3.1 Distributed Computing

Acknowledgements

- Much of this tutorial uses slide material from William Gropp, University of Illinois and Lisandro Dalcin, CONICET
- mpi4py is a Cythonized wrapper around MPI originally developed by Lisandro Dalcin, CONICET

Notebook Engine Setup

Following the recommendations in PEP 8, we import all Python modules at the beginning of the notebook.

In [5]:
```
%load_ext parallelmagic
%pylab inline --no-import-all
```

```
The parallelmagic extension is already loaded. To reload it, use:
  %reload_ext parallelmagic
Populating the interactive namespace from numpy and matplotlib
```

In [6]:
```
import os
from mpi4py import MPI
import numpy as np
from matplotlib import pyplot
```

Connecting to MPI via IPython

To run the examples in parallel, you must run the command:

```
ipcluster start --engines=MPI --n 4
```

Or use notebook Appendix_Launch_MPI_Engines (if you are using the VMs or have this configured for your environment).

Then execute the next cell:

In [7]:
```
from IPython.parallel import Client
c = Client()
view = c[:]

view.activate()
view.block = True
```

There are now 5 IPython Engines (also sometimes called kernels) running: 1 directly connected to the Notebook and 4 started by `ipcluster` and connected via the Client interface.

`%autopx` and the `ipcluster` Engines

For interactive convenience, we will use the `autopx` magic from the `parallelmagic` extensions. We can use the `autopx` magic to execute cells on the ipcluster Engines instead of the Notebook Engines.

In [8]:
```
os.getpid()
```

Out[8]:
```
22158
```

In [9]:
```
%autopx
```

```
%autopx enabled
```

Recall that when we used `import` earlier it was on the Notebook Engine. Before we can call `os.getpid` on the ipcluster Engines, we need to import `os` and any other modules we would like to use.

In [11]:
```
import os
#We will use mpi4py, numpy, and math later
from mpi4py import MPI
import numpy as np
import math
```

In [12]:
```
os.getpid()
```

Out[0:3]: 22398

Out[1:3]: 22399

Out[2:3]: 22400

Out[3:3]: 22397

A Quick Review of Concepts of Scalability

The Multiple Forms of Parallelism

- **instruction** - multiple program instructions are simultaneously dispatched in a pipeline or to multiple execution units (superscalar)
- **data** - the same program instructions are carried out simultaneously on multiple data items (SIMD)
- **task** - different program instructions on different data (MIMD)
- **collective** - single program, multiple data, not necessarily synchronized at individual operation level (SPMD)

This part of the tutorial focuses on data and collective parallelism

Parallel Programming Paradigms

- a parallel programming paradigm is a specific approach to exploiting parallelism in hardware
- many programming paradigms are very tightly coupled to the hardware beneath!
  - CUDA assumes large register files, Same Instruction Multiple Thread parallelism, and a mostly flat, structured memory model, matching the underlying GPU hardware
  - OpenMP exposes loop level parallelism with a fork/join model, assumes the presence of shared memory and atomics
  - OpenCL tries to generalize CUDA, but still assumes a 'coprocessor' approach, where kernels are shipped from a master core to worker cores

The Message Passing Model

- a process is (traditionally) a program counter for instructions and an address space for data
- processes may have multiple threads (program counters and associated stacks) sharing a single address space
- message passing is for communication among processes, which have separate address spaces
- interprocess communication consists of
  - synchronization
  - movement of data from one process's address space to another's

Why MPI?

- **communicators** encapsulate communication spaces for library safety
- **datatypes** reduce copying costs and permit heterogeneity
- multiple **communication modes** allow more control of memory buffer management
- extensive **collective operations** for scalable global communication
- **process topologies** permit efficient process placement, user views of process layout
- **profiling interface** encourages portable tools

It Scales!

MPI - Quick Review

- processes can be collected into **groups**
- each message is sent in a **context**, and must be received in the same context
- a **communicator** encapsulates a context for a specific group
- a given program may have many communicators with any level of overlap
- two initial communicators
  - `MPI_COMM_WORLD` (all processes)
  - `MPI_COMM_SELF` (current process)

In Python, these communicators are `MPI.COMM_WORLD and MPI.COMM_SELF`

Communicator, Rank, and Size Setup

We'll be using the `MPI.COMM_WORLD` communicator as `comm` for the remainder of this notebook. It's also very common to use the communicator's associated rank and size attributes as `rank` and `size`. We'll assign these variables now to simplify the readability of the code.

