MHPC
Master in High Performance Computing

Message Passing Programming Paradigm

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What is MPI?

- A standard, i.e. there is a document describing how the API are named and should behave; multiple “levels”, MPI-1 (basic), MPI-2 (advanced), MPI-3/4 (new) http://www.mpi-forum.org
- A library or API to hide the details of low-level communication hardware and how to use it
- Implemented by multiple vendors
  - Open source and commercial versions
  - Vendor specific versions for certain hardware
  - Not binary compatible between implementations

Goals of MPI

- Allow to write software (source code) that is portable to many different parallel hardware. i.e. agnostic to actual realization in hardware
- Provide flexibility for vendors to optimize the MPI functions for their hardware
- No limitation to a specific kind of hardware and low-level communication type. Running on heterogeneous hardware is possible.
- Fortran77 and C style API as standard interface

MPI Program Design

- Multiple and separate processes (can be local and remote) concurrently that are coordinated and exchange data through “messages”
  - ➢ a “share nothing” parallelization
- Best for coarse grained parallelization
- Minimize communication or overlap communication and computing for efficiency
  - ➢ Amdahl's law: speedup is limited by the fraction of serial code plus communication

MPI in C versus MPI in Fortran

The programming interface (“bindings”) of MPI in C and Fortran are closely related (wrappers for many other languages exist)

MPI in C:

- Use '#include <mpi.h>' for constants and prototypes
- Include only once at the beginning of a file

MPI in Fortran:

- Use 'include “mpif.h”' for constants
- Include at the beginning of each module
- All MPI functions are “subroutines” with the same name and same order and type of arguments as in C with return status added as the last argument

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A Fundamental Reference (list of the MPI-1 functions calls)

http://mpi-forum.org/docs/mpi-1.1/mpi-11-html/node182.html - Node182

When next writing an MPI program check all MPI function interfaces you introduce in your code at the above link

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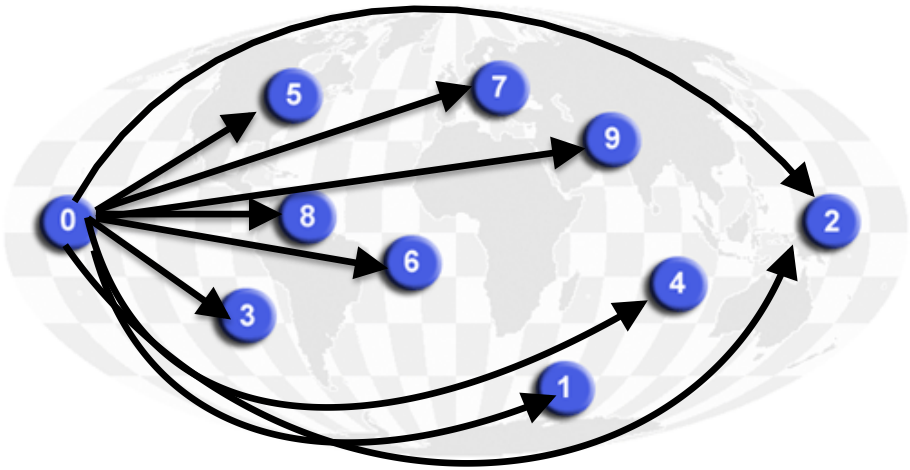
MPI Communicators

- Is the fundamental communication facility provided by MPI library. Communication between 2 processes
- Communication take place within a communicator: Source/s and Destination/s are identified by their rank within a communicator

MPI_COMM_WORLD



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Communicator Size & Process Rank

A “communicator” is a label identifying a group of processors that are ready for parallel computing with MPI

By default the **MPI_COMM_WORLD** communicator is available and contains all processors allocated by mpirun

Size: How many MPI tasks are there in total?

CALL MPI_COMM_SIZE(comm, size, status)

After the call the integer variable **size** holds the number of processes on the given communicator

Rank: What is the ID of “me” in the group?

CALL MPI_COMM_RANK(comm, rank, status)

After the call the integer variable **rank** holds the ID or the process. This is a number between **0** and **size-1**.

Fortran

```
PROGRAM hello
   INCLUDE `mpif.h`
   INTEGER :: ierr, rank, size
   CALL MPI_INIT(ierr)
   CALL MPI_COMM_RANK(MPI_COMM_WORLD,rank,ierr)
   CALL MPI_COMM_SIZE(MPI_COMM_WORLD,size,ierr)
   PRINT*, 'I am ', rank, ' of ', size
   CALL MPI_FINALIZE(ierr)
END
```

Important: call MPI_INIT before parsing arguments

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Phases of an MPI Program

1. Startup

- Parse arguments (mpirun may add some!)
- Identify parallel environment and rank of process
- Read and distribute all data

2. Execution

- Proceed to subroutine with parallel work (can be same of different for all parallel tasks)

3. Cleanup

CAUTION: this sequence may be run only once!

