Lecture 18 - MPI Part 1

DSE 512

Drew Schmidt
2022-03-31

From Last Time

- New homework is out
- Due April 9
- Questions?

Parallel Programming Models

- So far we've seen
  - implicit
  - manager/worker
- One process is in charge; tells workers what to do
- Natural extension of interactive programming
- Pros:
  - supports interactivity
  - ubiquitous
- Cons:
  - *not scalable*
  - not the most natural!

Non-Scalability of Manager/Worker

- Imagine an organization with 10, 100, 1000, 10,000 workers
  - Imagine *every* time *anyone* does *anything* it has to go through the CEO
  - Which organizations will get *anything* done?
- Parallel programs with 10, 100, 1000, 10,000 processes
  - If *all* tasks have to go through a manager process…

SPMD

- Single Program Multiple Data
- How *all* big programs are run in HPC
- Designed for batch computing
- No process is in charge

Other Parallel Programming Techniques

- Implicit
- Manager/worker
- MapReduce

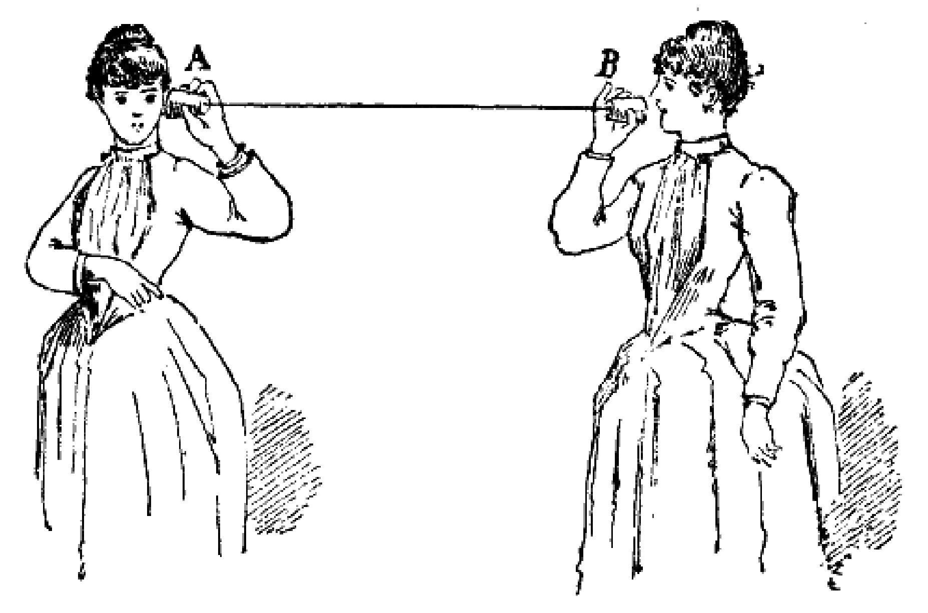
SPMD: How It Works

- One program is written
- All processes execute the single program
- Operates on *collectives*
- Some blocks may break this
  - I/O
  - Some point-to-points
  - In-situ/sub-communicators
  - ...

Message Passing Interface

MPI

- Message Passing Interface
- Distributed programming standard
- Implementations
  - OpenMPI
  - MPICH
  - MPT
  - Spectrum



Interfaces

- Bindings exist for almost every language
- The C interface (libmpi)
- Python: mpi4py
- R: pbdMPI (also Rmpi)

Installing

- Need a system installation of MPI
  - Linux: e.g. `apt install openmpi-bin libopenmpi-dev`
  - Mac: Build it from source; best of luck!
  - Windows: Download and install MSMPI
- *You don't need to do this* because you have ISAAC

Launching MPI Programs

- MPI programs *run in batch*
- Launched with a special launcher
- Many systems: `mpirun -np 2 my_mpi_program`
- ISAAC: `srun my_mpi_program`
- Launchers accept *many* arguments

Recall: MPI Hello World

https://github.com/wrathematics/mpi-hello

- Step 1: Download on ISAAC (`git clone`, `wget`, whatever)
- Step 2: Extract the archive as necessary
- Step 3: Compile it (do `less README.md` for instructions)
- Step 4: Do a quick test with `./mpi-hello`

