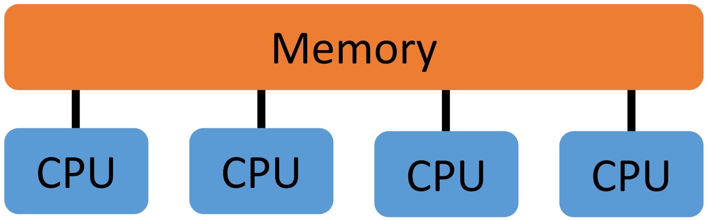
Introduction to MPI

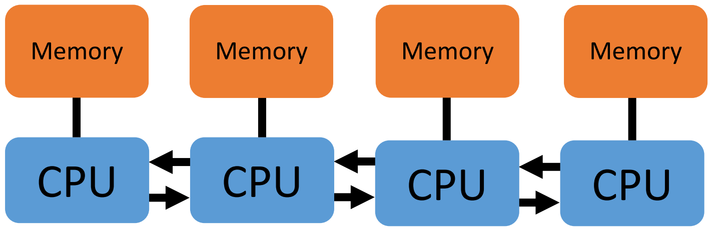
CDP

Shared Memory vs. Message Passing

- **Shared Memory**
  - Implicit communication via memory operations (load/store/lock)
  - Global address space



- **Message Passing**
  - Communicate data among a set of processors without the need for a global memory
  - Each process has its own local memory and communicated with others using messages



Shared Memory

- Advantages
  - **User Friendly:** global address space provides a user-friendly programming
  - **Fast and Uniform:** data sharing between tasks is both fast and uniform due to proximity of memory to CPUs
- Disadvantages
  - **Scalability:** primary disadvantage is the lack of scalability between memory and CPUs.
    Adding more CPUs can increase traffic on the shared memory CPU path.
  - **Responsibility:** Programmer responsibility for synchronization constructs that ensure “correct” access of global memory
  - **Hardware:** it becomes increasingly difficult and expensive to design and produce a shared memory machines with increasing number of processors

Message Passing

- Advantages
  - **Scalability:** adding more CPUs won't harm CPU-memory bandwidth
  - **Responsibility:** elimination of the need for synchronization constructs such as semaphores, monitors, etc…
  - **Distributed:** naturally supports distributed computation
- Disadvantages
  - **Copy Overhead:** data exchanged among processors cannot be shared; it is rather copied (using send/receive messages, not without a cost)
  - **Complicated:** less natural transition from serial implementation

Overview - What is MPI?
Message Passing Interface

- MPI is a message-passing library
- Industry Standard
  - Developed by a consortium of corporations, government labs and universities
  - "Standard" by consensus of MPI Forum participants from over 40 organizations
- The first standard and portable message passing library with good performance
- MPI consists of 128 functions for
  - Point-to-Point message passing
  - User defined datatypes
  - Collective communication
  - Communicator and group management
  - Process topologies
  - Environmental management
- Finished and published in May 1994, updated in June 1995.
- MPI v2 is now becoming the standard
  - Extends (does not change) MPI

What does MPI offer?

- **Standardization**
  - Rely on your MPI code to execute under any MPI implementation running on your architecture.
- **Portability**
  - Designed to supports most environments; very low resource requirements
  - Today your code is parallel; tomorrow it is distributed
- **Performance**
  - Meet industry’s performance demands
- **Richness**
  - 128 functions that allows many different communication methods

What is missing in MPI?

- **Dynamic process management**
  - All the processes created at initiation; cannot be changed.
  - MPI v2 already support dynamic processes
- **Shared memory operations**
  - Share data only via message passing
- **Multi-threading issues**
  - Threads are not supported by MPI (no shared memory)
  - Can use OpenMP with MPI

Design and Implement an MPI Program

- **Serial**
  - When possible, start with a debugged serial version
  - Much easier to debug when running serial
- **Design**
  - Design parallel algorithm
- **Implement**
  - Write code, making calls to MPI library
  - Compile
- **Start Slow**
  - Run with a few nodes first, increase number gradually
  - Easier to debug with small amount of processes

Basic Outline of an MPI Program

- **Initialization**
  - Initialize communications
- **Algorithm**
  - Communicate to share data between processes
  - The logic of your program
- **Finalize**
  - Exit in a "clean" fashion from the message-passing system when done communicating

