Introduction to parallel computing with MPI and Python

Robert Klöfkorn

2021

Question?

Who has used a parallel computer?

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```
blade ~ $ lscpu -e
CPU NODE SOCKET CORE L1d:L1i:L2:L3 ONLINE    MAXMHZ   MINMHZ
  0    0      0    0 0:0:0:0          yes 4500.0000 800.0000
  1    0      0    1 1:1:1:0          yes 4500.0000 800.0000
  2    0      0    2 2:2:2:0          yes 4500.0000 800.0000
  3    0      0    3 3:3:3:0          yes 4500.0000 800.0000
  4    0      0    4 4:4:4:0          yes 4500.0000 800.0000
  5    0      0    5 5:5:5:0          yes 4500.0000 800.0000
  6    0      0    0 0:0:0:0          yes 4500.0000 800.0000
  7    0      0    1 1:1:1:0          yes 4500.0000 800.0000
  8    0      0    2 2:2:2:0          yes 4500.0000 800.0000
  9    0      0    3 3:3:3:0          yes 4500.0000 800.0000
 10    0      0    4 4:4:4:0          yes 4500.0000 800.0000
 11    0      0    5 5:5:5:0          yes 4500.0000 800.0000
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```

Why Parallelization?

Moore's law is the observation that the number of transistors in a dense integrated circuit (IC) doubles about every two years. Taking into account various factors that meant that computer chip performance would roughly double every 18 months.

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- Problem size may exceed a single processors memory
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MIMD – multiple instruction, multiple data

Machines using MIMD have a number of processors that function asynchronously and independently. At any time, different processors may be executing different instructions on different pieces of data.

- Shared Memory
- Distributed Memory

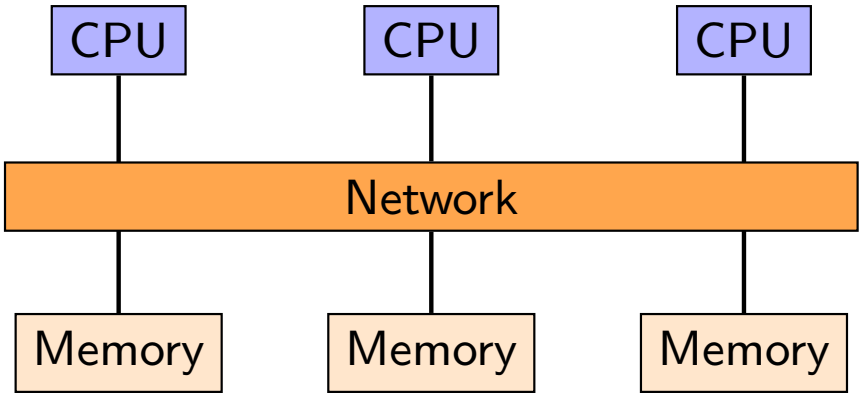
Programming paradigms: Shared memory

Shared memory

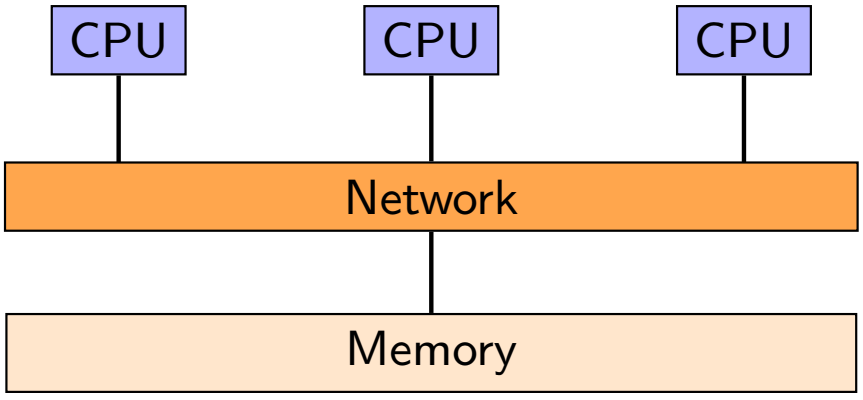
- each CPU has it's own processes and these can share memory
- necessity to ensure correct memory access, i.e. order access to same memory address (race condition)
- easy to program at first (for small code sections), race conditions can be a real nightmare in larger codes

Today's commonly used is for example **Open Multi Processing (OpenMP)** or Intel's **Thread Building Blocks (TBB)**.

