Advanced MPI

Erwin Laure
Director PDC-HPC

1

What we know already

- Everything to write typical MPI programs
  - Program structure
  - Point-to-point communication
  - Communication modes
  - Blocking/non-blocking communication
  - Collective Communication
  - Data types
  - Groups and communicators
  - Performance considerations

2

MPI provides additional, advanced features

- Virtual topologies
- MPI-IO
- One-sided communication
- Profiling Interface

- Very useful in special cases – go beyond an introductory lecture

- We will touch these issues only on the surface

3

MPI Profiling Interface

4

Profiling Interface Overview

- To understand program performance it is important to understand what the program is actually doing
- Simple printf's are not sufficient to understand the complex behavior of message passing programs
  - Where does synchronization occur?
  - Which process is waiting for input when?
  - Etc.

5

A side note: Timing in MPI

- To simply understand how long a program/a certain part of a program took MPI provides an interface to system timer:

```
double MPI_Wtime();
DOUBLE PRECISION MPI_WTIME()
```

- Timing resolution can be explored by

```
Double MPI_Wtick();
```

  - Resolution on the Cray is 1 microsecond
- Not enough to understand complex behavior

6

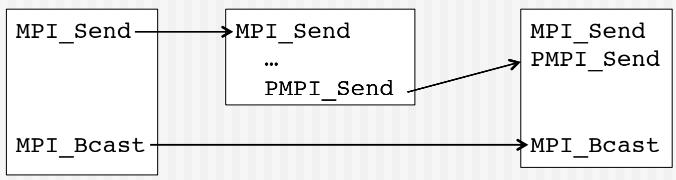
Profiling Interface

- MPI allows to log certain events to a log file that can be analyzed post-mortem
- Part of the MPI MultiProcessing Environment
  - Prefix MPE
  - **Tracing Library** This traces all MPI calls. Each MPI call is preceded by a line that contains the rank in MPI_COMM_WORLD of the calling process, and followed by another line indicating that the call has completed..
  - **Animation Library** This is a simple form of real-time program animation and requires X window routines.
  - **Logging Library** This is the most useful and widely used profiling libraries in MPE. They form the basis to generate log files from user MPI programs. There are currently 3 different log file formats allowed in MPE.

7

MPI Profiling Interface

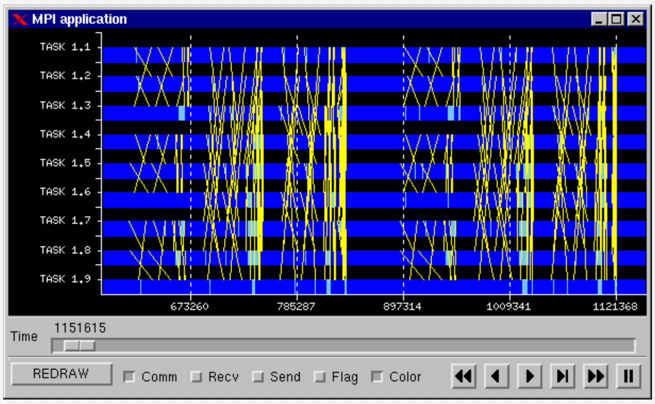
- You normally don't instrument and log events in your MPI program directly
- MPI provides a mechanism for tool developer to dynamically replace (at link time) standard MPI routines with instrumented ones through a nameshift
  - Each MPI call is also defined as PMPI



8

Using MPI Profiling

- Link against profiled MPI implementation
- This will produce a trace file
- Use performance tools (see performance lecture) to analyze the data