MPI Startup / Cleanup

Initializing the MPI environment:

CALL MPI_INIT(STATUS)

Status is integer set to MPI_SUCCESS, if operation was successful; otherwise to error code

Releasing the MPI environment:

CALL MPI_FINALIZE(STATUS)

NOTES:

All MPI tasks have to call **MPI_INIT** & **MPI_FINALIZE**

MPI_INIT may only be called once in a program

No MPI calls allowed outside of the region between calling **MPI_INIT** and **MPI_FINALIZE**

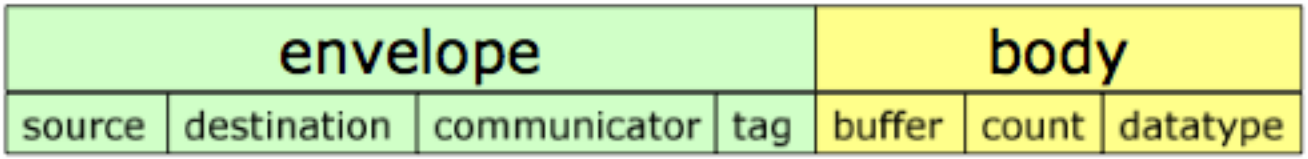
The Message

A message is an array of elements of some particular MPI data type

MPI defines a number of constants that correspond to language *datatypes* in Fortran and C

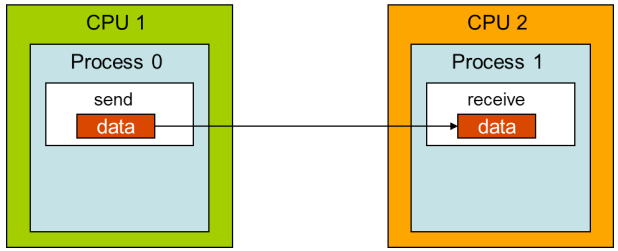
When an MPI routine is called, the Fortran (or C) datatype of the data being passed must match the corresponding MPI integer constant

Message Structure

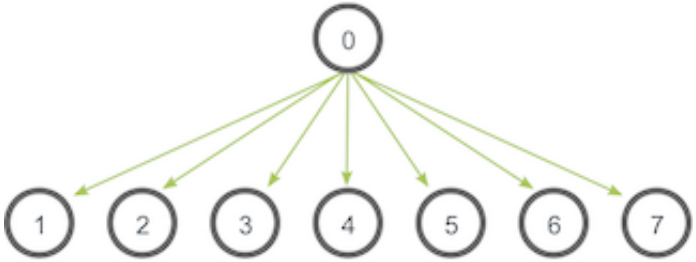


Communication Models in MPI

Point-to-Point Communication



Collective Communication



MPI DATA TYPES

MPI datatype handle	C datatype
MPI_INT	int
MPI_SHORT	short
MPI_LONG	long
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_CHAR	char
MPI_BYTE	unsigned char

Calling MPI_BCAST

MPI_BCAST(buffer, count, type, sender, comm, err)

buffer:	buffer with data
count:	number of data items to be sent
type:	type (=size) of data items
sender:	rank of sending processor of data
comm:	group identifier, MPI_COMM_WORLD
err:	error status of operation

NOTES:

- buffers must be large enough (can be larger)
- Data type must match (MPI does not check this)
- all ranks that belong to the communicator must call this

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)
  call MPI_COMM_RANK(comm, myrank, ierr)
  call MPI_COMM_SIZE(comm, ncpus, ierr)

  imesg = myrank
  print *, "Before Bcast operation I'm ", myrank, " and my message content is ", imesg

  call MPI_BCAST(imesg, 1, MPI_INTEGER, 0, comm, ierr)

  print *, "After Bcast operation I'm ", myrank, & " and my message content is ", imesg

  call MPI_FINALIZE(ierr)

end program bcast
```

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD
```

P_0

myrank = ??
ncpus = ??
imesg = ??
ierr = ??
comm = MPI_C...

P_1

myrank = ??
ncpus = ??
imesg = ??
ierr = ??
comm = MPI_C...

P_2

myrank = ??
ncpus = ??
imesg = ??
ierr = ??
comm = MPI_C...