Shared Memory MIMD – Example 1



Shared Memory MIMD – Example 2



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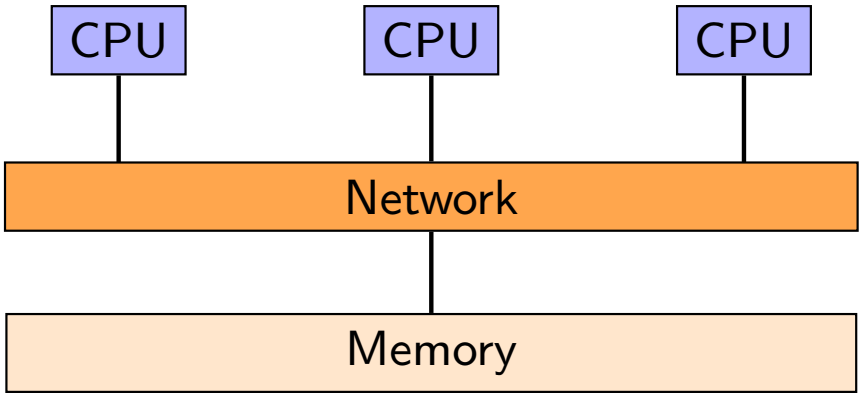

- Usually limited to smaller number of CPUs (< 1000)

Programming paradigms: Distributed memory

Distributed memory

- each CPU has it's own process but also it's own memory
- processes communicate by passing messages to each other (Message Passing)
- synchronization

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Today's standard is the so-called **Message Passing Interface (MPI)**.
Variants of MPI implementations

- MPICH, first implementation 1994, many forks exists
- OpenMPI, open source implementation to prevent forking
  OpenMPI != OpenMP
- MVAPICH, Intel MPI, MS MPI, and many more

Issues to keep in mind

- Communication is much slower than Computation! Thus avoid communication as much as possible (communication avoiding algorithms)
- Memory per core will decrease
- Degree of parallelism will increase
- Memory access is also slow compared to computations (FLOPs are for free)

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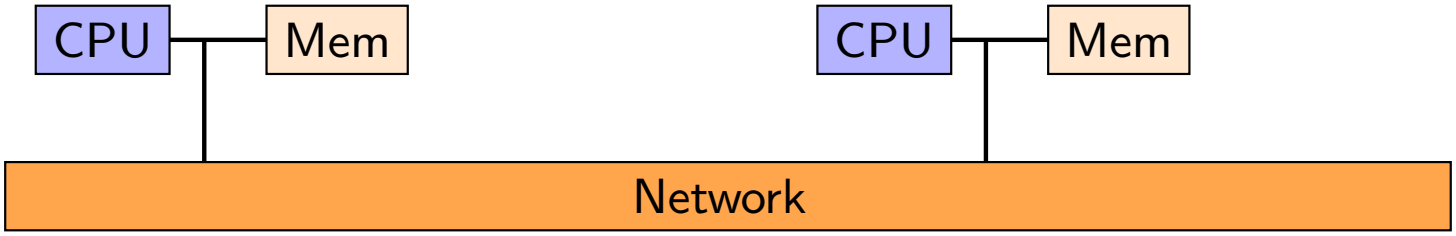
Distributed Memory architecture