9

Virtual Topologies

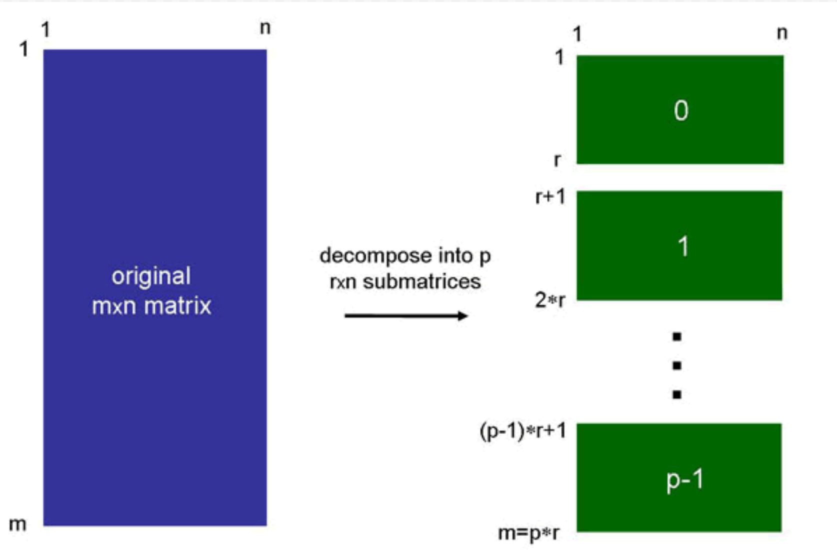
10

Ordering of Processes

- So far we have worked with a flat process space
  - Rank 0 … n-1
- Many application have however an inherent structure of their data
  - E.g. 2D or 3D matrices
- Likewise, the underlying network has a specific structure
  - E.g. fat tree, 3d torus (Cray)
- Can we take advantage of this and map processes in a similar fashion?

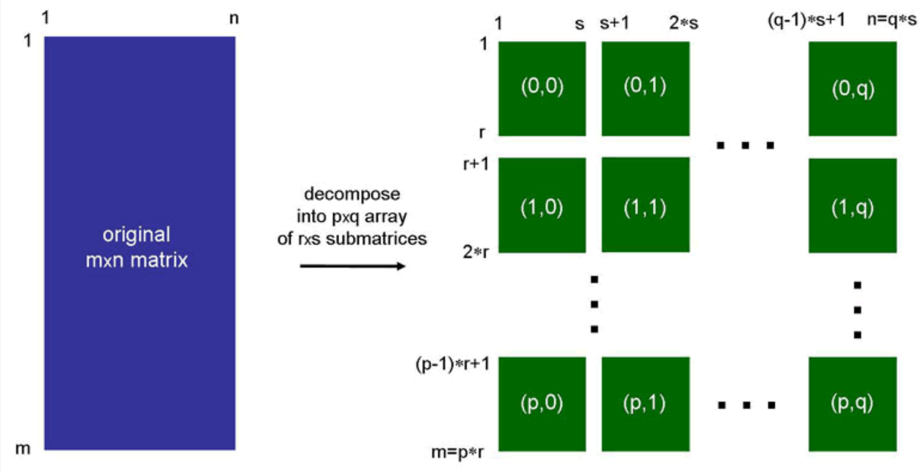
11

Example – Simple (flat) topology



12

Example – 2D Topology



- Can still use flat process space but requires tedious and error prone mapping

13

MPI Virtual Topologies

- MPI provides 2 types of virtual topologies
  - Cartesian
  - Graphs
- Cartesian topology (generalization of a grid function)
  - Each process is connected to its neighbors in a virtual grid
  - Boundaries can be cyclic (or not)
  - Processes are identified by (discrete) Cartesian coordinates
    - Eg. x,y,z
- Graph topology
  - Describe communication patterns by means of graphs
  - The most general description of communication patterns
  - Not covered here

14

Benefits of Virtual Topologies

- Convenient process naming
- Naming scheme to fit communication pattern
- Simplifies writing code
- Can allow MPI to optimize communications
  - Vendors can optimize mappings on their network topology

15

How do Virt. Topologies work?

- Creating a virtual topology produces a new communicator
- MPI provides mapping functions between the serial process enumeration and the virtual topology
- Mapping functions compute processor ranks based on the topology naming scheme

Virtual Grid

0,0 (0)	0,1 (1)
1,0 (2)	1,1 (3)
2,0 (4)	2,1 (5)

16

Main Cartesian Commands

- **MPI_CART_CREATE**: creates a new communicator using a Cartesian topology
- **MPI_CART_COORDS**: returns the corresponding Cartesian coordinates of a (linear) rank in a Cartesian communicator.
- **MPI_CART_RANK**: returns the corresponding process rank of the Cartesian coordinates of a Cartesian communicator.
- **MPI_CART_SUB**: creates new communicators for subgrids of up to (N-1) dimensions from an N-dimensional Cartesian grid.
- **MPI_CART_SHIFT**: finds the resulting source and destination ranks, given a shift direction and amount.