In [18]:
```
comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()
```

First Example: Hello World

In [19]:
```
# set up basic variables
name = MPI.Get_processor_name()
pid = os.getpid()
```

In [20]:
```
print("Hello World! I am process %d of %d on %s with pid %d.\n" % (rank, size, name, pid))
```

```
[stdout:0]
Hello World! I am process 1 of 4 on Arons-MacBook-Pro.local with pid 22398.

[stdout:1]
Hello World! I am process 2 of 4 on Arons-MacBook-Pro.local with pid 22399.

[stdout:2]
Hello World! I am process 3 of 4 on Arons-MacBook-Pro.local with pid 22400.

[stdout:3]
Hello World! I am process 0 of 4 on Arons-MacBook-Pro.local with pid 22397.
```

Note that the MPI rank is not necessarily synchronized with the IPython view rank.

Communicators

- processes can be collected into **groups**
- each message is sent in a **context**, and must be received in the same context
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- two initial communicators
  - `MPI_COMM_WORLD` (all processes)
  - `MPI_COMM_SELF` (current process)

Datatypes

- the data in a message to send or receive is described by address, count and datatype
- a datatype is recursively defined as:
  - predefined, corresponding to a data type from the language (e.g., `MPI_INT`, `MPI_DOUBLE`)
  - a contiguous, strided block, or indexed array of blocks of MPI datatypes
  - an arbitrary structure of datatypes
- there are MPI functions to construct custom datatypes

Tags

- messages are sent with an accompanying user-defined integer tag to assist the receiving process in identifying the message
- messages can be screened at the receiving end by specifying the expected tag, or not screened by using `MPI_ANY_TAG`

mpi4py Functionality

- Implements up to MPI-3 with underlying MPI implementation support
- Generic API with lowercase function names, e.g. `Comm.send`
- Efficient API with titlecase function names, e.g. `Comm.Send`
  - The efficient API can still handle default arguments and type discovery for NumPy arrays and PEP-3118 buffers

Job Startup

- To launch: mpirun --np NP python script_name
- IPython automatically handles calling `mpirun` for you with the `ipcluster` command

Initialization

`mpi4py` automatically calls `MPI_Init()` and `MPI_Finalize()`

- `MPI_Init()` is called when you import the `MPI` module from `mpi4py`
- `MPI_Finalize()` is called before the Python process ends
- If you need explicit control, use the `mpi4py.rc` module to configure before importing `MPI`

MPI Basic (Blocking) Send

C

```
   int MPI_Send(void* buf, int count, MPI_Datatype type,
   int dest, int tag, MPI_Comm comm)
```

mpi4py

```
  Comm.Send(self, buf, dest=0, tag=0)
  Comm.send(self, obj=None, dest=0, tag=0)
```

MPI Basic (Blocking) Recv

C

```
   int MPI_Recv(void* buf, int count, MPI_Datatype type,
   int source, int tag, MPI_Comm comm, MPI_Status status)
```

mpi4py

```
  comm.Recv(self, buf, source=0, tag=0, status=None)
  comm.recv(self, obj=None, source=0, tag=0, status=None)
```

Send/Receive Example

Generic

In [23]:
```
if rank == 0:
   data = {'a': 7, 'b': 3.14}
   comm.send(data, dest=1, tag=11)
elif rank == 1:
   data = comm.recv(source=0, tag=11)
   print data
```

```
[stdout:0] {'a': 7, 'b': 3.14}
```

Efficient

Explicit MPI Datatypes

In [27]:
```
if rank == 0:
    data = np.arange(10, dtype='i')
    comm.Send([data, MPI.INT], dest=1, tag=77)
elif rank == 1:
    data = np.empty(10, dtype='i')
    comm.Recv([data, MPI.INT], source=0, tag=77)
    print data
```

```
[stdout:0] [0 1 2 3 4 5 6 7 8 9]
```

Automatic MPI Datatype Discovery (NumPy arrays)

In [29]:
```
if rank == 0:
    data = np.arange(10, dtype=np.float64)
    comm.Send(data, dest=1, tag=13)
elif rank == 1:
    data = np.empty(10, dtype=np.float64)
    comm.Recv(data, source=0, tag=13)
    print data
```

```
[stdout:0] [ 0.  1.  2.  3.  4.  5.  6.  7.  8.  9.]
```