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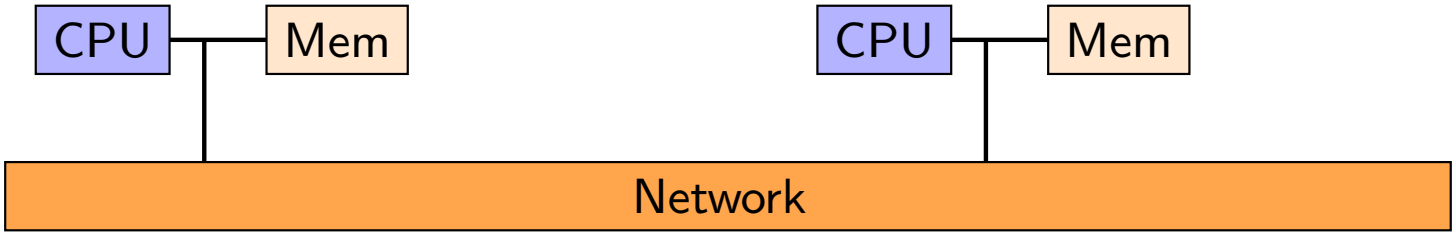

- A CPU–Memory pair is called a (work) node.
- Common model is the SPMD (single program multiple data)
- A node could be a SIMD (single instruction multiple data) or shared memory MIMD node.

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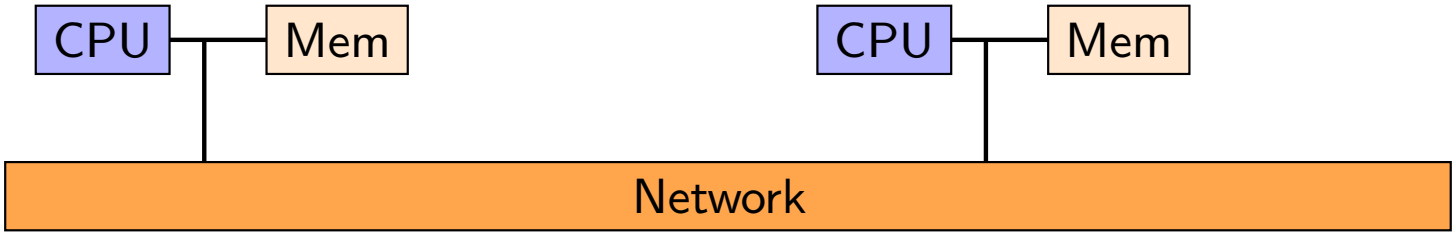

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How does the network look like?

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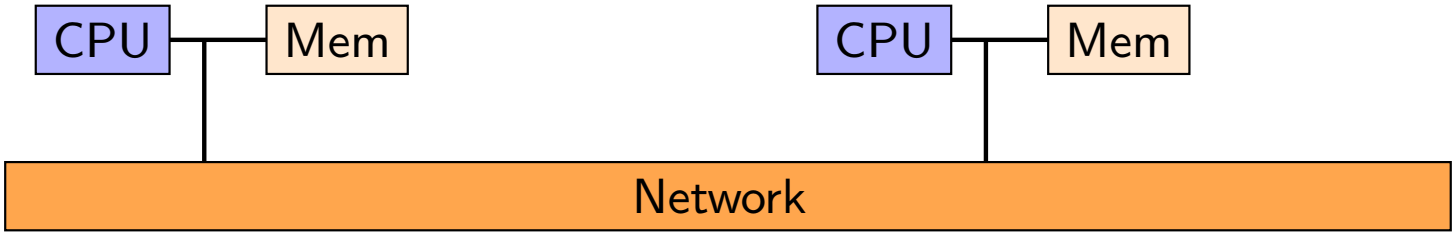

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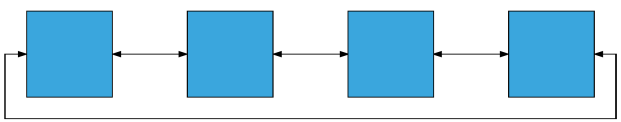
Network topology



1d torus (from Wikipedia)

