MPI-2 Overview

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Acknowledgements

Parts of this course is based on MPI-2 tutorial on the MPIDC 2000:

MPI-2: Extensions to the Message Passing Interface

Anthony Skjellum
Purushotham Bangalore, Shane Hebert
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MPI-2 Outlook

- MPI-2, standard since July 18, 1997
- Chapters:
  - Version 1.2 of MPI (Version number, Clarifications)
  - Miscellany (Info Object, Language Interoperability, New Datatype Constructors, Canonical Pack & Unpack, C macros)
  - Process Creation and Management (MPI_Spawn, ...)
  - One-Sided Communications
  - Extended Collective Operations
  - External interfaces (..., MPI and Threads, ...)
  - I/O
  - Language Binding (C++, Fortran 90)
- All documents from http://www.mpi-forum.org/
  (or from www.hlrs.de/mpi/)

MPI-1.2

- New function to obtain version of the MPI Standard implemented
- Compile time information
  - integer MPI_VERSION=1, MPI_SUBVERSION=2
- Runtime information
  - MPI_GET_VERSION( version, subversion )
- MPI_GET_VERSION can be called before MPI_INIT and after MPI_FINALIZE
- Clarifications and corrections to MPI-1.1
  - pointer to MPI-2 Chapter 10.2.2
  Problems with Fortran Bindings for MPI
MPI 1.2 — Clarifications to MPI 1.1

- **MPI_INITIALIZED**
  - behavior not affected by MPI_FINALIZE
- **MPI_FINALIZE**
  - user must ensure the completion of all pending communications (locally) before calling finalize
  - is collective on MPI_COMM_WORLD
  - may abort all processes except “rank==0” in MPI_COMM_WORLD
- Status object after MPI_WAIT/MPI_TEST
- **MPI_INTERCOMM_CREATE**
- **MPI_INTERCOMM_MERGE**

MPI 1.2 — Clarifications to MPI 1.1 (continued)

- Bindings for MPI_TYPE_SIZE
  - output argument in C is of type `int`
- **MPI_REDUCE**
  - the `datatype` and `op` for predefined operations must be same for all processes
- **MPI_PROBE and MPI_IPROBE**
- Attribute callback functions error behavior
- Other minor corrections
  - with nonblocking & persistent communications and MPI_Address:
    - Fortran problems with data copying and sequence association
    - Fortran problems with register optimization
Dynamic Process Management

• Goals
  – starting new MPI processes
  – connecting independently started MPI processes

• Issues
  – maintaining simplicity, flexibility, and correctness
  – interaction with operating systems, resource manager, and process manager

• Spawn interfaces:
  – at initiators (parents):
    • Spawning new processes is collective, returning an intercommunicator.
    • Local group is group of spawning processes.
    • Remote group is group of spawned processes.
  – at spawned processes (children):
    • New processes have own MPI_COMM_WORLD
    • MPI_Comm_get_parent() returns intercommunicator to parent processes

Dynamic Process Management — Get the intercomm, I.
Dynamic Process Management — Get the intercomm, II.

Parents:
MPI_COMM_SPAN
   _MULTIPLE (0, root, comm, intercomm, ...)

Children:
MPI_Init(...)
MPI_COMM_GET_PARENT(intercomm)

Dynamic Process Management — Multi-merging, a Challenge

- If a comm. P spawns A and B sequentially, how can P, A and B communicate in a single intracomm?
- The following sequence supports this:
  - P+A merge to form intracomm PA
  - P+B merge to form intracomm PB
  - PA and B create intercomm PA+B
    [using PB as peer, with p, b as leaders]
  - PA+B merge to form intracomm PAB
- This is not very easy, but does work
Dynamic Process Management — MPI_Info Object

- An MPI_Info is an opaque object that consists of a set of (key,value) pairs
  - both key and value are strings
  - a key should have a unique value
  - several keys are reserved by standard / implementation
  - portable programs may use MPI_INFO_NULL as the info argument, or sets of vendor keys
  - Several sets of vendor-specific keys may be used
- Allows applications to pass environment-specific information
- Several functions provided to manipulate the info objects
- Used in: Process Creation, Window Creation, MPI-I/O