P_3

myrank = ??
ncpus = ??
imesg = ??
ierr = ??
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)
```

P_0

myrank = ??
ncpus = ??
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = ??
ncpus = ??
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = ??
ncpus = ??
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = ??
ncpus = ??
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)

  call MPI_COMM_SIZE(comm, ncpus, ierr)

  call MPI_COMM_RANK(comm, myrank, ierr)
```

P_0

myrank = ??
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = ??
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = ??
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = ??
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)

  call MPI_COMM_SIZE(comm, ncpus, ierr)

  call MPI_COMM_RANK(comm, myrank, ierr)
```

P_0

myrank = 0
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = ??
ierr = MPI_SUC...
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)
  call MPI_COMM_RANK(comm, myrank, ierr)
  call MPI_COMM_SIZE(comm, ncpus, ierr)

  imesg = myrank
  print *, "Before Bcast operation I'm ", myrank, &
       " and my message content is ", imesg
```

P_0

myrank = 0
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = 1
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = 2
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = 3
ierr = MPI_SUC...
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)
  call MPI_COMM_RANK(comm, myrank, ierr)
  call MPI_COMM_SIZE(comm, ncpus, ierr)

  imesg = myrank
  print *, "Before Bcast operation I'm ", myrank, &
       " and my message content is ", imesg

  call MPI_BCAST(imesg, 1, MPI_INTEGER, 0, comm, ierr)
```

P_0

myrank = 0
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = 1
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = 2
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = 3
ierr = MPI_SUC...
comm = MPI_C...

call MPI_BCAST(imesg, 1, MPI_INTEGER, 0, comm, ierr)

P_0

myrank = 0
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = 1
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = 2
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = 3
ierr = MPI_SUC...
comm = MPI_C...

call MPI_BCAST(imesg, 1, MPI_INTEGER, 0, comm, ierr)

P_0

myrank = 0
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)
  call MPI_COMM_RANK(comm, myrank, ierr)
  call MPI_COMM_SIZE(comm, ncpus, ierr)

  imesg = myrank
  print *, "Before Bcast operation I'm ", myrank, &
       " and my message content is ", imesg

  call MPI_BCAST(imesg, 1, MPI_INTEGER, 0, comm, ierr)

  print *, "After Bcast operation I'm ", myrank, &
       " and my message content is ", imesg
```

P_0

myrank = 0
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)
  call MPI_COMM_RANK(comm, myrank, ierr)
  call MPI_COMM_SIZE(comm, ncpus, ierr)

  imesg = myrank
  print *, "Before Bcast operation I'm ", myrank, &
       " and my message content is ", imesg

  call MPI_BCAST(imesg, 1, MPI_INTEGER, 0, comm, ierr)

  print *, "After Bcast operation I'm ", myrank, &
       " and my message content is ", imesg

  call MPI_FINALIZE(ierr)
```

P_0

myrank = 0
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

```
program bcast

  implicit none

  include "mpif.h"

  integer :: myrank, ncpus, imesg, ierr
  integer, parameter :: comm = MPI_COMM_WORLD

  call MPI_INIT(ierr)
  call MPI_COMM_RANK(comm, myrank, ierr)
  call MPI_COMM_SIZE(comm, ncpus, ierr)

  imesg = myrank
  print *, "Before Bcast operation I'm ", myrank, &
       " and my message content is ", imesg

  call MPI_BCAST(imesg, 1, MPI_INTEGER, 0, comm, ierr)

  print *, "After Bcast operation I'm ", myrank, &
       " and my message content is ", imesg

  call MPI_FINALIZE(ierr)

end program bcast
```

P_0

myrank = 0
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_1

myrank = 1
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

P_2

myrank = 2
ncpus = 4
imesg = 0
ierr = MPI_SUCC
comm = MPI_C...

P_3

myrank = 3
ncpus = 4
imesg = 0
ierr = MPI_SUC...
comm = MPI_C...

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STANDARD BLOCKING SEND - RECV

MPI_SEND(buf, count, type, dest, tag, comm, ierr)

MPI_RECV(buf, count, type, dest, tag, comm, status, ierr)

Buf array of MPI type **type**.

Count (INTEGER) number of element of **buf** to be sent/recv

Type (INTEGER) MPI type of **buf**

Dest (INTEGER) rank of the destination process

Tag (INTEGER) number identifying the message

Comm (INTEGER) communicator of the sender and receiver

*** Status** (INTEGER) array of size **MPI_STATUS_SIZE** containing communication status information

Ierr (INTEGER) error code

**** used only for receive operations***

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Wildcards

Both in Fortran and C **MPI_RECV** accept wildcard:

- To ignore the receiving status object: MPI_STATUS_IGNORE
- To receive from any source: MPI_ANY_SOURCE
- To receive with any tag: MPI_ANY_TAG
- Actual source and tag are returned in the receiver's status parameter => status.MPI_SOURCE, status.MPI_TAG

MPI_GET_COUNT(status, datatype, count)

[IN status] return status of receive operation (Status)

[IN datatype] datatype of each receive buffer entry (handle)

[OUT count] number of received entries (integer)