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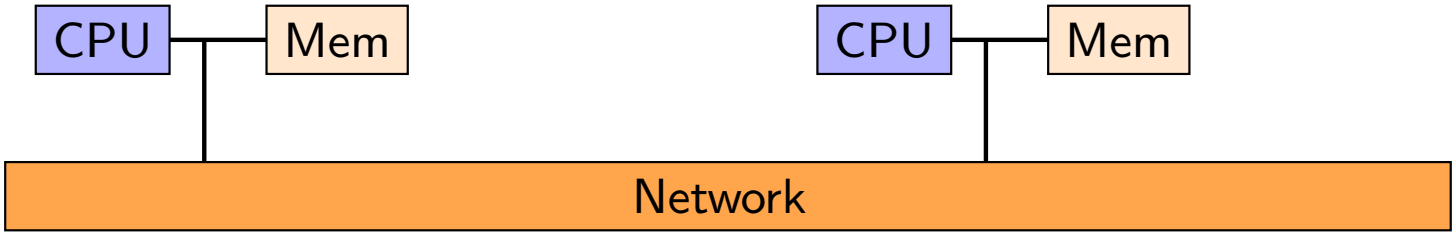

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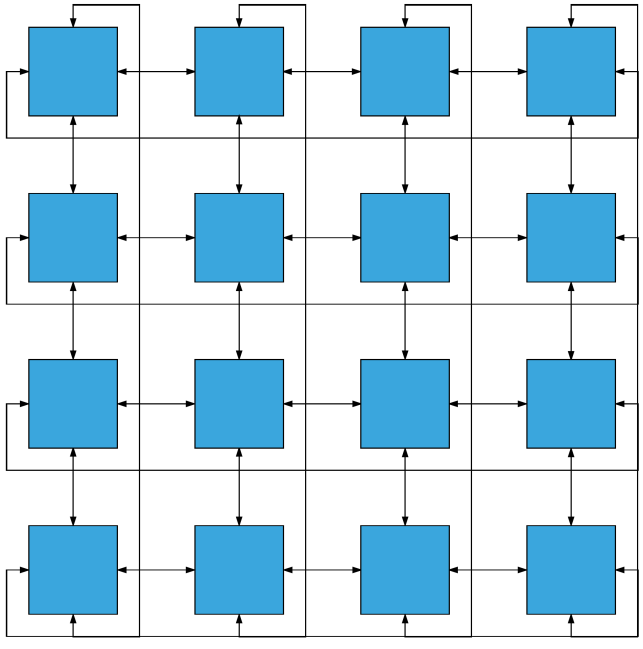
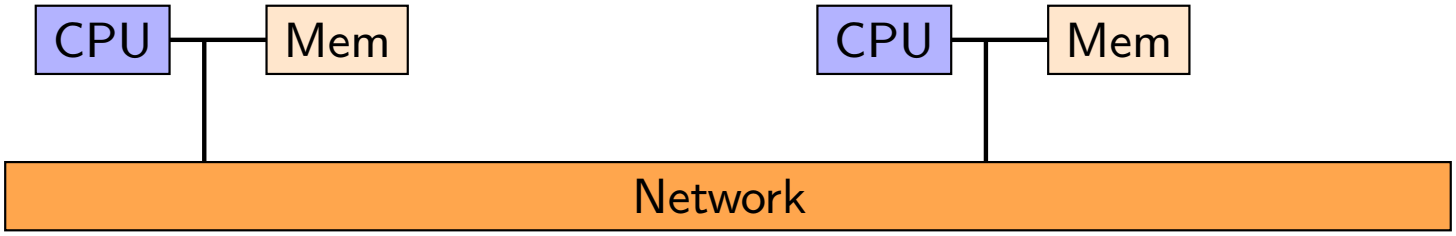


2d torus (from Wikipedia)