Synchronization

C

```
int MPI_Barrier(MPI_Comm comm)
```

mpi4py

```
comm.Barrier(self)
comm.barrier(self)
```

In [30]:
```
for r_id in range(comm.Get_size()):
    if rank == r_id:
        print "Hello from proc:", rank
    comm.Barrier()
```

```
[stdout:0] Hello from proc: 1
[stdout:1] Hello from proc: 2
[stdout:2] Hello from proc: 3
[stdout:3] Hello from proc: 0
```

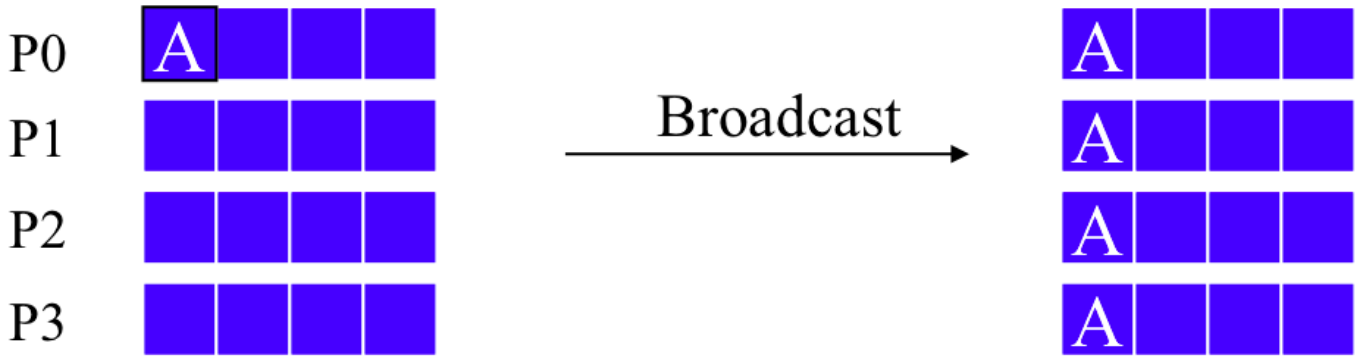
Timing and Profiling

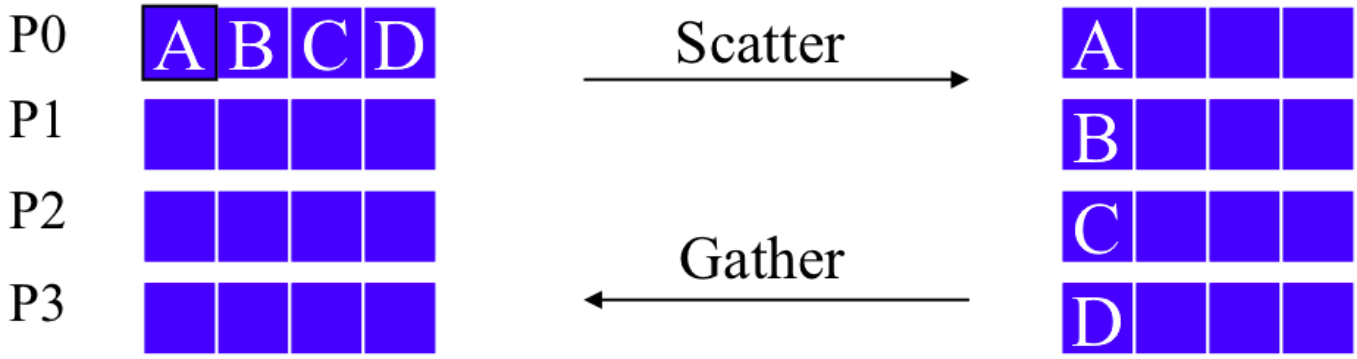
The elapsed (wall-clock) time between two points in an MPI program can be computed using MPI_Wtime:

In [31]:
```
t1 = MPI.Wtime()
t2 = MPI.Wtime()
print("time elapsed is: %e\n" % (t2-t1))
```

```
[stdout:0]
time elapsed is: 9.230500e-05

[stdout:1]
time elapsed is: 9.876500e-05

[stdout:2]
time elapsed is: 9.861000e-05

[stdout:3]
time elapsed is: 4.349900e-05
```

Basic Collectives: Broadcast, Scatter, and Gather





C

```
   int MPI_Bcast(void *buf, int count, MPI_Datatype type,
   int root, MPI_Comm comm)
```

mpi4py

```
  comm.Bcast(self, buf, root=0)
  comm.bcast(self, obj=None, root=0)
```

