Programming with MPI

Communicators etc.

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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 processors together

MPI_COMM_SELF is just the local processor

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

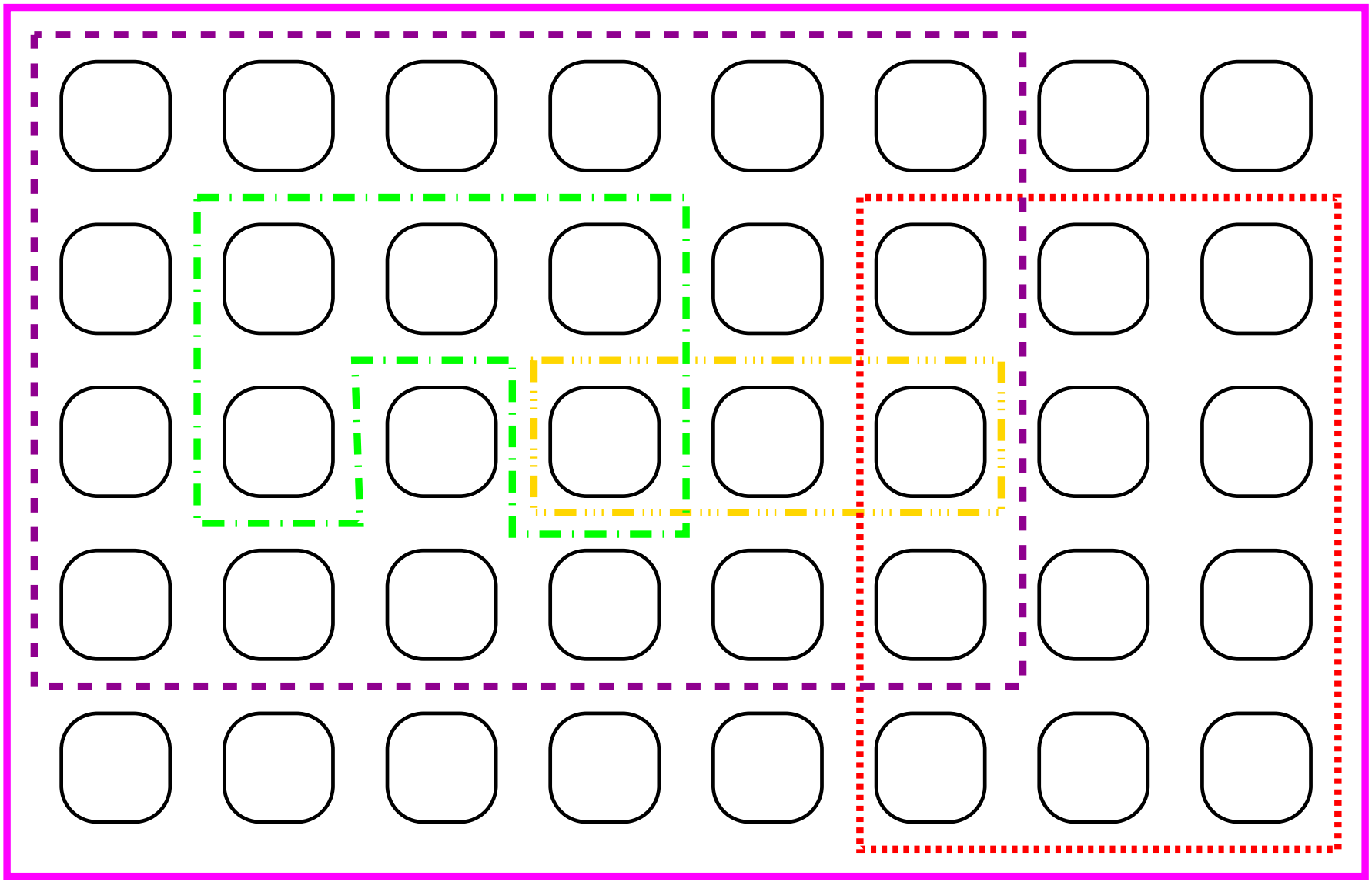
- MPI won't get confused – but you and I will

And don't even think of trying to tune such a mess!