Distributed Memory architecture



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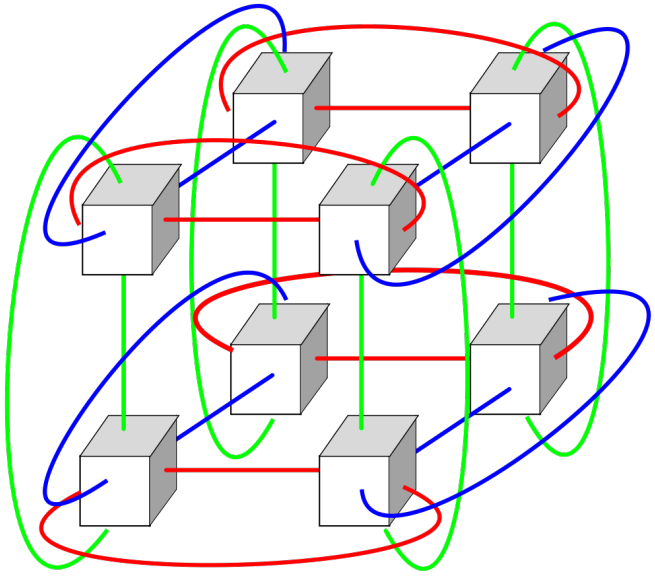
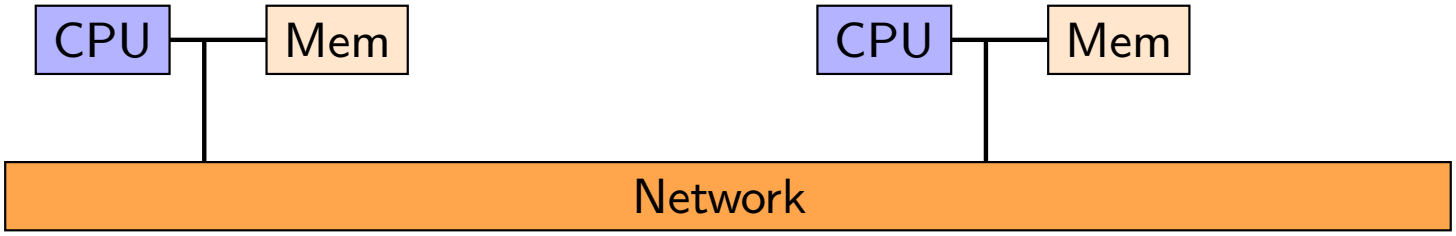


3d torus (from Wikipedia)

Distributed Memory architecture



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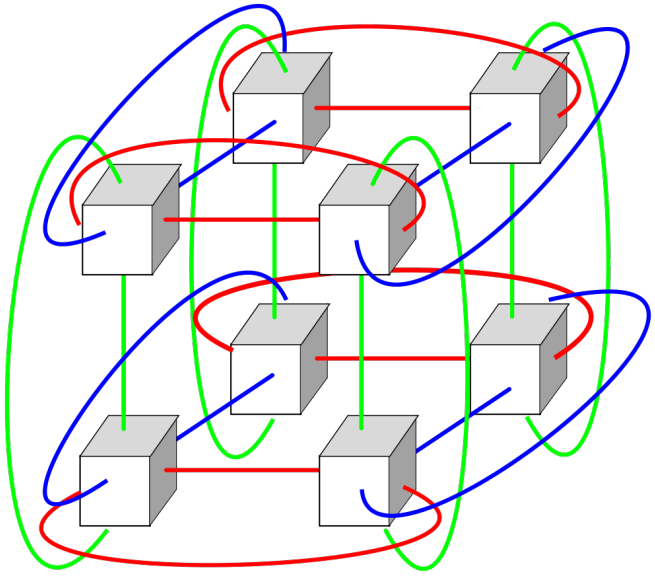

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Also HyperCube networks and mesh networks.

The mpi4py module

- Python interface to MPI
- Based on MPI-2 C/C++ bindings
- Almost all MPI calls supported
- Popular on Linux clusters and in the SciPy community
- Operations are primarily methods on communicator objects
- Supports communication of pickled (serializable) Python objects
- Optimized communication of NumPy arrays
- API docs: `https://mpi4py.readthedocs.io/en/stable/`

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Installation of mpi4py

Easy to install with Anaconda:

```
$ conda create -n mpi mpi4py numpy scipy
```

or pip

```
$ pip install mpi4py
```

Simple example

helloworlddeprecated.py

```
from mpi4py import MPI
""" Get a communicator:
    The most common communicator is the
    one that connects all available processes
    which is called COMM_WORLD
"""
comm = MPI.COMM_WORLD

# print rank (the process number) and overall number of processes
print("Hello World: process", comm.Get_rank(), " out of
    ",comm.Get_size()," is reporting for duty!")
```

On Linux/Mac OS run

```
mpirun -np 4 python helloworld.py
```

On Windows install MSMPI and then set %PATH% environment variable

```
mpiexec /np 4 python helloworld.py
```

to execute the script using 4 processes.