Format of MPI routines

- **bindings:**
  - **xxxx**(parameter, ...)
- All MPI routines for point-to-point communication and collective communication have integer return type.
- Header file required
  - from mpi4py import MPI
  - for Python programs

6 Basic MPI calls

- **Init**
- **Finalize**
- **Get_rank**
- **Get_size**
- **Send/send**
- **Recv/recv**

Initializing an MPI process

- **MPI_Init**
  - Initialize environment for communication
  - The first MPI call in any MPI process
  - One and only one call to **MPI_Init** per process
  - MPI_Init is **automatically** called when you import the module.
- Process creation is done by the call to
  - **mpirun** -np <num_processes> python <executable>

Exiting from MPI

- **MPI_Finalize**
  - Exit in a "clean" fashion when done communicating
  - Cleans up state of MPI.
  - The last call of an MPI process
  - Must be called only when there is no more pending communications
  - MPI_Finalize is **automatically** called before the Python process ends.

Basic MPI Definitions

- **Group**
  - An ordered set of processes
  - Has its own unique identifier (handle)
    - Assigned by the system
    - Unknown to the user
  - Associated with a communicator
  - Initially, all processes are members of the group given by the predefined communicator **COMM_WORLD**
- **Rank**
  - Unique, integer identifier for a process within a group
  - Sometimes called a "process ID"
  - Contiguous and begin at zero
  - Used to specify the source and destination of messages

Communicator

- Defines the collection of processes (group) which may communicate with each other (context)
- Possesses its own unique identifier (handle)
- Most MPI subroutines require you to specify the communicator as an argument
- We can create and remove groups/communicators during the program runtime
- **COMM_WORLD** is the predefined communicator which includes all processes in the MPI application

Rank and size within a communicator

- **Proccess Rank**
  - Gets a process' rank within a communicator
  - Get_rank()
- **Cluster Size**
  - Gets the number of processes within a communicator
  - Get_size()

MPI Communicator Rank/Size Example

```
import mpi4py.MPI as MPI
# MPI.Init()

comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()
print("Helloworld! I am process %d of %d
processes." % (rank, size))

# MPI.Finalize()
```

Sending and receving messages

- **MPI_Send**
  - Basic blocking send operation
  - Called "standard" send mode
  - **Send**(obj, dest=0, tag=0)

- **MPI_Recv**
  - Basic blocking receive operation
  - **Recv**(buf, source=0, tag=0, status=None)

Sending and receving messages

- **Send/Recv** - uses Numpy arrays, **fast**
- **send/recv** - uses any python object (pickle), **slow**

- **Communication of buffer-like objects [data, count, datatype]**
  - Automatic MPI datatype discovery for NumPy arrays and PEP-3118 buffers is supported, but limited to basic C types (all C/C99-native signed/unsigned integral types and single/double precision real/complex floating types) and availability of matching datatypes in the underlying MPI implementation. In this case, the buffer-provider object can be passed directly as a buffer argument, the count and MPI datatype will be inferred.

MPI messages

- **Message** = **data** + **envelope**

$$\textbf{Send}\ (\underbrace{[\text{data, count, datatype}]}_{\textbf{DATA}},\ \underbrace{\text{dest, tag}}_{\textbf{ENVELOPE}})$$

Data

- **data:** starting location of data
- **count:** number of elements
  - receiver >= sender
- **datatype**: basic or derived
  - receiver == sender

$$\textbf{Send}\ (\underbrace{[\text{data, count, datatype}]}_{\textbf{DATA}},\ \underbrace{\text{dest, tag}}_{\textbf{ENVELOPE}})$$

Envelope

- **dest:** Destination or source
  - Rank in a communicator of sender/receiver respectively
  - Must match or receiver may use **ANY_SOURCE**
- **tag:** Message identifier
  - Integer chosen by programmer
  - Must match or receiver may use **ANY_TAG**

$$\textbf{Send}\ (\underbrace{[\text{data, count, datatype}]}_{\textbf{DATA}}, \underbrace{\text{dest, tag}}_{\textbf{ENVELOPE}})$$