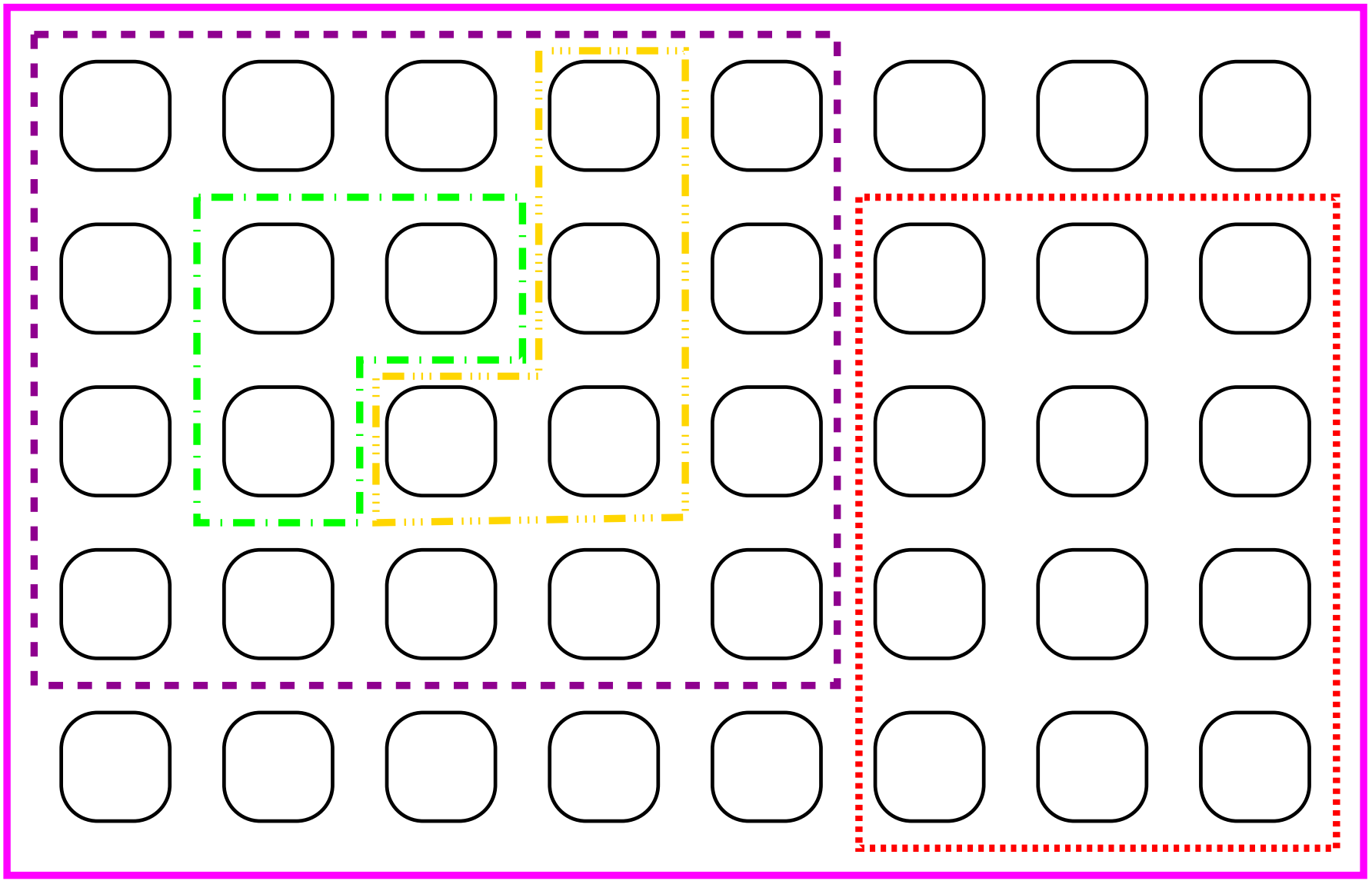
Design your communicator use to be hierarchical
Like recursion in groups of processors