Dynamic Process Management — Establishing Communication

1. A: Open port: returns portname “ppp”
2. A: tell “ppp” to appl. B (e.g. via a name service)
3. B: get portname “ppp”
4. B: connect to “ppp”
5. A: accept the connection

Result: An intercommunicator between both original communicators
Dynamic Process Management — Another way

- Another way to establish MPI communication
- `MPI_COMM_JOIN(fd, intercomm)`
- joins by an intercommunicator
- two independent MPI processes
- that are connected with Berkley Sockets of type SOCK_STREAM

Dynamic Process Management — Singleton INIT

- High quality MPI’s will allow single processes to start, call `MPI_INIT()`, and later join in with other MPI programs
- This approach supports parallel plug-ins to sequential APPs
  - other transparent uses of MPI
- Provides a means for using MPI without having to have the “main” program be MPI specific.
One-Sided Operations

- **Goals**
  - PUT and GET data to/from memory of other processes
- **Issues**
  - Synchronization is separate from data movement
  - Automatically dealing with subtle memory behavior: cache coherence, sequential consistency
  - Balancing efficiency and portability across a wide class of architectures
    - shared-memory multiprocessor (SMP)
    - clusters of SMP nodes
    - NUMA architecture
    - distributed-memory MPP’s
    - workstation networks
- **Interface**
  - PUTs and GETs are surrounded by special synchronization calls

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One-Sided Operations — Origin and Target

- Communication parameters for both the sender and receiver are specified by one process (origin)
- User must impose correct ordering of memory accesses

Origin Process

Target Process (the owner of the memory)
One-Sided Operations — An Example

- The target process declares a window with
  - `MPI_WIN_CREATE(base_addr, win_size, disp_unit, info, comm, win)`
- Synchronization necessary between
  - remote memory access (RMA)
    - `MPI_PUT`
    - `MPI_GET`
    - `MPI_ACCUMULATE`
  - and local memory access
    - loads and stores, generated by the compiler
- Three synchronization methods:
  - `MPI_FENCE` (like a barrier)
  - Post / start / wait / complete (point-to-point synchronization)
  - Lock / unlock (allows passive target communication)

Extended Collective Operations

- In MPI-1, collective operations are restricted to ordinary (intra) communicators.
- In MPI-2, most collective operations are extended by an additional functionality for intercommunicators
  - e.g., Bcast on a parents-children intercommunicator: sends data from one parent process to all children.
- Provision to specify "in place" buffers for collective operations on intracommunicators.
- Two new collective routines:
  - generalized all-to-all
  - exclusive scan
Extended Collective Operations — MPI_Bcast on intercomm.

- root = MPI_ROOT
- broadcast communication

Extended Collective Operations — MPI_Allgather on intercomm.

- remember: allgather = gather + broadcast
- allgather communication
Extended Collective Operations —
“In place” Buffer Specification

The **MPI_IN_PLACE** has two meanings:
- to prohibit the local copy:
  - GATHER(V), SCATTER(V) at root node
  - ALLGATHER(V) at any node
- to overwrite input buffer with the result:
  (sendbuf=**MPI_IN_PLACE**, input is taken from recvbuf, which is then overwritten)
  - REDUCE at root
  - ALLREDUCE, REDUCE_SCATTER, SCAN at any node

Extended Collective Operations —
Generalized All-to-all

- The most general form of all-to-all
- Allows separate specification of count, displacement, and **datatype**
- Displacement is specified in terms of no. of bytes to allow maximum flexibility
- Useful for matrix transpose and corner-turn operations

**MPI_Alltoall**(sendbuf, sendcounts, sdispls, **sendtypes**, recvbuf, recvcounts, rdispls, **recvtypes**, comm)

- recvtypes, sendtypes now both arrays
MPI - I/O

- Goals:
  - reading and writing files in parallel
- Rich set of features:
  - Basic operations: open, close, read, write, seek
  - noncontiguous access in both memory and file
  - logical view via filetype and element-type
  - physical view addressed by hints, e.g. "striping_unit"
  - explicit offsets / individual file pointers / shared file pointer
  - collective / non-collective
  - blocking / non-blocking or split collective
  - non-atomic / atomic / explicit sync
  - “native” / “internal” / “external32” data representation

