Session 12: Introduction to MPI (4PY)

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Overview

• Introduction
  • Basic concepts
  • mpirun

• Hello world
• Wrapping numpy arrays
• Common Pitfalls
Introduction

• MPI: de facto standard for parallel programming in HPC systems since 1994 (MPI 1.0)
• Currently at MPI 3.1
• MPI is a standard with different implementation
  • OpenMPI
  • MPICH
  • Mvapich
  • ...
• Distributed memory systems (process parallel)
• Message-passing
• Goals: performance, scalability, portability
  • Shared memory, sockets, Infiniband...
• Standard is C (C++ bindings deprecated)
• MPI4PY: Layer above in Python

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Getting started

• Requires an MPI Installation + mpi4py
• **Communicator**: The “context” processes use to talk with each other
  • groups processes
  • Separation of concerns
• Process can be in more than one communicator
  rank = comm.Get_rank()
size = comm.Get_size()
• **MPI_COMM_WORLD (MPI.COMM_WORLD)**
  • Basic communicator, created at start time
Introduction: mpirun

- MPI programs are started with a specialized runner application
  - Sets up the environment and starts the instances
  - Distributes processes across nodes

`mpirun --np 2 python hello_world.py <args>`

`mpirun` : MPI runner applications
- `np 2` : number of parallel mpi processes to start
`python hello_world.py` : Your application
`<args>` : Arguments (argv and argc stay the same.)

**Note:** On clusters with SLURM use `srun` instead on `mpirun`
Hello world

from mpi4py import MPI

# Communicator that contains all mpi processes
comm = MPI.COMM_WORLD

rank = comm.Get_rank()
size = comm.Get_size()
name = MPI.Get_processor_name()

print("Rank {0} out of {1} on {2}".format(rank, size, name))

$ srun -np 2 python3 hello_world.py
Rank 0 out of 2 on ANDREASPC
Rank 1 out of 2 on ANDREASPC
Blocking Point-to-Point

• Simple principle:
  • One process sends a message (comm.send)
  • Another process receives the message (comm.recv)
• Blocking, until **locally** completed
• Tag for matching (Should always be set, if possible)

```python
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=1)
elif rank == 1:
    data = comm.recv(source=0, tag=11)
    print(data)
```
MPI4Py: *pickle based vs. arrays*

- MPI4Py supports both:
  - generic Python objects
  - buffer-like objects (e.g. numpy)

- Generic objects
  - Data are pickled before transfer
  - Needs time and memory

- Buffer-like objects
  - Send(), Recv()
  - Tuple/triple for the data
    - [data, MPI.DOUBLE]
    - [data, count, MPI.DOUBLE]
Example: Send/Recv with numpy

```python
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank is 0:
    data = np.array([1,2,4,5], dtype='int')
    comm.send(data, dest=1, tag=1)
elif rank is 1:
    data = comm.recv(source=0, tag=1)
    print(data)
```
Example: Send/Recv with numpy

```python
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank is 0:
    data = np.array([1, 2, 4, 5], dtype='int')
    comm.Send([data, MPI.INT], dest=1, tag=11)
elif rank is 1:
    data = np.zeros(4, dtype='int')
    comm.Recv([data, MPI.INT], source=0, tag=11)
print(data)
```
Performance Comparison

MPI4Py Latency

Python Array
Numpy Array + send()
Numpy Array + Send()
Non-Blocking Point to Point

- Non-blocking version of Send/Recv
- Start a send/recv operations
- Completed later (wait)
- Used to overlap computation and communication
- Avoiding Deadlocks

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

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
req = {}

if rank == 0:
    data = np.array([1,2,4,5], dtype='int')
    req[0] = comm.Isend([data, MPI.INT], dest=1, tag=11)
elif rank == 1:
    data=np.zeros(4, dtype='int')
    req[0] = comm.Irecv([data, MPI.INT],source=0, tag=11)
req[0].wait()
#MPI.Request.waitall(req)
```
Exercise 1: Deadlocks