This is easier to show using pictures

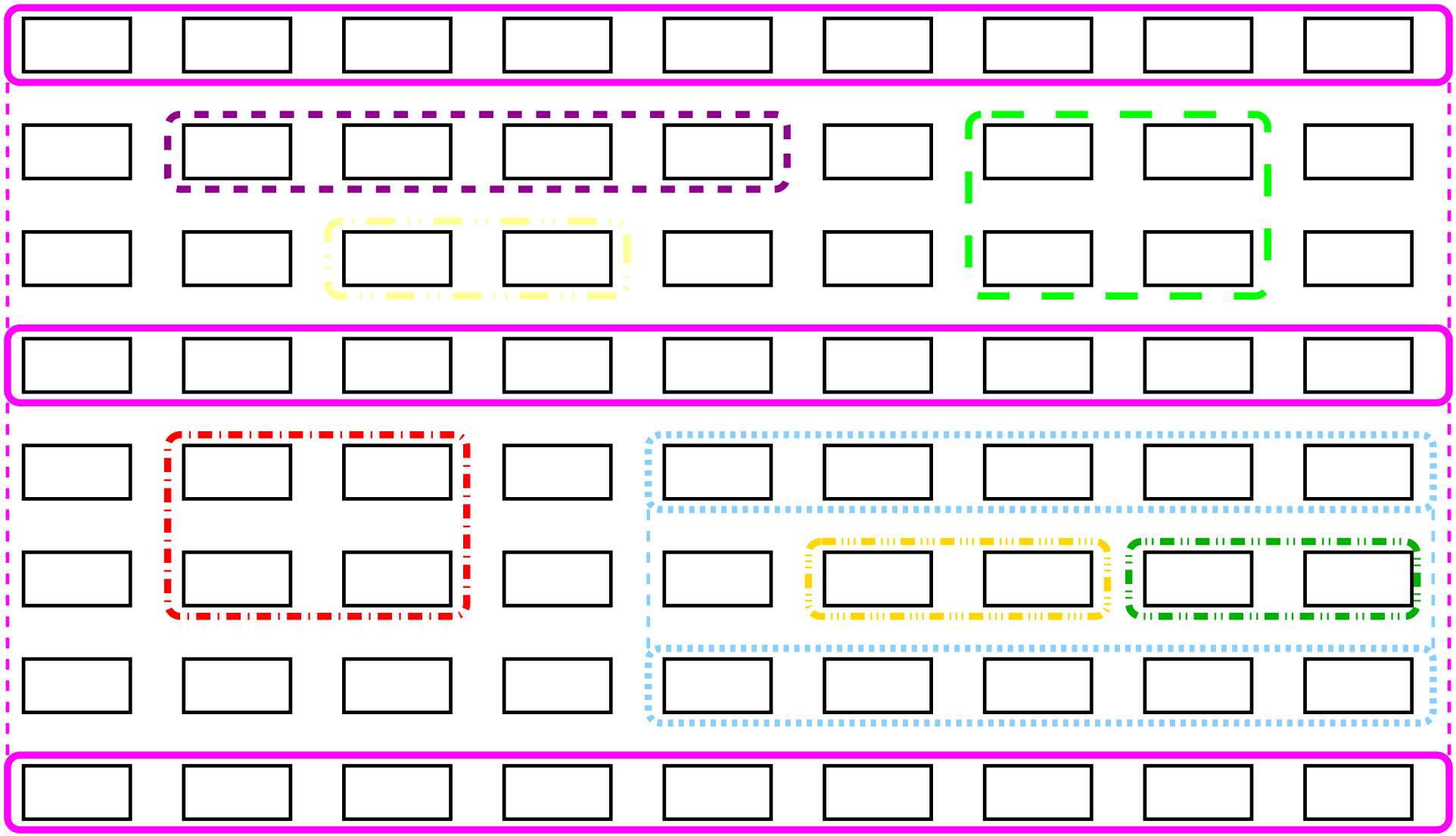
General Communicators



Hierarchical Communicators



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

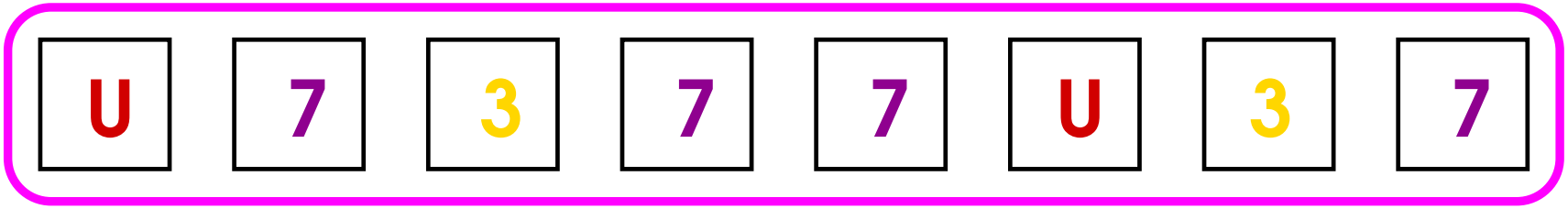
That is an unspecified negative integer

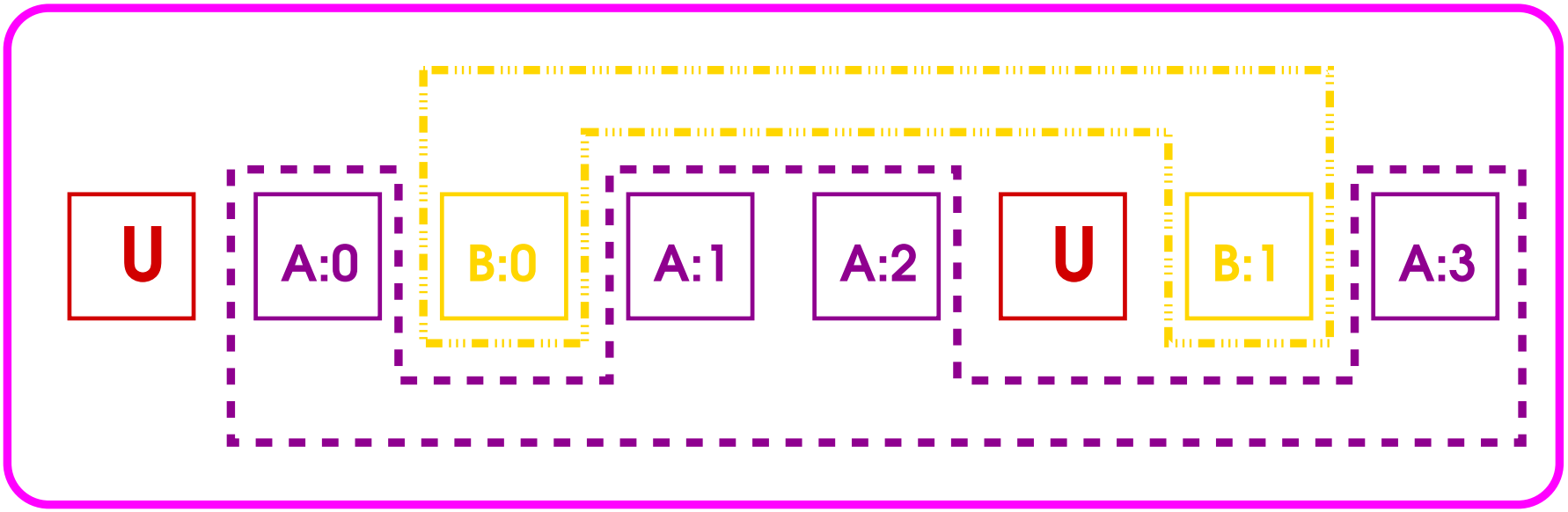
Note that zero is a valid colour

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 ) ;
}
```

Split (3)

C++ example:

```
int colour , error ;
// 'colour' is set to an appropriate value
MPI::Comm newcomm ;

newcomm = MPI::COMM_WORLD . Split ( colour , 0 ) ;
if ( newcomm != MPI::COMM_NULL ) {
        // Not a member function to avoid subclassing
        My_collective ( newcomm , ... ) ;
        MPI::COMM_WORLD . 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