My Workstation Example

```
mpirun -np 4 ./mpi-hello
```

```
Hello from rank 0/4 global 0/4 local
Hello from rank 1/4 global 1/4 local
Hello from rank 2/4 global 2/4 local
Hello from rank 3/4 global 3/4 local
```

ISAAC Example

```bash
#!/bin/bash
#SBATCH --account=ACF-UTK0188
#SBATCH --job-name=MPI_hello_world
#SBATCH --nodes=2
#SBATCH --ntasks=4
#SBATCH --ntasks-per-node=2
#SBATCH --time=00:00:30
#SBATCH --partition=condo-dse512
#SBATCH --qos=condo

cd ~/mpi-hello
srun ./mpi-hello
```

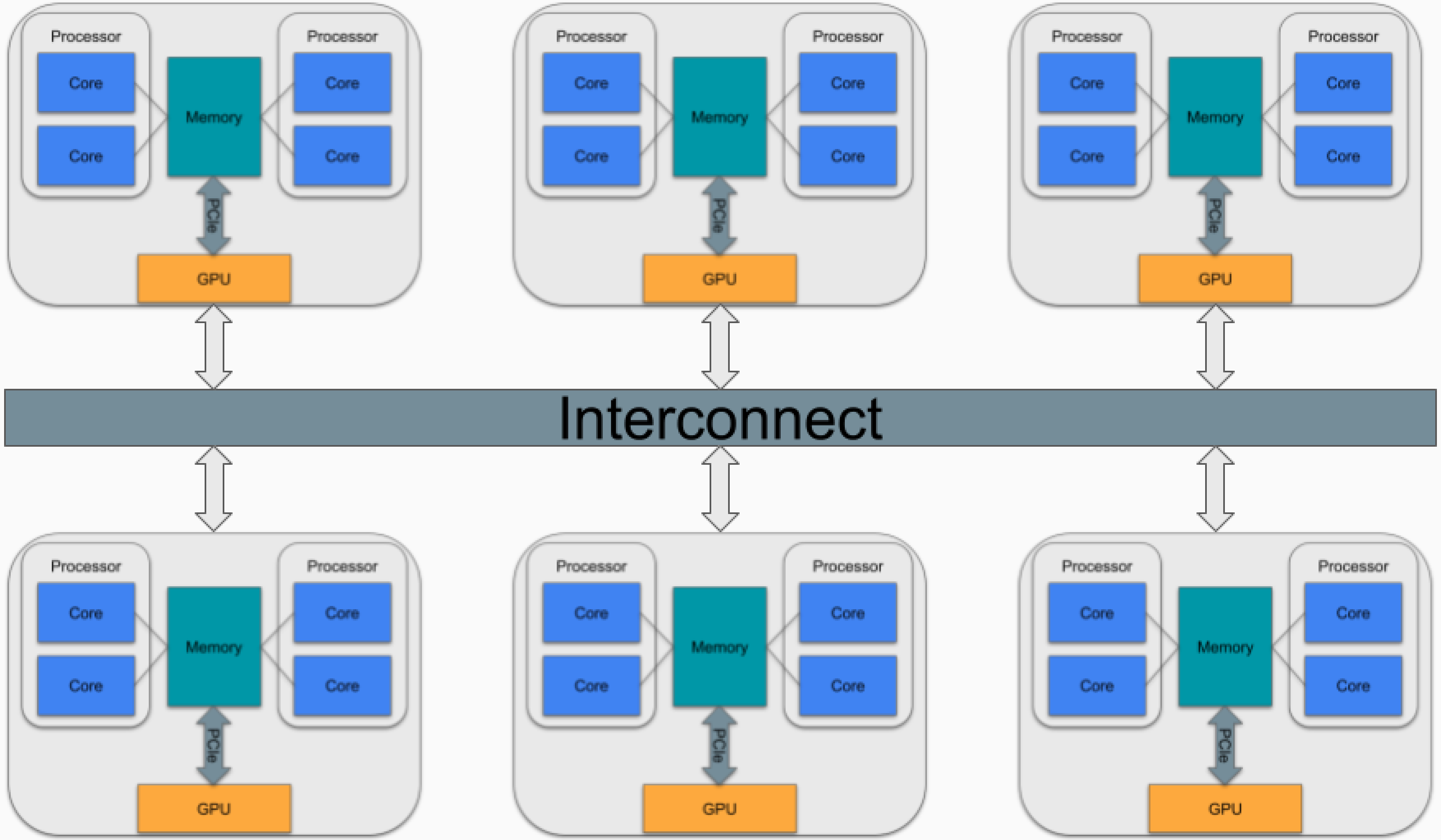
```
Hello from rank 0/4 global 0/2 local
Hello from rank 1/4 global 1/2 local
Hello from rank 2/4 global 0/2 local
Hello from rank 3/4 global 1/2 local
```