17

MPI_CART_CREATE

```
int MPI_Cart_create(MPI_Comm old_comm, int ndims,
    int *dim_size, int *periods, int reorder,
    MPI_Comm *new_comm)

MPI_CART_CREATE(OLD_COMM, NDIMS, DIM_SIZE, PERIODS,
                REORDER, NEW_COMM, IERR)
```

`periods:` Array of size ndims specifying periodicity status of each dimension

`reorder:` whether process rank reordering by MPI is permitted

`New_comm:` Communicator handle

18

Example

```
#include "mpi.h"
MPI_Comm old_comm, new_comm;
int ndims, reorder, periods[2], dim_size[2];

old_comm = MPI_COMM_WORLD;
ndims = 2;           /*  2-D matrix/grid */
dim_size[0] = 3;     /* rows */
dim_size[1] = 2;     /* columns */
periods[0] = 1;      /* row periodic (each column forms a
                        ring) */
periods[1] = 0;      /* columns nonperiodic */
reorder = 1;         /* allows processes reordered for
                        efficiency */

MPI_Cart_create(old_comm, ndims, dim_size,
                periods, reorder, &new_comm);
```

19

Example Cont'd

	-1,0 (4)	-1,1 (5)	
0,-1(-1)	0,0 (0)	0,1 (1)	0,2(-1)
1,-1(-1)	1,0 (2)	1,1 (3)	1,2 (-1)
2,-1(-1)	2,0 (4)	2,1 (5)	2,2 (-1)
	3,0 (0)	3,1 (1)	

periods(0)=.true.;periods(1)=.false.

20

Note

- `MPI_CART_CREATE` is a collective communication function so it must be called by all processes in the group. Like other collective communication routines, `MPI_CART_CREATE` uses blocking communication. However, it is not required to be synchronized among processes in the group and hence is implementation dependent.
- If the total size of the Cartesian grid is smaller than available processes, those processes not included in the new communicator will return `MPI_COMM_NULL`.
- If the total size of the Cartesian grid is larger than available processes, the call results in error.

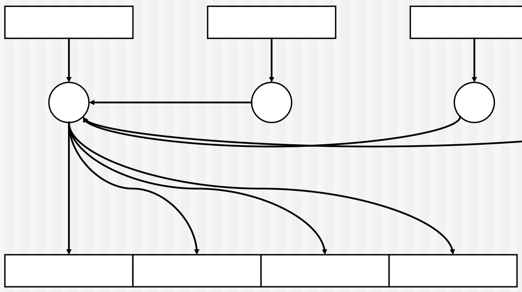
21

MPI-IO

22

Common Ways of Doing I/O in Parallel Programs

- Sequential I/O:
  - All processes send data to process 0, and 0 writes it to the file

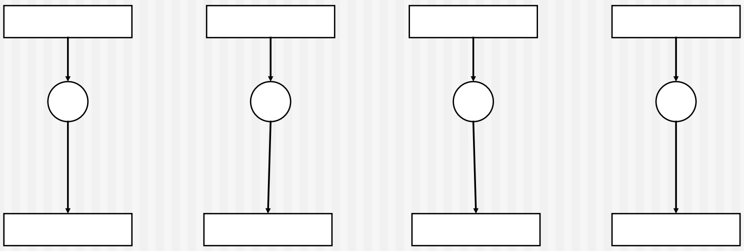


Pros and Cons of Sequential I/O

- Pros:
  - parallel machine may support I/O from only one process
    - (e.g., no common file system)
  - Some I/O libraries (e.g. HDF-4, NetCDF) not parallel
  - resulting single file is handy for **`ftp`**, **`mv`**
  - big blocks improve performance
  - short distance from original, serial code
- Cons:
  - lack of parallelism limits scalability, performance (single node bottleneck)

Another Way

- Each process writes to a separate file

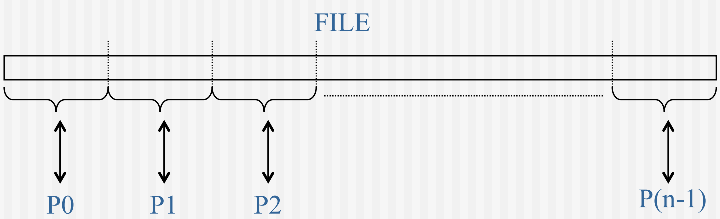


- Pros:
  - parallelism, high performance
- Cons:
  - lots of small files to manage
  - difficult to read back data from different number of processes
  - Lots of requests can make trouble to the file system

25

What is Parallel I/O?

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



26

Why Parallel I/O?

