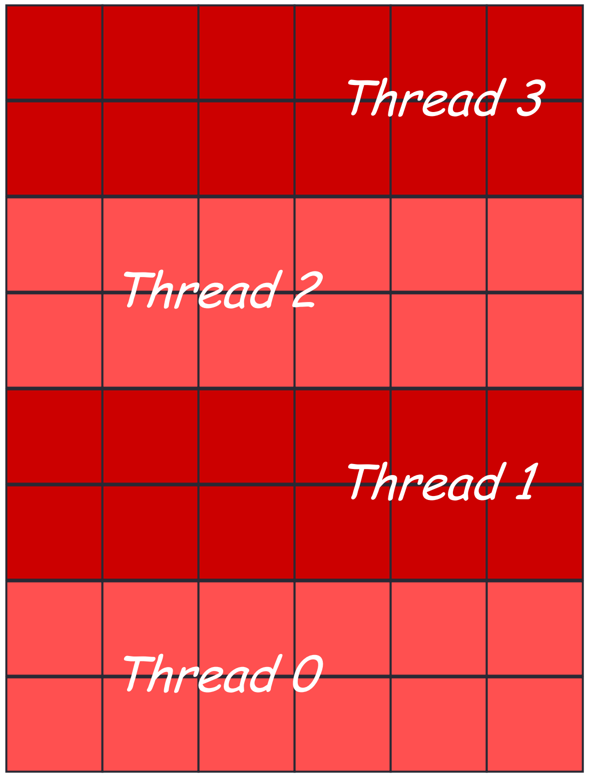


Solution Contour Plot

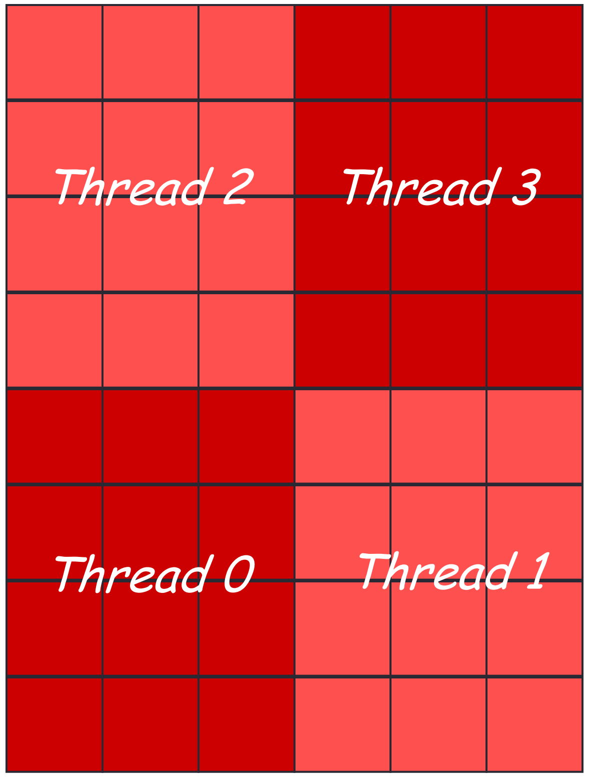


Domain Decompositions

1D Domain Decomposition



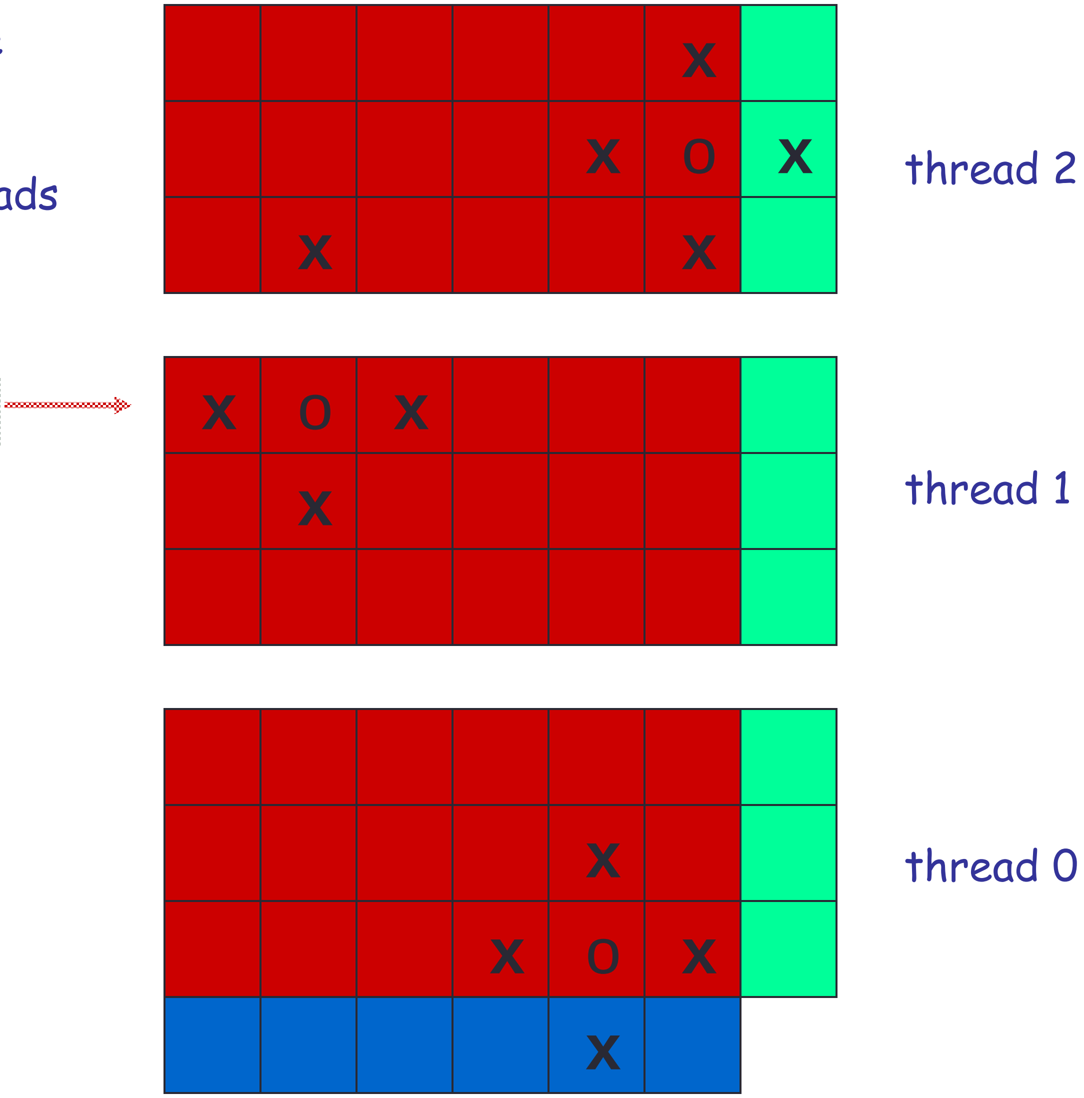