Broadcast Example

In [54]:
```
if rank == 0:
   data = {'key1' : [7, 2.72, 2+3j],
           'key2' : ( 'abc', 'xyz')}
else:
   data = None
data = comm.bcast(data, root=0)
print "bcast finished and data \
 on rank %d is: "%comm.rank, data
```

```
[stdout:0] bcast finished and data  on rank 0 is:  {'key2': ('abc', 'xyz'), 'key1': [7, 2.72, (2+3j)]}
[stdout:1] bcast finished and data  on rank 1 is:  {'key2': ('abc', 'xyz'), 'key1': [7, 2.72, (2+3j)]}
[stdout:2] bcast finished and data  on rank 3 is:  {'key2': ('abc', 'xyz'), 'key1': [7, 2.72, (2+3j)]}
[stdout:3] bcast finished and data  on rank 2 is:  {'key2': ('abc', 'xyz'), 'key1': [7, 2.72, (2+3j)]}
```

Scatter Example:

In [55]:
```
if rank == 0:
   data = [(i+1)**2 for i in range(size)]
else:
```

```
   data = None
data = comm.scatter(data, root=0)
assert data == (rank+1)**2
print "data on rank %d is: "%comm.rank, data
```

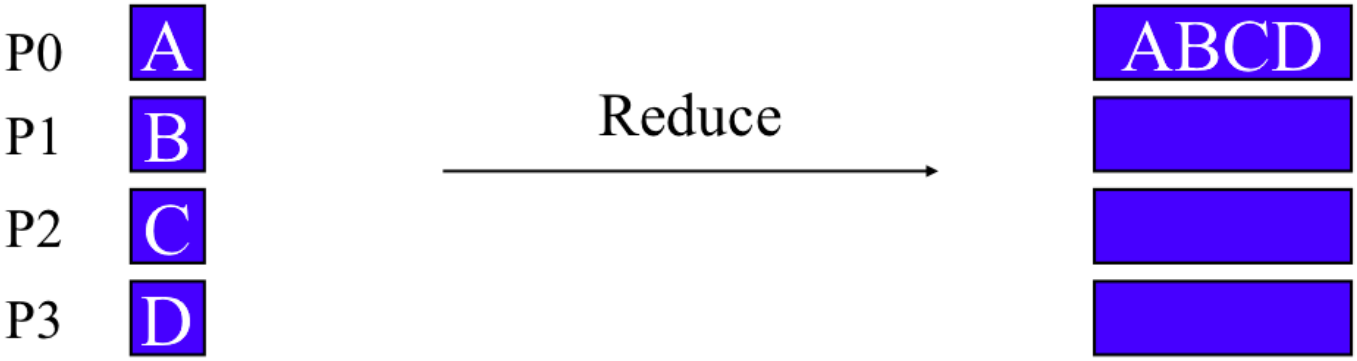
```
[stdout:0] data on rank 0 is:  1
[stdout:1] data on rank 1 is:  4
[stdout:2] data on rank 3 is:  16
[stdout:3] data on rank 2 is:  9
```

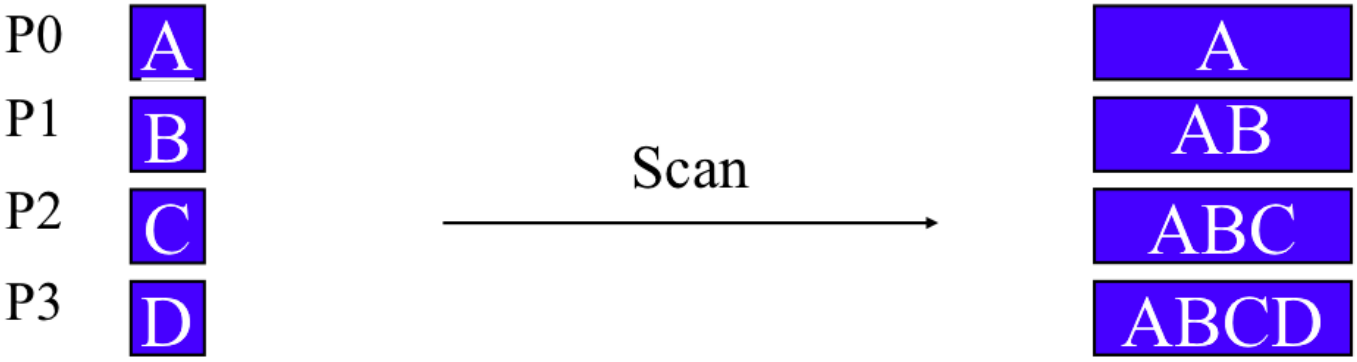
Gather (and Barrier) Example:

In [56]:
```
data = (rank+1)**2
print "before gather, data on \
  rank %d is: "%rank, data

comm.Barrier()
data = comm.gather(data, root=0)
if rank == 0:
   for i in range(size):
       assert data[i] == (i+1)**2
else:
   assert data is None
print "data on rank: %d is: "%rank, data
```

```
[stdout:0]
before gather, data on   rank 0 is:  1
data on rank: 0 is:  [1, 4, 9, 16]
[stdout:1]
before gather, data on   rank 1 is:  4
data on rank: 1 is:  None
[stdout:2]
before gather, data on   rank 3 is:  16
data on rank: 3 is:  None
[stdout:3]
before gather, data on   rank 2 is:  9
data on rank: 2 is:  None
```

Reduce and Scan





Reduce Example

The lower-case `reduce` implemented in `mpi4py` is not designed to be particularly scalable. If you need to perform a reduce on thousands of processes or more, it is recommended that you either switch to the non-generic Reduce, or utilize the scalable reduce provided in `mpi4py/demo/reductions/reductions.py`

In [57]:
```
sendmsg = comm.rank
recvmsg1 = comm.reduce(sendmsg, op=MPI.SUM, root=0)
recvmsg2 = comm.allreduce(sendmsg)
print recvmsg2
```

```
[stdout:0] 6
[stdout:1] 6
[stdout:2] 6
[stdout:3] 6
```

Compute Pi Example

The following example is completely self-contained to simplify reuse in another script. You can switch between running the code in parallel and serial by executing an %autopx cell.

In [33]:
```
from mpi4py import MPI
import math

def compute_pi(n, start=0, step=1):
    h = 1.0 / n
    s = 0.0
    for i in range(start, n, step):
        x = h * (i + 0.5)
        s += 4.0 / (1.0 + x**2)
    return s * h
```

```
comm = MPI.COMM_WORLD
nprocs = comm.Get_size()
myrank = comm.Get_rank()
if myrank == 0:
    n = 10
else:
    n = None

n = comm.bcast(n, root=0)

mypi = compute_pi(n, myrank, nprocs)

pi = comm.reduce(mypi, op=MPI.SUM, root=0)

if myrank == 0:
    error = abs(pi - math.pi)
```

```
[stdout:3]
pi is approximately 3.1424259850010983
error is 0.0008333314113051
```

Mandelbrot Set Example

The following example is completely self-contained to simplify reuse in another script.

In [41]:
```
from mpi4py import MPI
import numpy as np

def mandelbrot (x, y, maxit):
    c = x + y*1j
    z = 0 + 0j
    it = 0
    while abs(z) < 2 and it < maxit:
        z = z**2 + c
        it += 1
    return it

x1, x2 = -2.0, 1.0
y1, y2 = -1.0, 1.0
w, h = 250, 200
maxit = 127

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

# number of rows to compute here
N = h // size + (h % size > rank)

# first row to compute here
start = comm.scan(N)-N

# array to store local result
Cl = np.zeros([N, w], dtype='i')

# compute owned rows

dx = (x2 - x1) / w
dy = (y2 - y1) / h

for i in range(N):
    y = y1 + (i + start) * dy
    for j in range(w):
        x = x1 + j * dx
        Cl[i, j] = mandelbrot(x, y, maxit)

# gather results at root (process 0)
counts = comm.gather(N, root=0)
C = None
if rank == 0:
    C = np.zeros([h, w], dtype='i')

# here we create a custom datatype for sending/receiving rows of data.
rowtype = MPI.INT.Create_contiguous(w)
rowtype.Commit()
```

```
comm.Gatherv(sendbuf=[Cl, MPI.INT], recvbuf=[C, (counts, None), rowtype],root=0)
```

We can't inline plots from the `ipcluster` Engines where we just performed the computations. Instead, we use the Notebook Engine to get a copy of the data on MPI rank 0, then plot as before.

First, we switch off `%autopx` to enable computing on the Notebook Engine.

In [42]:
```
%autopx
```

```
%autopx disabled
```

Then we collect the array and rank data from the `ipcluster` Engines using the `view` object.

In [43]:
```
# CC is a list of C from all ranks
CC = view['C']
# Similarly, ranks is a list of MPI ranks from all ipcluster processes
ranks = view['rank']

# Do the plotting
# We use the IPython index of the ipcluster process with rank 0 as
# the index into CC
pyplot.imshow(CC[ranks.index(0)])
pyplot.spectral()
pyplot.show()
```