- Non-parallel I/O is simple but
  - Poor performance (single process writes to one file) or
  - Awkward and not interoperable with other tools (each process writes a separate file)
- Parallel I/O
  - Provides high performance
  - Can provide a single file that can be used with other tools (such as visualization programs)

27

What is MPI-IO

- I/O interface specification for use in MPI applications
- Data model is a stream of bytes in a file
  - Same as POSIX and stdio
- Features
  - Noncontiguous I/O with MPI datatypes and file views
  - Collective I/O
  - Nonblocking I/O
  - Language bindings

28

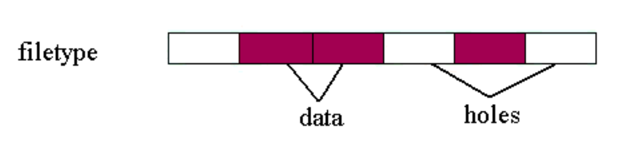
MPI File Structure

- MPI defines how multiple processes access and modify data in a shared file.
- Necessary to think about how data is partitioned within this file
  - Similar to how derived datatypes define data partitions within memory
- MPI-IO works with simple datatypes and derived datatypes
  - Derived datatypes are preferred because of performance benefits
- A view defines the current set of data, visible and accessible, from an open file.
  - Each process has its own view of the shared file that defines what data it can access.
  - A view can be changed by the user during program execution.

29

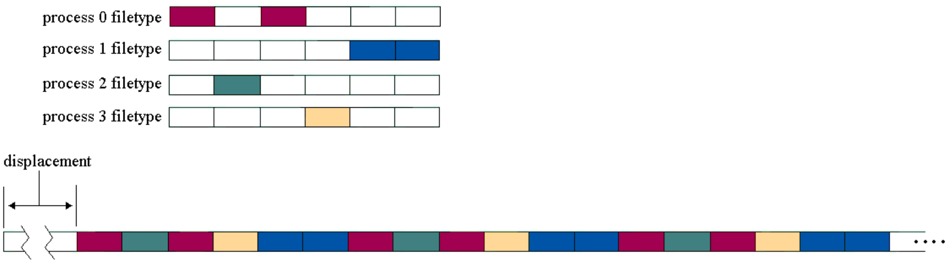
Essential Concepts

- Displacement
  - describes where to start in the file
- Elementary datatype (etype)
  - the type of data that is to be written or read
  - Basic or derived datatype
- Filetype
  - the pattern of how the data is partitioned in the file
  - A filetype is a defined sequence of etypes, which can have data or be considered blank



30

Example: File views



31

Simple Example

```
MPI_File fh;
MPI_Status status;
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
bufsize = FILESIZE/nprocs;
nints = bufsize/sizeof(int);

MPI_File_open(MPI_COMM_WORLD, "/pfs/datafile",
              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);
MPI_File_close(&fh);
```

offset

32

More about MPI-IO

- See for instance

*www.npaci.edu/ahm2002/ahm_ppt/**Parallel_IO_MPI_2**.ppt*
Rajeev Thakur. Mathematics and Computer Science Division. Argonne National Laboratory

33

One-sided Communication

34

Recap: Point-to-point Communication

- Both sender and receiver must issue matching MPI calls
  - Depending on buffering semantics may require handshake
- Sometimes it is difficult to know in advance when messages have to be sent/received and what characteristics these messages have
  - Could solve such situations with extra control messages
    - Requires polling, introduces overhead, and is cumbersome
- MPI provides Remote Memory Access (RMA), or one-sided communication
  - Allows one process to specify all communication parameters for both the sender and receiver

35

One-sided Communication

- Communication and Synchronization are separated
- Allows remote processes to
  - Write into local memory (**put**)
  - Read local memory (**get**)
- Accessible memory areas are called “windows”
- Communication can happen without synchronization
- Access to windows is synchronized