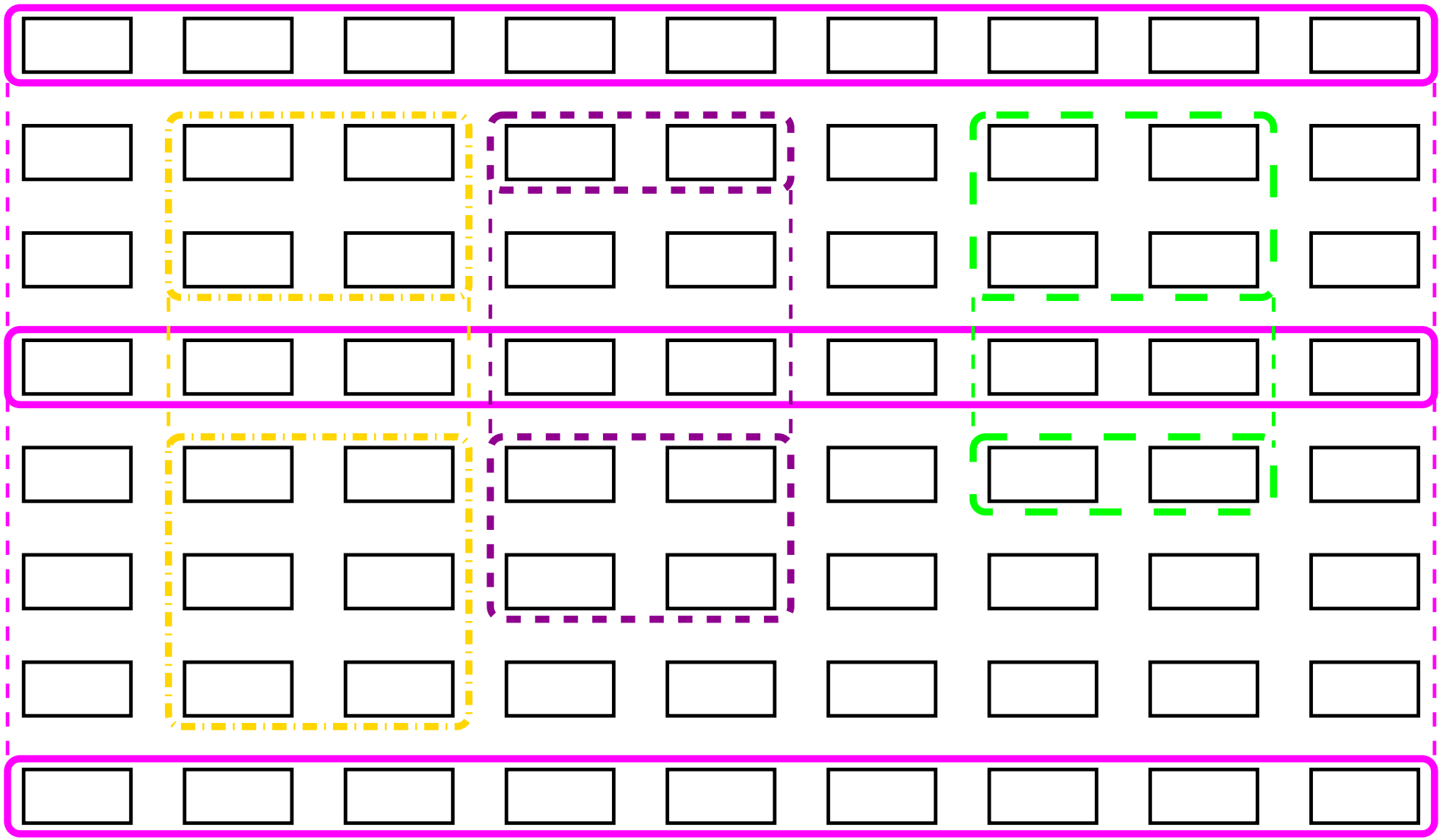
Inactive communicators aren't a problem

- 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)

```
My_global_collective ( MPI::COMM_WORLD ) ;
newcomm = MPI::COMM_WORLD . Split ( colour ) ;
if ( newcomm != MPI::COMM_NULL )
        My_split_collective ( newcomm , ... ) ;
My_global_collective ( MPI::COMM_WORLD ) ;
if ( newcomm != MPI::COMM_NULL )
        My_split_collective ( newcomm , ... ) ;
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!

```
My_global_collective ( MPI::COMM_WORLD ) ;
newcomm = MPI::COMM_WORLD . Split ( colour ) ;
if ( newcomm != MPI::COMM_NULL ) {
        My_split_collective ( newcomm , ... ) ;
        newcomm . Barrier ( ) ;
}
MPI::COMM_WORLD . Barrier ( ) ;
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

Other Facilities

- That’s more–or–less all you need to know!

You can add names to communicators in MPI–2
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/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

Some of the C++ names are slightly different

Orphan Topic

Following topic doesn’t fit naturally anywhere

Relevant only to Fortran 90 programmers

But it’s almost trivial to use, so here it is

Fortran Precisions (1)

Fortran 90 allows selectable precisions
KIND=SELECTED_INTEGER_KIND(precision)
KIND=SELECTED_REAL_KIND(precision[,range])

Can create a MPI derived datatype to match these
Then can use it just like a built–in datatype

Surprisingly, it is a predefined datatype
Do NOT commit or free it
[Don’t worry if that makes no sense to you]

Fortran Precisions (2)

```
INTEGER ( KIND =        &
          SELECTED_INTEGER_KIND ( 15 ) ) ,      &
       DIMENSION ( 100 ) :: array
INTEGER :: root , integertype , error

CALL MPI_Type_create_f90_integer (      &
       15 , integertype , error )
CALL MPI_Bcast ( array , 100 ,      &
       integertype , root ,      &
       MPI_COMM_WORLD , error )
```

Fortran Precisions (3)

REAL and COMPLEX are very similar

```
REAL ( KIND =       &
         SELECTED_REAL_KIND ( 15 , 300 ) ) ,     &
      DIMENSION ( 100 ) :: array
CALL MPI_Type_create_f90_real (       &
      15 , 300 , realtype , error )

COMPLEX ( KIND =       &
         SELECTED_REAL_KIND ( 15 , 300 ) ) ,     &
      DIMENSION ( 100 ) :: array
CALL MPI_Type_create_f90_complex (       &
      15 , 300 , complextype , error )
```

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
And one on Fortran 90 allows selectable precisions