MPI Basics

Communicator

- Comms managed by a *communicator*
  - special/magical object
  - it's a little complicated...
- Enables parallelism
  - lets different processes "talk" to each other
  - can send/receive essentially any kind of data
  - how it actually works is complicated...
- Primary motivation: distributed computing

Hardware



Basic Communicator Jargon

- init - initialize
- finalize - shut down
- rank - "who am I?"
- size - "how many of us are there?"

Communicators

- "world"
  - default communicator
  - contains *all* processes
- sub-communicators

Reasons for Sub-Communicators

- It's a bit complicated...
- Why would you even want to?
- In-situ analysis
  - One set of processes simulating/generating data
  - Another analyzing generated data
- Running one task per node
  - Usually a job for the scheduler
  - Use case: getting local rank in "hello world"

Basic Communicator Example

R

```r
suppressMessages(library(pbdMPI))

rank = comm.rank()
print(rank)

finalize()
```

```
mpirun -np 2 Rscript example.r
```

```
[1] 0
[1] 1
```

Python

```python
from mpi4py import MPI
comm = MPI.COMM_WORLD

rank = comm.rank
print(rank)

MPI.Finalize()
```

```
mpirun -np 2 python example.py
```

```
0
1
```

Some Language Comments

- R (pbdR)
  - main interface is very simplified compared to MPI standard
  - offers *many* high-level helpers
    - `comm.print()`
    - `get.jid()`
    - `pbdLapply()`
- Python (mpi4py)
  - offers a very MPI-like interface
  - its "high-level" functions look more like R's interface
  - *Be very careful* with non-numpy data
- Often need (or receive!) a "placeholder" value
  - `NULL` in R
  - `None` in Python

MPI Operations

MPI Operations

- Many operations supported by MPI
- We will focus on a few *collectives*
  - all processes "contribute"
  - each calls the operation
  - generally one or all receive the result
  - if you need something else, use a sub-communicator
- Point-to-point also possible
  - send/receive
  - who calls what is very problem-dependent

Blocking vs Non-Blocking

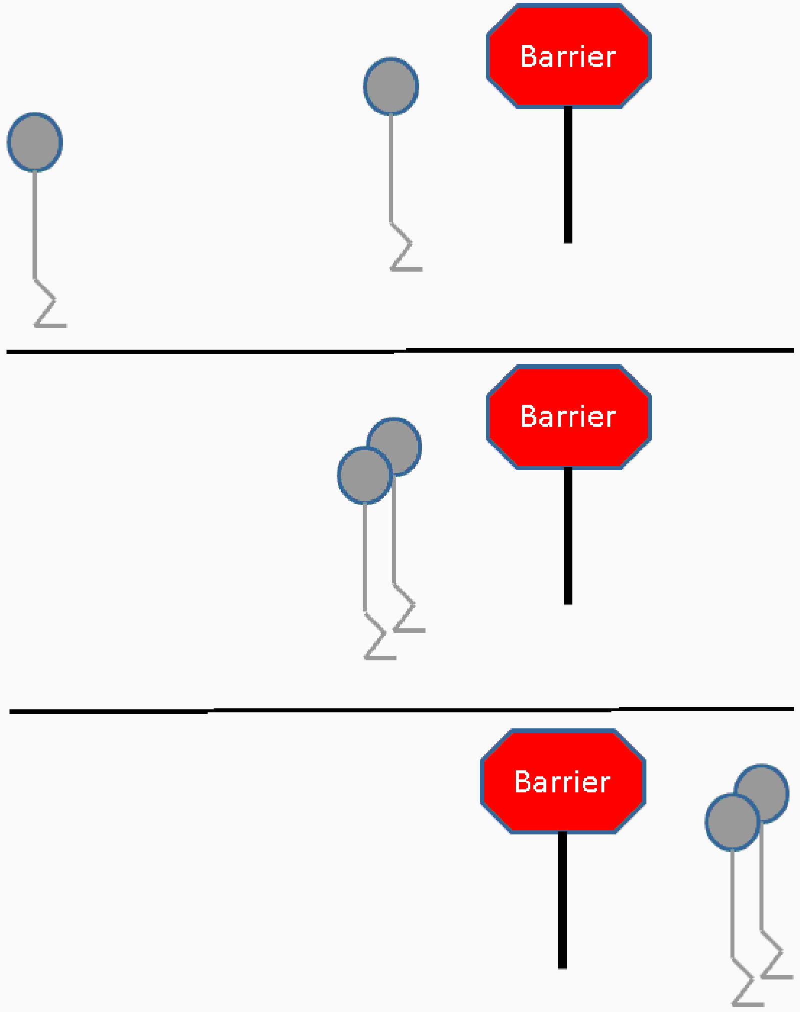
- We will only focus on blocking ops
- Blocking: do not return until communication completes
- Explanation:
  - Consider `ret = my_expensive_operation()`
  - Blocking: does not proceed until `ret` is set
  - Non-blocking: continues whether it's done or not!
  - No serial analogue! *All* computation is blocking in serial
  - Non-blocking can work with forks
- Non-blocking analogues exist (prefaced by `i`)
  - `send` becomes `isend`
  - `recv` becomes `irecv`