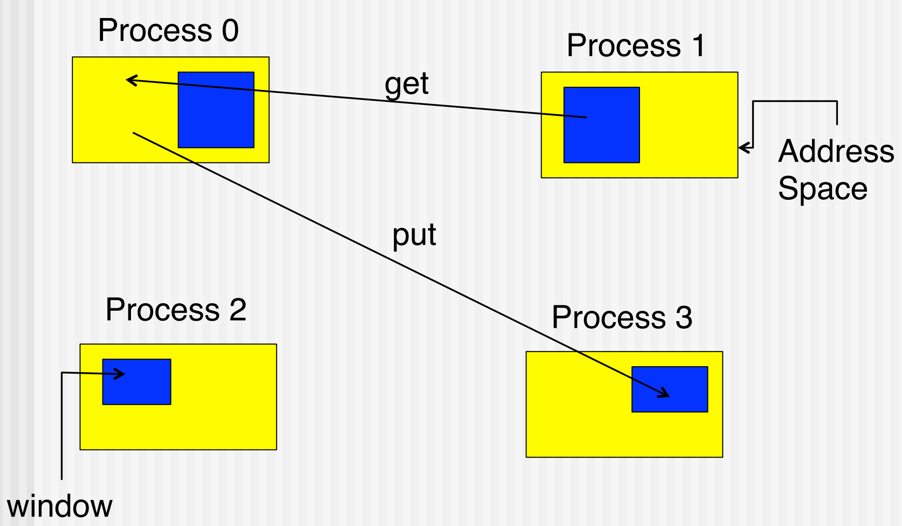
36

Looks a bit like shared-memory programming?

- In fact, tries to bring the advantages of shared-memory programming to MPI programs
- Effective implementation needs shared memory or hardware support for RDMA
  - Available e.g. in infiniband or Cray networks
- Need synchronization to ensure correct behavior
  - Same issues as in shared-memory programming
  - MPI provides **window objects** for synchronization
- How to implement synchronization is a great optimization field

37

Window Objects



38

Main Commands

- `MPI_Win_create` exposes local memory to RMA operation by other processes in a communicator
  - Collective operation
  - Creates window object
- `MPI_Win_free` deallocates window object
- `MPI_Put` moves data from local memory to remote memory
- `MPI_Get` retrieves data from remote memory into local memory
- `MPI_Accumulate` updates remote memory using local values
- Data movement operations are non-blocking
- **Subsequent synchronization on window object needed to ensure operation is complete**

39

Advantages of one-sided communication

- Can do multiple data transfers with a single synchronization operation
- Bypass tag matching
  - effectively precomputed as part of remote offset
- Some irregular communication patterns can be more economically expressed
- Can be significantly faster than send/receive on systems with hardware support for remote memory access, such as shared memory systems
  - **BUT**: can also be significantly slower depending on synchronization need and access patterns!

40

Synchronization

- `Put/Get/Accumulate` are non-blocking
  - Subsequent synchronization on window object is needed to ensure operations are complete
- MPI_Win_fence is used to synchronize access to windows
  - Should be called before and after RMA
  - Similar to a barrier in shared memory

Process 0	Process 1
`MPI_Win_fence(win)`	`MPI_Win_fence(win)`
`MPI_Put`	
`MPI_Put`	
`MPI_Win_fence(win)`	`MPI_Win_fence(win)`

41

Summary

- One-sided communication provides convenient means for irregular applications
- Communication can be more efficient with proper hardware support
- Great care needs to be put on (efficient) synchronization

42

And finally …

- The top MPI Errors according to

Advanced MPI: I/O and One-Sided Communication, presented at SC2005, by William Gropp, Rusty Lusk, Rob Ross, and Rajeev Thakur
http://www.mcs.anl.gov/research/projects/mpi/tutorial/advmpi/sc2005-advmpi.pdf)

43

Top MPI Errors

- Fortran: missing ierr argument
- Fortran: missing MPI_STATUS_SIZE on status
- Fortran: Using integers where MPI_OFFSET_KIND or MPI_ADDRESS_KIND integers are required (particularly in I/O)
- Fortran 90: Using array sections to nonblocking routines (e.g., MPI_Isend)
- All: MPI_Bcast not called collectively (e.g., sender bcasts, receivers use MPI_Recv)
- All: Failure to wait (or test for completion) on MPI_Request
- All: Reusing buffers on nonblocking operations
- All: Using a single process for all file I/O
- All: Using MPI_Pack/Unpack instead of Datatypes
- All: Unsafe use of blocking sends/receives
- All: Using MPI_COMM_WORLD instead of comm in libraries
- All: Not understanding implementation performance settings
- All: Failing to install and use the MPI implementation according to its documentation.

44

Summary

- MPI allows to write portable parallel code across many different architectures
- Writing simple MPI programs is easy (6 commands)
- Writing efficient MPI programs is difficult
  - Need also to understand MPI implementation and underlying hardware
  - Experiment with different options
  - Also experiment with hybrid approaches: use Open-MP within a nodes and MPI across nodes

45