```
PROGRAM send_recv
      INCLUDE ‘mpif.h‘
      INTEGER :: ierr, myid, nproc, status(MPI_STATUS_SIZE)
      REAL A(2)
      CALL MPI_INIT(ierr)
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nproc, ierr)
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
      IF( myid .EQ. 0 ) THEN
            A(1) = 3.0
            A(2) = 5.0
            CALL MPI_SEND(A, 2, MPI_REAL, 1, 10, MPI_COMM_WORLD, ierr)
      ELSE IF( myid .EQ. 1 ) THEN
            CALL MPI_RECV(A, 2, MPI_REAL, 0, 10, MPI_COMM_WORLD, status, ierr)
            WRITE(6,*) myid,’: a(1)=’,a(1),’ a(2)=’,a(2)
      END IF
      CALL MPI_FINALIZE(ierr)
END
```

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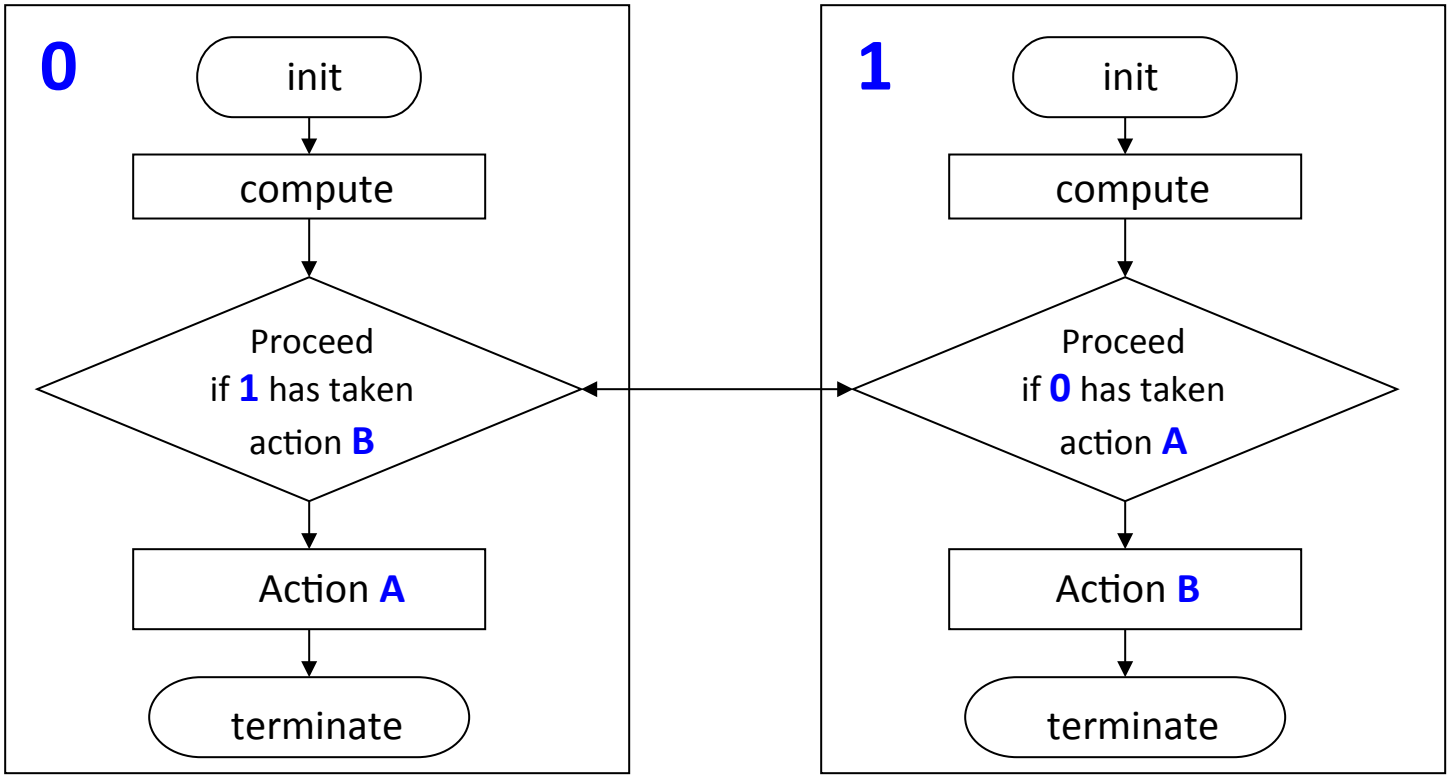
DEADLOCK

Deadlock occurs when 2 (or more) processes are blocked and each is waiting for the other to make progress.



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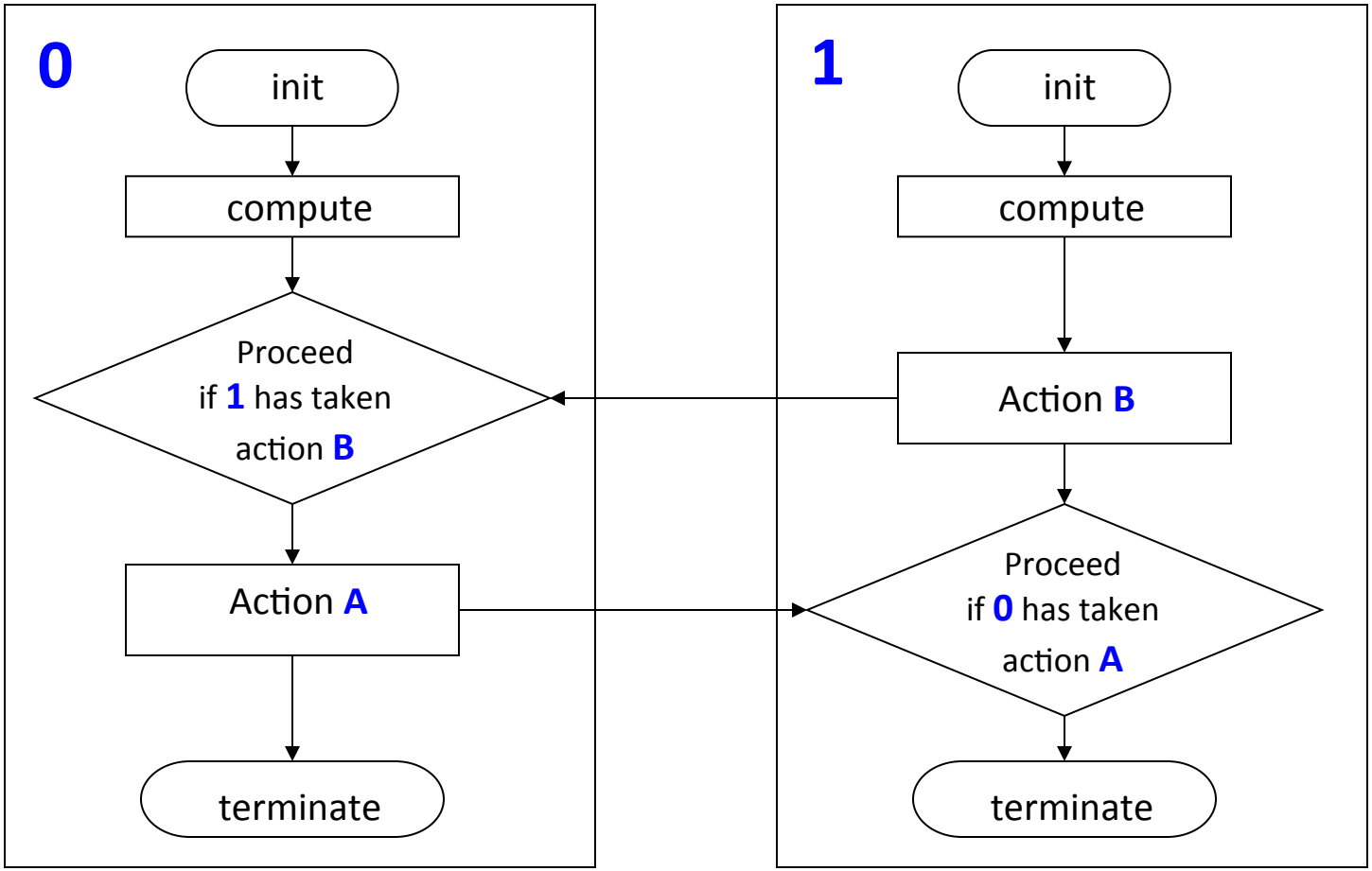
Avoiding DEADLOCK



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