Marjor Collective Operations

- Barrier
- Reduce
- Gather
- Broadcast

Barrier

- Computation wall
- All processes in the communicator "synchronize"
- No process can proceed until *all* can proceed
- Can destroy performance!



Barrier Example

R

```r
suppressMessages(library(pbdMPI))

Sys.sleep(comm.rank())
barrier()

finalize()
```

```
mpirun -np 2 Rscript example.r
```

```
real    0m1.874s
user    0m2.044s
sys     0m0.264s
```

Python

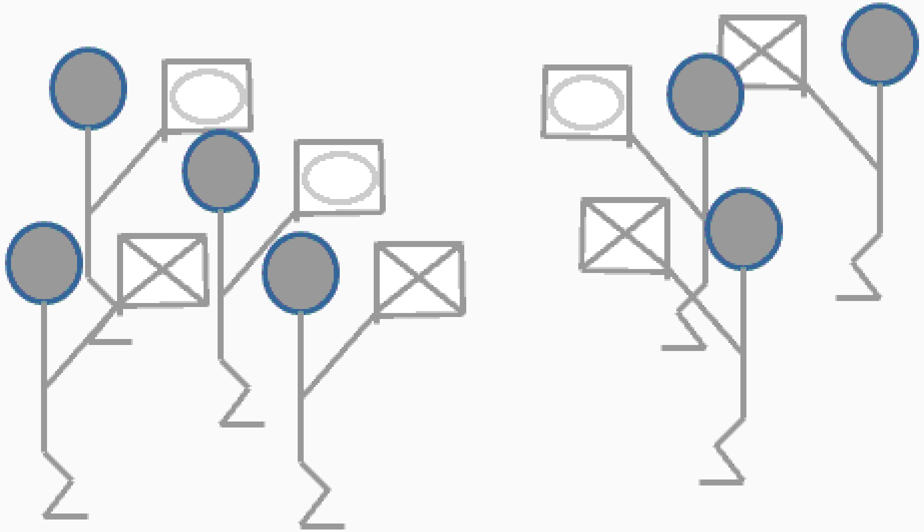
```python
import time
from mpi4py import MPI
comm = MPI.COMM_WORLD

time.sleep(comm.rank)
comm.Barrier()

MPI.Finalize()
```

```
time mpirun -np 2 python example.py
```

```
real    0m1.400s
user    0m1.120s
sys     0m0.079s
```

Reduce

- One of the main MPI workhorses
- *Shockingly* useful
- What it does:
  - each processor has a number
  - add all of them up, find the largest/smallest, …
- `reduce` - reduce to one
- `allreduce` - reduce to all