2D Domain Decomposition



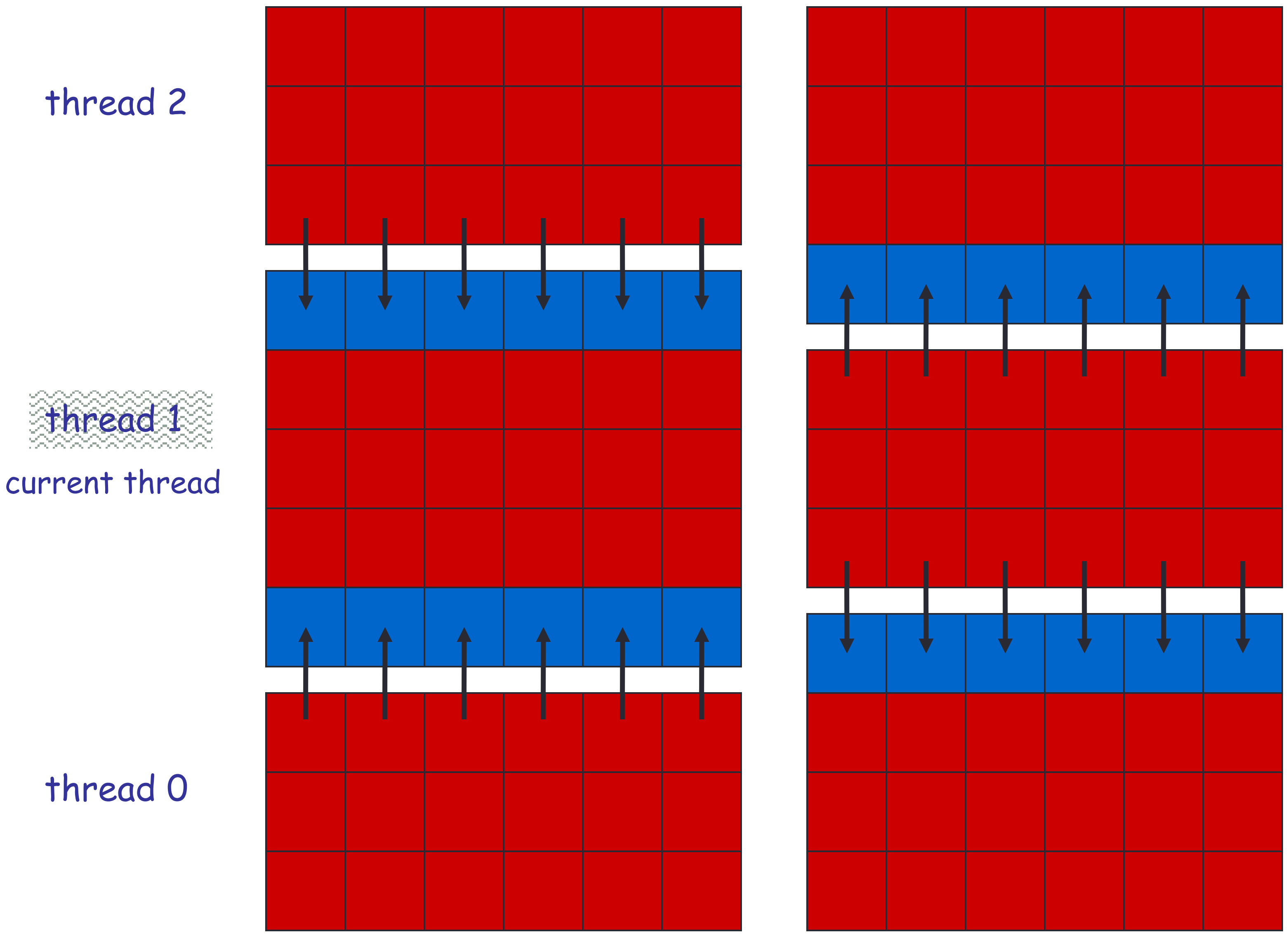
Unknowns At Border Cells – 1D

Five-point finite-difference stencil applied at thread domain border cells require cells from neighboring threads and/or boundary cells.