MPI - I/O — Logical view / Physical view

mpi processes of a communicator

file, logical view

file, physical view

addressed only by hints

scope of MPI-I/O
MPI - I/O — Definitions

- etype (elementary datatype)
- filetype
  - filetype process 0
  - filetype process 1
  - filetype process 2
- file
- displacement
- logical view

 MPI - I/O — Example with Subarray: Reads and distributes a matrix

```fortran
!! real garray(20, 30) ! these HPF-like comment lines
!! PROCESSORS P(2, 3) ! explain the data distribution
!! DISTRIBUTE garray(BLOCK,BLOCK) ! used in this MPI program

real larray(10, 10) ; integer (kind=MPI_OFFSET_KIND) disp ; disp=0
ndims=2 ; psizes(1)=2 ; period(1)=.false. ; psizes(2)=3 ; period(2)=.false.
call MPI_CART_CREATE(MPI_COMM_WORLD, ndims, psizes, period, .TRUE., comm,ierror)
call MPI_COMM_RANK(comm, rank, ierror)
call MPI_CART_COORDS(comm, rank, ndims, coords, ierror)
gsizes(1)=20 ; lsizes(1)=10 ; starts(1)=coords(1)*lsizes(1)
gsizes(2)=30 ; lsizes(2)=10 ; starts(2)=coords(2)*lsizes(2)
call MPI_TYPE_CREATE_SUBARRAY(ndims, gsizes, lsizes, starts, MPI_ORDER_FORTRAN, MPI_REAL, subarray_type, ierror)
call MPI_TYPE_COMMIT(subarray_type , ierror)
call MPI_FILE_OPEN(comm, 'exa_subarray_testfile', MPI_MODE_CREATE + MPI_MODE_RDONLY, MPI_INFO_NULL, fh, ierror)
call MPI_FILE_SET_VIEW(fh, disp, MPI_REAL, subarray_type, 'native', MPI_INFO_NULL, ierror)
call MPI_FILE_READ_ALL(fh, larray, lsizes(1)*lsizes(2), MPI_REAL, status, ierror)
```
Other MPI-2 Features (1)

- Standardized Process Startup: `mpiexec`
- C / C++ / Fortran language interoperability
- Datatypes:
  - New constructors:
    - `MPI_Type_create_darray / ..._subarray / ..._indexed_block`
  - new routines due to incorrect Fortran binding in MPI-1:
    - `INTEGER (KIND=MPI_ADDRESS_KIND) ...` in MPI-2
  - new predefined datatypes:
    - `MPI_WCHAR, MPI_SIGNED_CHAR, MPI_UNSIGNED_LONG_LONG`
- Null values:
  - `MPI_Init(NULL,NULL)`
  - `MPI_STATUS(ES)_IGNORE` instead of `(&)status`

Other MPI-2 Features (2)

- C/C++/Fortran Language interoperability support
  - between languages in same processes
  - messages transferred from one language to another
- `(P)MPI_Wtime and ..._Wtick may be implemented as macros in C`
- New values `VERSION=2, SUBVERSION=0`
### Deprecated Names/Functions

<table>
<thead>
<tr>
<th>Deprecated</th>
<th>MPI-2 Replacement</th>
</tr>
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<tbody>
<tr>
<td>MPI_ADDRESS</td>
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<tr>
<td>MPI UB</td>
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<tr>
<td>MPI LB</td>
<td>MPI_TYPE_CREATE_RESIZED</td>
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</tbody>
</table>

Motivation: Incorrect Fortran interface for Aint

### Process Startup

- Current MPI implementations provide the “mpirun” as a startup command which is not standard and not portable
- MPI-2 specifies an “mpiexec” startup command (recommended)

```bash
mpiexec {-n <maxprocs> -soft < > -host < > -arch < > -wdir < > -path < > -file < > ....... Command
```