MPI Status

- **Get_count()** - returns message size in Bytes
- **Get_elements(datatype)** - returns number of elements of type datatype
- **Get_source()** - returns message source
- **Get_tag()**- returns message tag
- **Get_error()** – returns the error code

MPI Send/Recv Simple Example

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank == 0:
    data = {'a': 7, 'b': 3.14}
    comm.send(data, dest=1, tag=11)
    print("Message sent, data is: ", data)
elif rank == 1:
    data = comm.recv(source=0, tag=11)
    print("Message Received, data is: ", data)
```

MPI Send/Recv Numpy Arrays

```python
from mpi4py import MPI
import numpy as np

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

# pass explicit MPI datatypes
if rank == 0:
    data = np.arange(1000, dtype= np.int32)
    comm.Send([data, 1000, MPI.INT], dest=1, tag=77)
elif rank == 1:
    data = np.empty(1000, dtype= np.int32)
    comm.Recv([data, 1000, MPI.INT], source=0, tag=77)
```

MPI Send/Recv Numpy Arrays

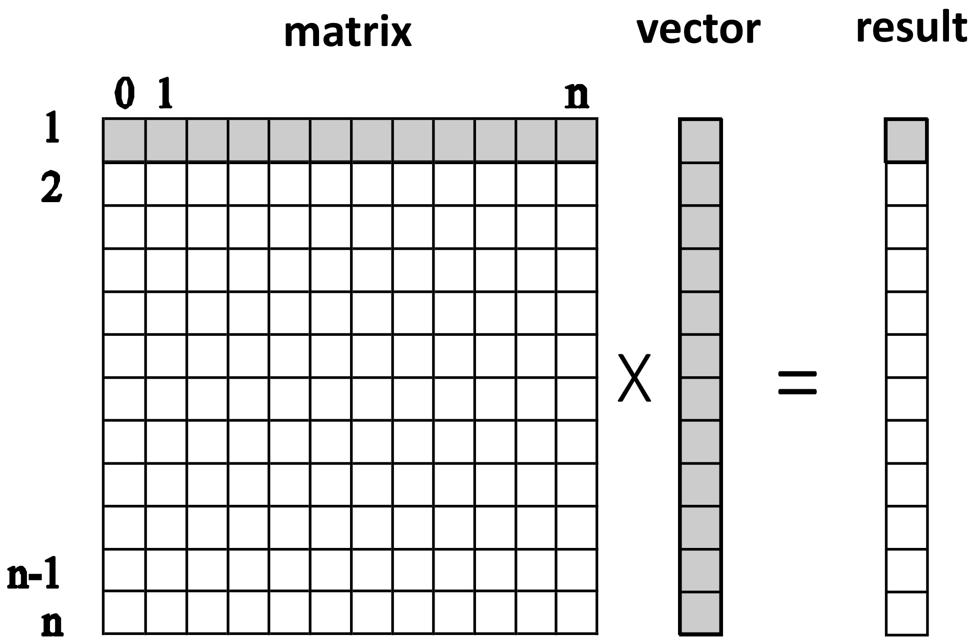
```
from mpi4py import MPI
import numpy as np

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

# automatic MPI datatype discovery
if rank == 0:
    data = numpy.arange(100, dtype=np.float64)
    comm.Send(data, dest=1, tag=13)
elif rank == 1:
    data = numpy.empty(100, dtype=np.float64)
    comm.Recv(data, source=0, tag=13)
```

Multiplying a Dense Matrix with a Vector

- Reminder
  - The computation of each cell in the output vector is independent of the others
  - We can divide the output cells between the processes



```python
from mpi4py import MPI
import numpy as np


RES_VECTOR_TAG = 5

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


matrix = np.ones((128,128))
vector = np.ones(128)

chunk_size = 128//size
```

```python
result = np.empty(chunk_size, dtype=np.int32)

for i in range(0,chunk_size):
    result[i] = np.matmul(matrix[i+rank*chunk_size],vector)

if rank != 0:
    comm.Send([result, chunk_size, MPI.INT], dest=0, tag=1)
else:
    for i in range(1, size):
        recv_res = np.empty(chunk_size, dtype=np.int32)
        comm.Recv(recv_res, source=i, tag=1)
        result = np.append(result,recv_res)
    print(result)
```