Message passing required



Message Passing to Fill Boundary Cells



For Individual Threads . . .

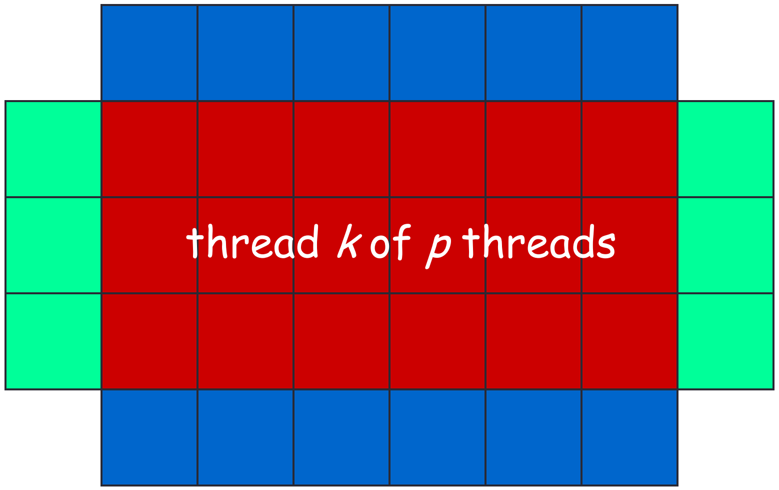
Recast 5-pt finite-difference stencil for individual threads