Reduce Example

R

```r
suppressMessages(library(pbdMPI))

x_local = 1:5 * 10^comm.rank()
x = reduce(x_local)
if (comm.rank() == 0)
  print(x)

finalize()
```

```
mpirun -np 2 Rscript example.r
```

```
[1] 11 22 33 44 55
```

Python

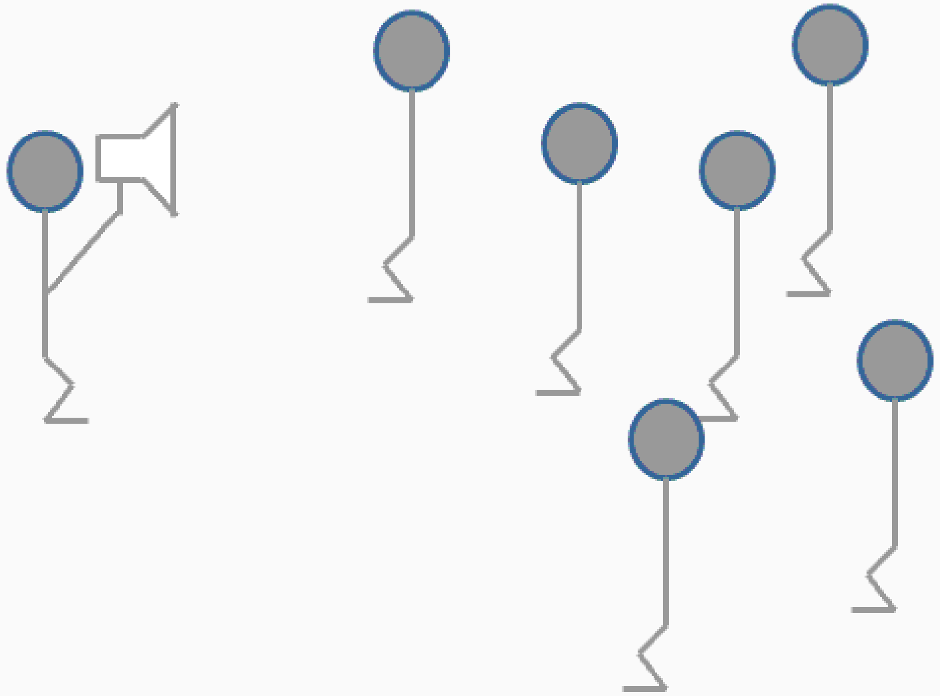
```python
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD

x_local = np.linspace(1, 5, 5) * 10**comm
x = comm.reduce(x_local, op = MPI.SUM)
if comm.rank == 0:
  print(x)

MPI.Finalize()
```

```
mpirun -np 2 python example.py
```

```
[11. 22. 33. 44. 55.]
```

Broadcast

-
- What it does:
  - one process has a number
  - give it to ever other process
- `bcast` - broadcast from one to all



Broadcast Example

R

```r
suppressMessages(library(pbdMPI))

if (comm.rank() == 0){
  x_local = matrix(1:4, nrow=2)
} else {
  x_local = NULL
}

x = bcast(x_local)
comm.print(x, rank.print=1)

finalize()
```

```
COMM.RANK = 1
     [,1] [,2]
[1,]    1    3
[2,]    2    4
```