...
**C++ Language Bindings**

- C++ bindings match the new C bindings
- MPI objects are C++ objects
- MPI functions are methods of C++ classes
- User must use MPI create and free functions instead of default constructors and destructors
- Uses shallow copy semantics (except MPI::Status objects)
- C++ exceptions used instead of returning error code
- declared within an MPI namespace (MPI::...)
- C++/C mixed-language interoperability

**Fortran 90 Support, I.**

- MPI-2 Fortran bindings are Fortran 90 bindings that are “Fortran 77 friendly” (most cases)
- Fortran 90 and MPI have several incompatibilities
  - strong typing vs. choice arguments
  - data copying vs. sequence association
  - special values vs. special constants
  - ...
- MPI-2 standard documents the “do’s” and “don’ts” while using Fortran 90 / 77 features
  - Chap. 10.2.2 “Problems with Fortran Bindings for MPI”
Problems Due to Data Copying and Sequence Association

- **Example 1:**

```fortran
real a(100)
call MPI_Irecv(a(1:100:2), MPI_REAL, 50, ...)
```

- First dummy argument of MPI_Irecv is an assumed-size array (`<type> buf(*)`)
- `a(1:100:2)` is copied into a scratch array, which is freed after the end of MPI_Irecv
- Afterwards, until MPI_Wait, there is no chance to store the results into `a(1:100:2)`

- **Example 2:**

```fortran
real a
call user1(a,rq)
call MPI_Wait(rq,status,ierr)
write (*,*) a
subroutine user1(buf,request)
call MPI_Irecv(buf, ..., request, ...)
end
```

- the compiler has to guarantee, that it makes no copy of the scalar `a`
  - neither in the calling procedure
  - nor in the called procedure
- check for compiler flags!
- guarantee is necessary for
  - `MPI_Get_address`
  - all non-blocking MPI routines
Fortran Problems with Register Optimization and 1-sided

- Fortran register optimization
- Result ccc=999, but expected ccc=777
- How to avoid: see MPI-2, Chap. 6.7.3
  - window memory declared in COMMON blocks
    - i.e. MPI_ALLOC_MEM cannot be used
  - declare window memory as_VOLATILE
    - (non-standard, disables compiler optimization)
  - Calling MPI_Address(buff, idummy_addr, ierror) after 2nd FENCE in process 2

Fortran 90 Support, II.

- Different support levels:
  - Basic Fortran support
    - mpif.h is valid with free-form and fixed-form
  - Extended Fortran support
    - an mpi module [use mpi] instead of [include mpif.h]
    - datatype generation routines for KIND-parameterized Fortran types:
      - MPI_TYPE_CREATE_F90_INTEGER
      - MPI_TYPE_CREATE_F90_REAL
      - MPI_TYPE_CREATE_F90_COMPLEX
    - alternative concept [not appropriate for heterogeneous platforms]:
      - MPI_SIZEOF, MPI_TYPE_MACH_SIZE
Summary of MPI-2

- MPI-2 standard document available since July 1997
- Provides extensions to MPI-1, does not replace MPI-1
- Provides a wide variety of functionality, some still untested
- Implementation of parts of the MPI-2 standard are available
- Nearly full implementations were available by mid-2000 on
  - Fujitsu
  - NEC
  - Hitachi
- Subset examples:
  - Cray: mpt.1.4.0.1 (MPI-I/O [romio], one-sided)
  - MPICH
  - LAM: with dynamic process start
- List of MPI-2 implementations and subsets: [www.mpi.nd.edu/MPI2/](http://www.mpi.nd.edu/MPI2/)

Other MPI Activities

- Metacomputing
  - MPI-PACX, MetaMPI, HARNESS, Globus, StaMPI, ...
  - IMPI (Interoperable Message Passing Interface)
- Real-time MPI
- Additional MPI Language Bindings
  - Java
  - Ada-95
  - COM
- The DARPA Data Reorganization Standard
- MPI on PC clusters

(see [www.hlrs.de/mpi/](http://www.hlrs.de/mpi/) )