$$v_{\xi,\eta}^{n+1,k} = \frac{v_{\xi+1,\eta}^{n,k} + v_{\xi-1,\eta}^{n,k} + v_{\xi,\eta+1}^{n,k} + v_{\xi,\eta-1}^{n,k}}{4}$$

$$\xi = 1,2,\dots,m; \quad \eta = 1,2,\dots,m'$$
$$m' = m/p; \quad k = 0,1,2,\dots,p-1$$

Boundary Conditions

- 🟦 $v_{\xi,m'+1}^{n,k} = v_{\xi,1}^{n,k+1}; \quad \xi = 0,\dots,m+1; \quad k = 0$
- 🟦 $v_{\xi,0}^{n,k} = v_{\xi,m'}^{n,k-1}; \quad \xi = 0,\dots,m+1; \; 0 < k < p-1$
- 🟦 $v_{\xi,m'+1}^{n,k} = v_{\xi,1}^{n,k+1}; \quad \xi = 0,\dots,m+1; \; 0 < k < p-1$
- 🟦 $v_{\xi,0}^{n,k} = v_{\xi,m'}^{n,k-1}; \quad \xi = 0,\dots,m+1; \; k = p-1$



- For simplicity, assume *m* divisible by *p*
- B.C. time-dependent
- B.C. obtained by message-passing
- Additional boundary conditions on next page

Relationship Between u and v

Physical boundary conditions

- 🟦 $v_{\xi,0}^{n,k} = u(x_i,0) = sin(\pi x_i);\quad \xi = i = 0,\dots,m+1;\quad k = 0$
- 🟦 $v_{\xi,m'+1}^{n,k} = u(x_i,1) = sin(\pi x_i)e^{-\pi};\quad \xi = i = 0,\dots,m+1;\ k = p-1$
- 🟩 $v_{0,\eta}^{n,k} = u(0,y_{\eta+k*m'}) = 0;\quad \eta = 1,\dots,m';\ 0 \le k \le p-1$
- 🟩 $v_{m+1,\eta}^{n,k} = u(1,y_{\eta+k*m'}) = 0;\quad \eta = 1,\dots,m';\ 0 \le k \le p-1$

Relationship between global solution *u* and thread-local solution *v*

$$u_{\xi,\eta+k*m'}^{n} = v_{\xi,\eta}^{n,k}$$

$$\xi = 1,2,\ \dots, m;\quad \eta = 1,2,\ \dots, m'$$
$$m' = m/p;\quad k = 0,1,2,\ \dots, p-1$$

MPI Functions Needed For Job

- *MPI_Sendrecv* (= *MPI_Send* + *MPI_Recv*) – to set boundary conditions for individual threads
- *MPI_Allreduce* – to search for global error to determine whether convergence has been reached.
- *MPI_Cart_Create* – to create Cartesian topology
- *MPI_Cart_Coords* – to find equivalent Cartesian coordinates of given rank
- *MPI_Cart_Rank* – to find equivalent rank of Cartesian coordinates
- *MPI_Cart_shift* – to find current thread's adjoining neighbor threads

Successive Over Relaxation

1. Make initial guess for *u* at all interior points *(i,j)*.
2. Define a scalar $\omega_n \quad (0 \le \omega_n < 2)$
3. Use 5-pt stencil to compute $u'_{i,j}$ at all interior points *(i,j)*.
4. Compute $u^{n+1}_{i,j} = \omega_n u'_{i,j} + (1-\omega_n) u^n_{i,j}$
5. Stop if prescribed convergence threshold is reached.
6. Update: $u^n_{i,j} = u^{n+1}_{i,j} \quad \forall \; i, j$
7. Go to step 2.

