Programming with MPI

Communicators etc.

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Programming with MPI – p. 1/??

Basic Concepts

A group is a set of process identifiers Programs view them as integers 0...(size-1)

A context is the communication environment Separate contexts are entirely independent Programs don't (and can't) view contexts directly

A communicator is a group plus a context So separate communicators are independent, too

Even if they have the same group of processes

Normally, we work solely on communicators

Predefined Communicators

There are several predefined communicators Use these when appropriate

MPI_COMM_WORLD is all processes together

MPI_COMM_SELF is just the local process

MPI_COMM_NULL is an invalid communicator Used as an error result from several functions

Use of Communicators (1)

Most people use only MPI_COMM_WORLD We covered information calls in the first lecture MPI_Comm_rank and MPI_Comm_size Why do we need to go beyond that?

- To use collectives on only some processes
- Need to do a task on only some processes
- Want to do several tasks in parallel

Can do those messily by using point-to-point Or by creating new, subset communicators

Use of Communicators (2)

Avoid using two communicators that overlap Including one together with a subset of itself Clean up the use of one before starting the other

• MPI won't get confused – but you and I will And don't even think of trying to tune such a mess!

Design your communicator use to be hierarchical Like recursion in groups of processes

This is easier to show using pictures

General Communicators

MPI_COMM_WORLD



Hierarchical Communicators

MPI_COMM_WORLD



Using Hierarchies



Splitting Communicators (1)

• You always start with an existing communicator And subdivide it to make one or more new ones A collective call on the existing communicator

 Each process specifies a non-negative integer The value is commonly called the colour
 Each new communicator corresponds to one colour
 E.g. all processes that specify the integer 42

If two processes specify different colours the call returns different communicators

• A communicator is a value not an identifier

Splitting Communicators (2)

Can also specify MPI_UNDEFINED to opt out That is an unspecified negative integer Note that zero is a valid colour

Call will return MPI_COMM_NULL

• This is an invalid communicator – don't use it

Splitting Communicators





Splitting Communicators (3)

Can also set the rank in the new communicator A key argument that has an integer value Any values are allowed, even negative ones

Processes have ranks in key order All keys to zero says you don't care

I recommend doing just that – one less detail

Doing anything else with keys is advanced use Comparable to operating on groups directly

Destroying Communicators

When you have finished with a communicator You should free (delete/destroy) it A collective call on the communicator

This will free any resources it uses

• You must tidy up all transfers first Some libraries and tools may check that is so

• You needn't free it if you only stop using it I.e. when you are going to reuse it later

Split (1)

Fortran example:

INTEGER :: colour , newcomm , error
! 'colour' is set to an appropriate value

CALL MPI_Comm_split (& MPI_COMM_WORLD, & colour, 0, newcomm, error) IF (newcomm /= MPI_COMM_NULL) THEN CALL My_collective (newcomm, ...) CALL MPI_Comm_free (newcomm, error) END IF

Split (2)

C example:

```
int colour, error;
/* 'colour' is set to an appropriate value */
MPI Comm newcomm;
error = MPI_Comm_split (MPI_COMM_WORLD,
    colour, 0, & newcomm);
if ( newcomm != MPI_COMM_NULL ) {
    My_collective (newcomm, ...);
    error = MPI_Comm_free ( newcomm );
```

More Complex Uses (1)

You can obviously do the above recursively Change MPI_COMM_WORLD to newcomm Change newcomm to evennewercomm

I said don't use overlapping communicators Inactive communicators aren't a problem

• Just tidy up all transfers before proceeding Suggest using barriers for tuning reasons

Will give just a very simple, C-style example

Using Two Levels



More Complex Uses (2)

```
errno = My_global_collective ( MPI_COMM_WORLD );
errno = Split ( MPI_COMM_WORLD , colour , 0 , & newcomm );
if ( newcomm != MPI_COMM_NULL )
    errno = My_split_collective ( newcomm , ... );
errno = My_global_collective ( MPI_COMM_WORLD ) ;
if ( newcomm != MPI_COMM_NULL )
    errno = My_split_collective ( newcomm , ... );
errno = My_global_collective ( MPI_COMM_WORLD ) ;
```

Note newcomm is actually three communicators They can't overlap, so the above use is safe Yes, that is parallel use of collectives

More Complex Uses (3)

And here is the first half, with some barriers Probably easier to tune, and possibly faster Note which communicator they are used with!

```
errno = My_global_collective ( MPI_COMM_WORLD );
errno = Split ( MPI_COMM_WORLD , colour , 0 , & newcomm );
if ( newcomm != MPI_COMM_NULL ) {
    errno = My_split_collective ( newcomm , ... );
    errno = Barrier ( newcomm );
}
errno = Barrier ( MPI_COMM_WORLD );
errno = My_global_collective ( MPI_COMM_WORLD );
```

Error Handling

• The error handler is inherited

You can change that subsequently I can't imagine many people wanting to

 Remember to set any error handler first obviously on MPI_COMM_WORLD
 Before creating any sub-communicators

Replication

You can make an exact copy of a communicator It is then completely independent of the first one The function is MPI_Comm_dup

• Could be useful to bypass implementation bugs Another possible use is mentioned in extra lectures But, in general, very few people will want it

FFTW and SPOOLES use MPI_Comm_dup I think only because they misunderstood MPI Possibly to fix up some broken implementation

Topologies

Topologies are how the processes are connected MPI's virtual topologies map the program structure

Independent of the actual hardware network

There is another lecture on Cartesian topologies May clarify code that uses an N-dimensional grid

That use is simple but omitted for brevity

Topologies are almost essential if: You are writing structure-generic libraries Your program has a variable graph structure

Other Facilities

• That's more–or–less all you need to know!

MPI 2 allowed adding names to communicators Might improve your diagnostics considerably MPI_Comm_get_name & MPI_Comm_set_name

One other function, useful for advanced use only MPI_Comm_compare

Groups (1)

There are facilities for operating on groups Not often used (though I have and CPMD does) So here is just a very brief summary

Operations on groups are entirely local Just operating on sets of integers, after all

For cleanliness, MPI hides them behind a handle This is called MPI_Group in C You should use only the facilities it provides

Take effect only when you create a communicator

Groups (2)

Alternative way of creating subset communicators

- MPI_Comm_group gets the current group
 I.e. it extracts it from the communicator
- MPI_Group_incl creates a subset group
 You pass it the ranks you want to keep
- MPI_Comm_create makes a new communicator using the new subset group
- MPI_Group_free releases the groups Highly desirable to avoid resource leaks
- MPI_Comm_free is used as earlier

Groups (3)

Strongly advised to program those collectively I.e. do identical group calculations on all processes Not because MPI needs that – but to avoid errors

Only two actual collectives:

MPI_Comm_create and MPI_Comm_free But group membership in all processes must match

You may find that easier than MPI_Comm_split It's purely a matter of personal preference

Other Group Functions

MPI_Group_compare MPI_Group_difference MPI_Group_excl MPI_Group_intersection MPI_Group_range_excl

MPI_Group_range_incl MPI_Group_rank MPI_Group_size MPI_Group_translate_ranks MPI_Group_union

Many of them are alternatives to MPI_Group_incl I doubt you will ever want to use the others

Epilogue

You now know what you can do with communicators Most of you will use only MPI_COMM_WORLD

One simple exercise using MPI_Comm_split