Simple example

helloworld.py

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from mpi4py import MPI
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# acts like COMM_WORLD but is a separate instance
comm = MPI.Comm.Clone( MPI.COMM_WORLD )

# print rank (the process number) and overall number of processes
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Note:

- `MPI_Initialize` is called upon `import` `mpi4py` and
- `MPI_Finalize` is called when the script exits

MPI: most basic send and receive commands

sendrecv.py

```
from mpi4py import MPI
import numpy as np
""" Get a communicator:
    The most common communicator is the
    one that connects all available processes
    which is called COMM_WORLD.
    Clone the communicator to avoid interference
    with other libraries or applications
"""
comm = MPI.Comm.Clone( MPI.COMM_WORLD )

rank = comm.Get_rank()
if rank == 0:
    # send 10 numbers to rank 1 (dest=1)
    data = np.array([range(1,10)])
    print("P[",rank,"] sent data =",data)
    # method 'send' for Python objects (pickle under the hood):
    comm.send(data, dest=1 )

if rank == 1:
    # receive 10 numbers from rank 0 (source=0)
    # method 'recv' for Python objects (pickle under the hood):
    data = comm.recv(source=0 )
    print("P[",rank,"] received data =",data)
```

MPI: optimized Send/Recv for numpy arrays

SendRecv.py

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comm = MPI.Comm.Clone( MPI.COMM_WORLD )

rank = comm.Get_rank()
if rank == 0:
    # send 10 numbers to rank 1 (dest=1)
    data = np.arange(10, dtype='f')
    comm.Send([data,MPI.INT], dest=1, tag=42 )
if rank == 1:
    # receive 10 numbers from rank 0 (source=0)
    data = np.empty(10, dtype='f')
    comm.Recv(data, source=0, tag=42 )
    print("P[",rank,"] received data =",data)
```

MPI: commonly made mistakes

failure.py

```
from mpi4py import MPI
comm = MPI.Comm.Clone( MPI.COMM_WORLD )
rank = comm.Get_rank()

import numpy as np
data = np.array([range(1,10)])

""" Make sure that every send has a matching recv! """

if rank == 0:
    # send 10 numbers to rank 1 (dest=1)
    # method 'send' for Python objects (pickle under the hood):
    comm.send(data, dest=1 )

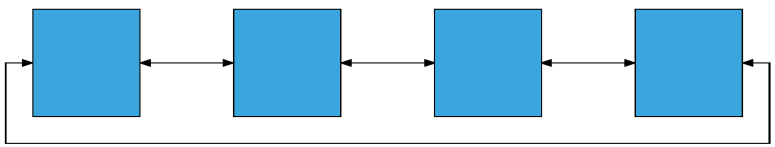
if np.linalg.norm( data ) > 1:
    # receive 10 numbers from rank 0 (source=0)
    # method 'recv' for Python objects (pickle under the hood):
    data = comm.recv(source=0 )
    print("P[",rank,"] received data =",data)
```

Exercise: Let's program a ring communication

Exercise: Lets program a ring where every process communicates with the neighboring processes only.
Let r be the rank of each process for $P \in I\!N$ proceses. Compute the sum of all ranks:

$$s = \sum_{i=0}^{P-1} r_i$$

Use the above mentioned `send` and `recv` commands.



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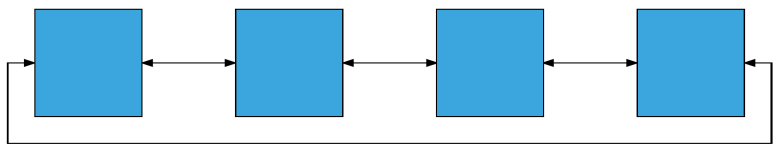

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Compare your result with the simple call

allreduce.py

```
s = comm.allreduce( rank, op=MPI.SUM )
```

Further Reading

mpi4py
https://mpi4py.readthedocs.io/en/stable/
Accessed 2021.

Open MPI
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Accessed 2021.

MPI Forum
https://www.mpi-forum.org
Accessed 2021.