$$\omega_0 = 0 \;\; ; \;\; \omega_1 = \frac{1}{1-\rho^2/2} \;\; ; \;\; \omega_2 = \frac{1}{1-\rho^2\omega_1/4}$$

$$\omega_n = \frac{1}{1-\rho^2\omega_{n-1}/4} ; \quad n > 2$$

$$\rho = 1 - \left(\frac{\pi}{2(m+1)}\right)^2$$

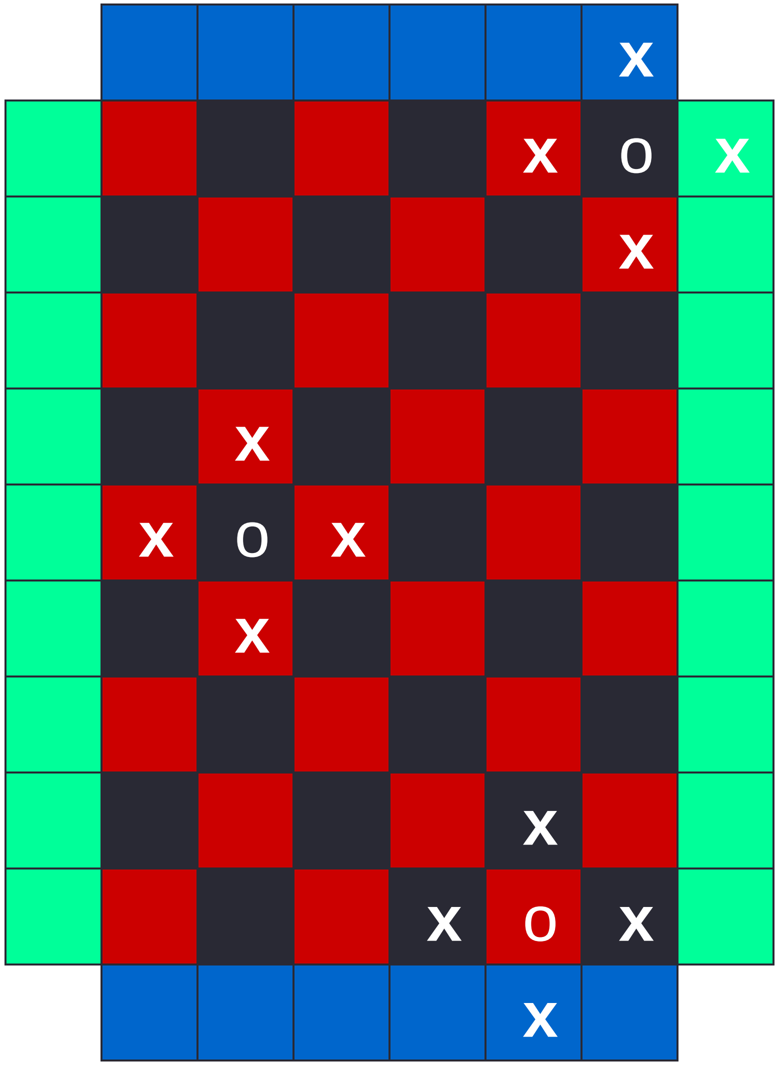
In Step 3, compute u' with u at time n+1 wherever possible to accelerate convergence. This inhibits parallelism.

Red-Black SOR Scheme

To enable parallelism, note that solution at black cells (by virtue of 5-pt stencil) depend on 4 neighbor red cells. Conversely, red solution cells depend only on 4 respective adjoining black cells.

1. Compute *v* at black cells at time *n+1* in parallel with *v* at red cells at time *n*.
2. Compute *v* at red cells at time *n+1* in parallel with *v* at black cells at time *n+1*.
3. Repeat steps 1 and 2 until converged

Can alternate order of steps 1 and 2.



Useful SCV Info

- **RCS home page** (http://www.bu.edu/tech/services/research/)
- **Resource Applications** http://www.bu.edu/tech/support/research/account-management/create-project/
- **Help**
  - **System**
    - **help@scc.bu.edu**
  - Web-based tutorials (http://www.bu.edu/tech/support/research/training-consulting/online-tutorials/)

    (MPI, OpenMP, MATLAB, IDL, Graphics tools)
  - HPC consultations by appointment
    - Kadin Tseng (kadin@bu.edu)