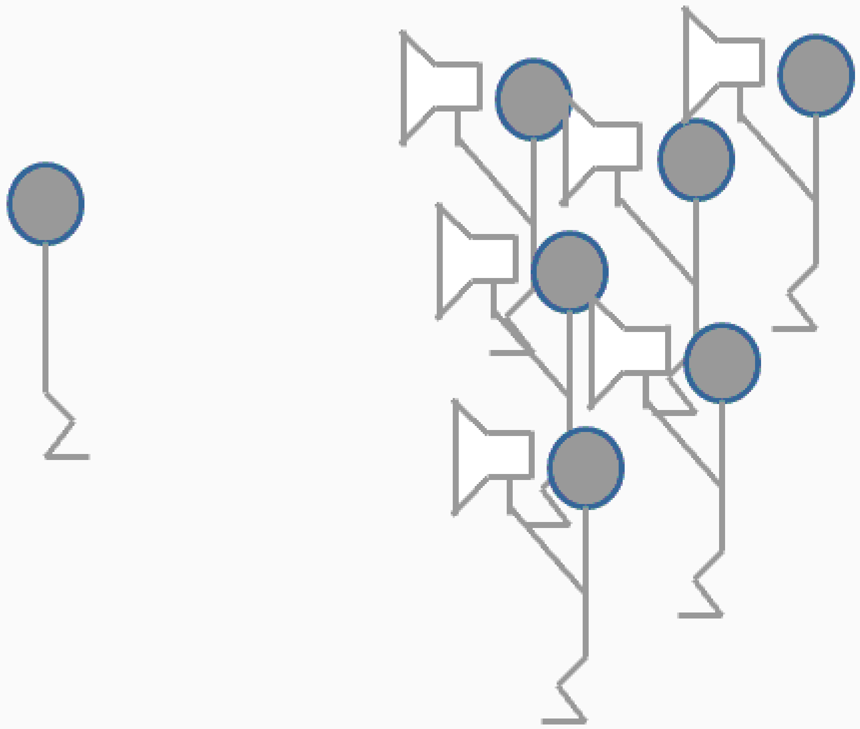
Python

```python
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD

if (comm.rank == 0):
  x_local = np.array([[1, 2], [3, 4]])
else:
  x_local = None

x = comm.bcast(x_local)
if comm.rank == 1:
  print(x)

MPI.Finalize()
```

```
[[1 2]
 [3 4]]
```

Gather

-
- What it does:
  - each process has a number
  - all processes should also have that number
- Reverse `bcast`
- `gather` - gather to one
- `allgather` - gather to all



Gather Example

R

```r
suppressMessages(library(pbdMPI))

x_local = comm.rank()
x = gather(x_local)
comm.print(x)

finalize()
```

```
COMM.RANK = 0
[[1]]
[1] 0

[[2]]
[1] 1
```

Python

```python
from mpi4py import MPI
comm = MPI.COMM_WORLD

x_local = comm.rank
x = comm.gather(x_local)
if comm.rank == 1:
  print(x)

MPI.Finalize()
```

```
[0, 1]
```

More MPI Examples

RNG

R

```r
suppressMessages(library(pbdMPI))
comm.set.seed(1234, diff=TRUE)

x_local = sample(1:10, size=1)
comm.print(x_local, all.rank=TRUE)

finalize()
```

```
COMM.RANK = 0
[1] 4
COMM.RANK = 1
[1] 6
```

Python

```python
from mpi4py import MPI
import random
comm = MPI.COMM_WORLD

random.seed(1234 + comm.rank)
x_local = random.randint(1, 10)
print(x_local)

MPI.Finalize()
```

```
7
8
```

Hello World: mpi4py

```python
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

comm_localrank = MPI.Comm.Split_type(comm, MPI.COMM_TYPE_SHARED, 0)
rank_local = comm_localrank.Get_rank()
size_local = comm_localrank.Get_size()

for p in range(0, size):
    if p == rank:
        print("Hello from rank ", end="")
        print(str(rank) + "/" + str(size) + " global ", end="")
        print(str(rank_local) + "/" + str(size_local) + " local")

    comm.Barrier()

MPI.Finalize()
```

Hello World: mpi4py

```
mpirun -np 2 python p.py
```

```
Hello from rank 0/2 global 0/2 local
Hello from rank 1/2 global 1/2 local
```

Hello World: pbdR

```r
suppressMessages(library(pbdMPI))

rank = comm.rank()
size = comm.size()
rank_local = comm.localrank()

hostname = system("uname -n", intern=TRUE)
hostnames = allgather(hostname) |> unlist() |> table()
size_local = hostnames[hostname] |> unname()

msg = paste0("Hello from rank ", rank, "/", size, " global ", rank_local, " local\n")
comm.cat(msg, all.rank=TRUE, quiet=TRUE)

finalize()
```

Hello World: pbdR

```
$ mpirun -np 2 Rscript x.r
```

```
Hello from rank 0/2 global 0 local
Hello from rank 1/2 global 1 local
```

Wrapup

Wrapup

- Be careful with RNG's in parallel!
- MPI collectives are very powerful.
- We'll see how to use them next time…
- Next time: task parallelism with MPI

Questions?