```python
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()
#modify this function so we don't have a deadlock
send_data1 = np.array([1, 2, 4, 5], dtype='int')
send_data2 = np.array([5, 7, 8, 9], dtype='int')
recv_data1 = np.zeros(4, dtype='int')
recv_data2 = np.zeros(4, dtype='int')
next = (rank + 1) % size
prev = (size + rank - 1) % size
comm.Send([send_data1, MPI.INT], dest=next, tag=11)
comm.Recv([recv_data2, MPI.INT], source=next, tag=12)
comm.Send([send_data2, MPI.INT], dest=prev, tag=12)
comm.Recv([recv_data1, MPI.INT], source=prev, tag=11)
```
Caution

- Send/Recv are only locally blocking
- Send may return, before the other process has received the data
- Depends on the Message size and the MPI-implementation
- (buffered send vs. rendezvous protocol)
- Using non-blocking communication does NOT necessarily mean that communication is handled in the background
- May require “poking” of the MPI Progress Engine
- Depends on MPI implementation and message size
- Req.test()
- Wait is usually busy wait (in HPC, we prefer our threads to sleep)
Collective Operations

• A communication call to collective send/recv messages in a communicator
  • Barrier
  • Bcast
  • Scatter
  • Gather
  • Allgather
  • Reduce/Allreduce

• Forces a synchronization between Processes
  • Can also be a reason for slow-down
  • Usually, a busy waiting model (HPC)
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
comm.Barrier()
#comm.barrriere()
Bcast and Scatter

```python
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank is 0:
    data = np.array([2, 2, 3, 4], dtype='int')
else:
    data = np.zeros(1, dtype='int')

comm.Bcast([data, MPI.INT], root=0)
print("bcast", rank, data)
if rank is 0:
    comm.Scatter([data, MPI.INT], [data, MPI.INT], root=0)
else:
    comm.Scatter(None, [data, MPI.INT], root=0)
print("scatter", rank, data)
```
Gather and Allgathер

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

data = (rank+1)**2
data = comm.gather(data, root=0)

print(rank, data)

data = np.array(rank, dtype='int')
gather = np.zeros(4, dtype='int')
comm.Allgathер([[data,MPI.INT],
                 [gather, MPI.INT]])
print(rank, gather)
```
Reduce/Allreduce

```python
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
data = np.array(rank, dtype='int')
result = np.zeros(1, dtype='int')
comm.Reduce([data, MPI.DOUBLE],
             [result, MPI.DOUBLE],
op=MPI.SUM, root=0)
print("reduce", rank, result)

comm.Allreduce([data, MPI.DOUBLE],
               [result,
                MPI.DOUBLE],
op=MPI.SUM)
print("allreduce", rank, result)
```
Reduce/Allreduce

```python
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
data = np.array(rank, dtype='int')
result = np.zeros(1, dtype='int')
comm.Reduce([data, MPI.DOUBLE],
            [result, MPI.DOUBLE],
            op=MPI.SUM, root=0)
print("reduce", rank, result)

comm.Allreduce([data, MPI.DOUBLE],
               [result,
                MPI.DOUBLE],
               op=MPI.SUM)
print("allreduce", rank, result)
```

reduce 1 [0]
reduce 3 [0]
reduce 2 [0]
reduce 0 [6]
allreduce 2 [6]
allreduce 3 [6]
allreduce 1 [6]
allreduce 0 [6]
Exercise 2: Computing Pi in Parallel

If rank is 0
    N = np.array(10000, 'i')

#Distribute N Across all nodes

start = time.time()
h = 1.0 / N; s = 0.0
for i in range(rank, N, size):
    x = h * (i + 0.5)
    s += 4.0 / (1.0 + x**2)
PI = np.array(s * h, dtype='d')

#collect result with the reduce function
end = time.time()
if rank is 0:
    print ("I get for PI {0}".format(PI_ALL))
    print("I needed {0} seconds").format(end-start)
Exercise 3: 2-D Stencil
Tips: Send/recv partial arrays

```python
req[0] = comm.Isend([grid1[1][:],MPI.DOUBLE], dest=top, tag=2)
req[1] = comm.Irecv([grid1[my_m+1][:],MPI.DOUBLE], source=btm, tag=2)
```
Further reading and resources used

https://en.wikipedia.org/wiki/Message_Passing_Interface

Thank you for your attention

References and further reading: