Python for High Performance Computing

Monte Lunacek

Research Computing, University of Colorado **Boulder**

University of Colorado

- Some tightly-coupled MPI codes
- Many **independent tasks**
- Diverse computing backgrounds
  - Geography
  - Ecology and Evolutionary Biology
  - Microbial Ecology
  - Astronomy
  - Geology
- Range of computational experience

High Throughout Computing

- Simulations
  - Monte Carlo
  - Parameter scan
  - Uncertainty Quantification
- Parameter Optimization
- Data Analysis (MapReduce)
- Parallel workflows

Supercomputing Without the Pain

- Accessible to anyone with:
  - Simulation or analysis to run
  - Desire to do it faster
- Remove barriers to entry

Success Stories

~500,000 simulations on ~7,000 cores with mpi4py (http://mpi4py.scipy.org/)

Parameter optimization on ~100 cores with Scoop (https://code.google.com/p/scoop/) and DEAP (https://code.google.com/p/deap/)

Improved biological workflow with IPython Parallel (http://ipython.org/ipython-doc/dev/parallel/)

Wrapped an engineering simulation with f2py (http://www.scipy.org/F2py) and IPython Parallel (http://ipython.org/ipython-doc/dev/parallel/)

Outline

- Python (http://python.org)
- Ipython Notebook (http://ipython.org/ipython-doc/dev/interactive/htmlnotebook.html)
- High Throughput Computing
    - IPython Parallel (http://ipython.org/ipython-doc/dev/parallel/)
    - Scoop (https://code.google.com/p/scoop/)
    - mpi4py (http://mpi4py.scipy.org/)
- Data Analysis with pandas (http://discoproject.org/)
- Conclude

What is Python?

Python

- Flexible, powerful programming language
  - Object oriented
  - Runs everywhere
- Easy, clean syntax
- Glue: Cython, F2py
- Large community of support
  - Consistent feel
- Free as in **free beer**
- Free as in **free speech**

Packages for Computational Science

- **python**: the base language
- **numpy**: arrays, fast operations on arrays
- **scipy**: higher level computational routines
- **matplotlib**: plotting
- **ipython**: notebooks, flexible shell, and parallel
- **pandas**: data analysis

What can you do with Python?

- OS support: manage files and directories
- Glue existing applications
- LAPACK and BLAS: access powerful C and Fortran libraries
- Parallel
- Data Analysis
- Visualization
- GUI programming
- Scrape websites
- Build websites
- **Anything!**

Distributions

- Enthought (http://www.enthought.com/products/epd.php)
- Python(x,y) (http://www.pythonxy.com/)
- Anaconda (https://store.continuum.io/cshop/anaconda)

IPython terminal

```
ipython --pylab
```

IPython notebook

```
ipython notebook --pylab=inline
```

Notebook

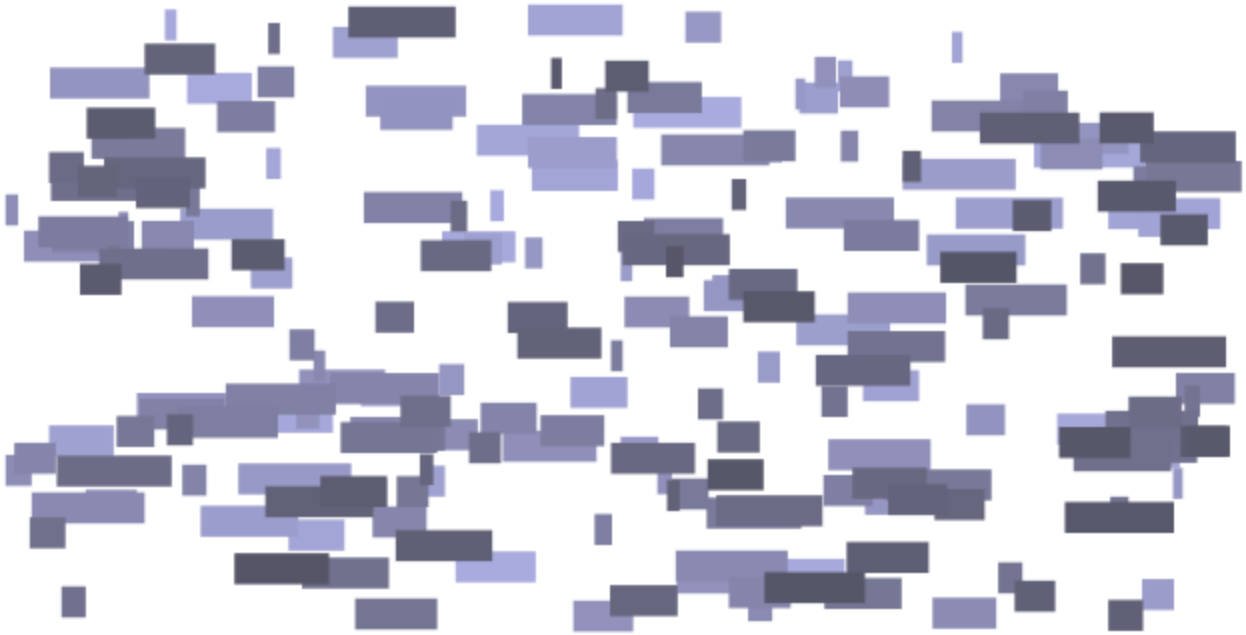
This webpage is not available

Google Chrome's connection attempt to **127.0.0.1** was rejected. The website may be down, or your network may not be properly configured.

Here are some suggestions:

- Reload this webpage later.
- Check your Internet connection. Restart any router, modem, or other network devices you may be using.
- Add Google Chrome as a permitted program in your firewall's or antivirus software's settings. If it is already a permitted program, try deleting it from the list of permitted programs and adding it again.
- If you use a proxy server, check your proxy settings or contact your network administrator to make sure the proxy server is working. If you don't believe you should be using a proxy server, adjust your proxy settings: Go to **Applications > System Preferences > Network > Advanced > Proxies** and deselect any proxies that have been selected.

Error 102 (net::ERR_CONNECTION_REFUSED): The server refused the connection.



High Throughput Computing

Bash

```
count_base=0
for i in {1..N}
do
  for j in {1..12}
  do
          b=$(($count_base + $j))
          ./simulator -s 5 -t $b &
        done
  wait
  count_base=$(( $count_base + $np))
done
```

Limited to a **single node**

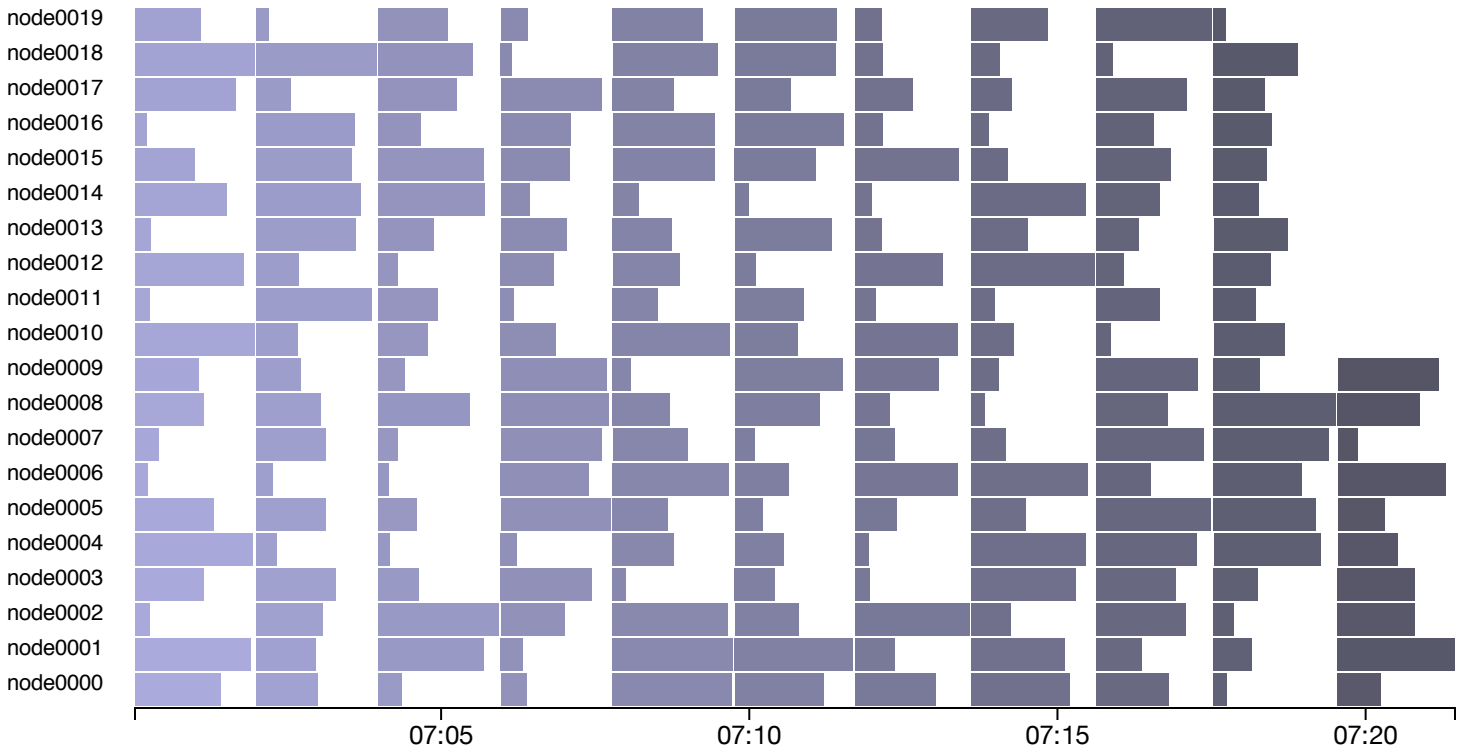
pbsdsh

```
#!/bin/bash
PATH=$PBS_O_WORKDIR:$PBS_O_PATH
TRIAL=$(($PBS_VNODENUM + $1))
python ./simulator.py -s 5 -t $TRIAL
```

```
for i in {1..N}
do
  pbsdsh wrapper.sh $count
  count=$(( $count + 12))
done
```

A little **painful**

A little inefficient



Objective Function

```
def simulation(x):
    value = x*x + 10
    return value
```

The functions name is **simulation**

Multiprocessing

Import

```
from multiprocessing import Pool
```

Map the values

```
if __name__ == '__main__':

    pool = Pool(12)  # workers
    data = range(200) # tasks

    results = pool.map(simulation, data)
```

Great for single node

Python's **threading** library

Scoop

Import

```
from scoop import futures
```

Map the values

```
if __name__ == '__main__':

    data = range(200) # tasks
    results = futures.map(simulation, data)
```

Launch

```
python -m scoop filename.py
```

Efficient startup!

IPython Parallel

```
from IPython.parallel import Client, require
```

Map the values

```
if __name__ == '__main__':

    data = range(200) # tasks
    rc = Client(profile='mpi')
    lview = rc.load_balanced_view()

    results = lview.map(simulation, data)
    results.wait()
```

Compare

```
results = pool.map(simulation, data)
```

```
results = futures.map(simulation, data)
```

```
results = lview.map(simulation, data)
```

It's the way you create the **object.map()** that separates these methods.

Compare

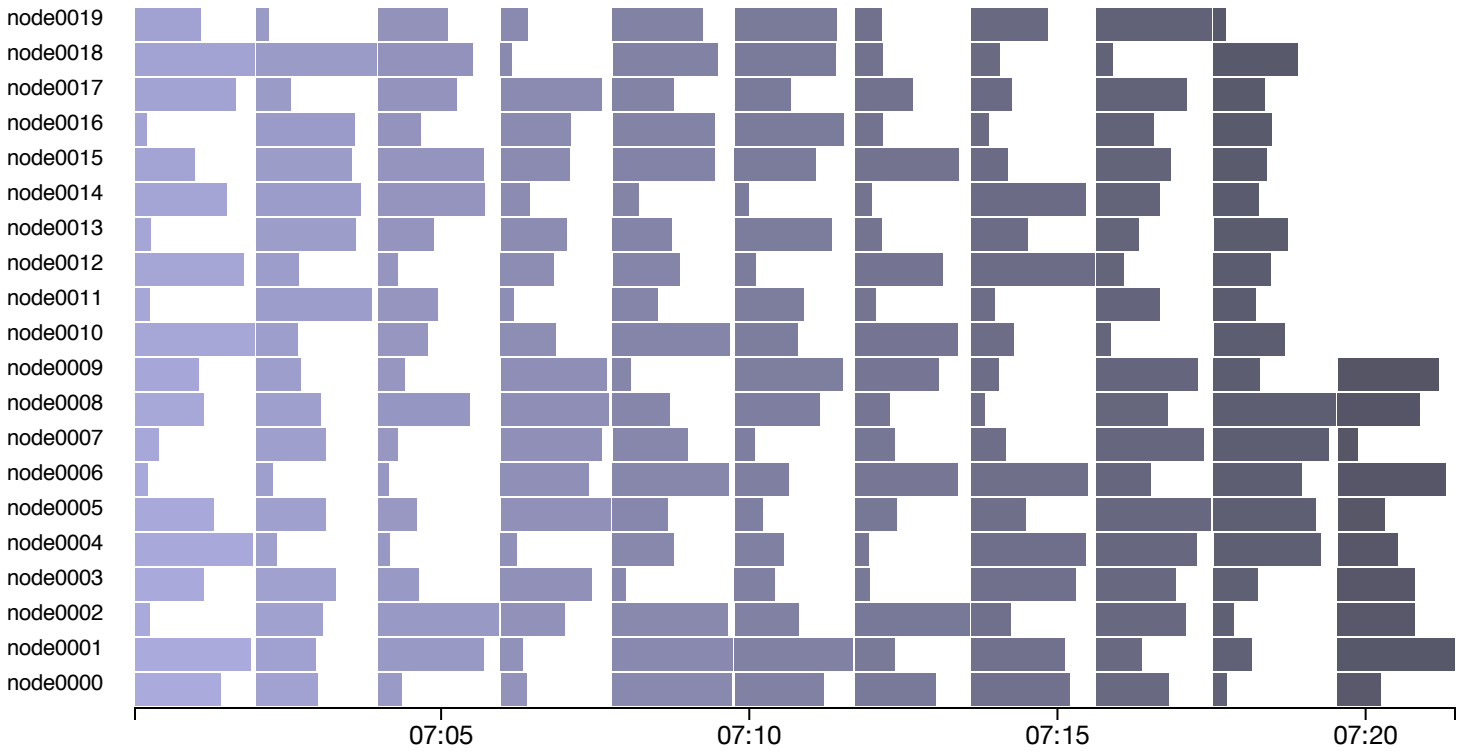
Good

IPython	Fault-tolerance
IPython	Schedule
IPython	Interactive
Scoop	Efficient launch
Multiprocessing	Included in the standard Library

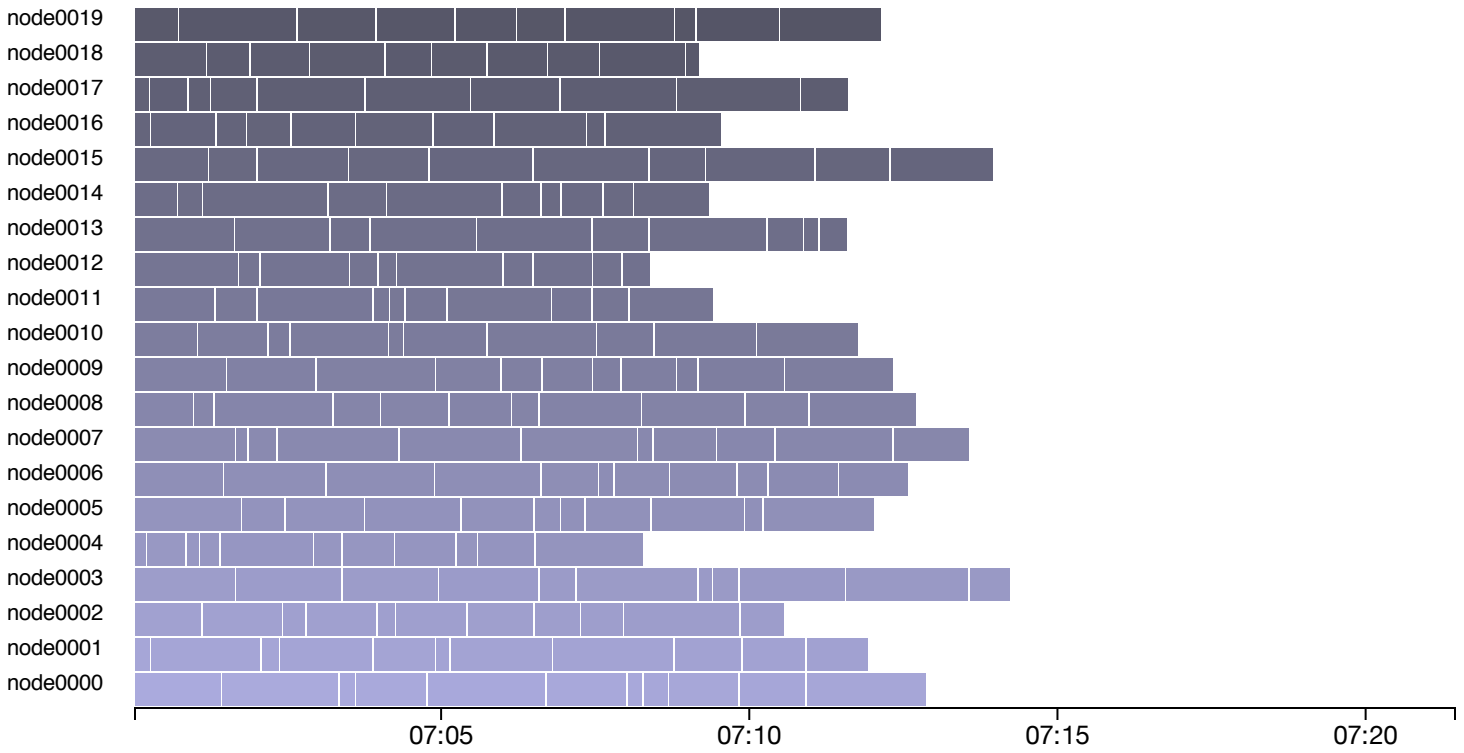
Needs work

All	Scaling unknown
IPython	Launcher (configuration)
Scoop and MP	__main__
Scoop	Schedule
Multiprocessing	One node (kind of)

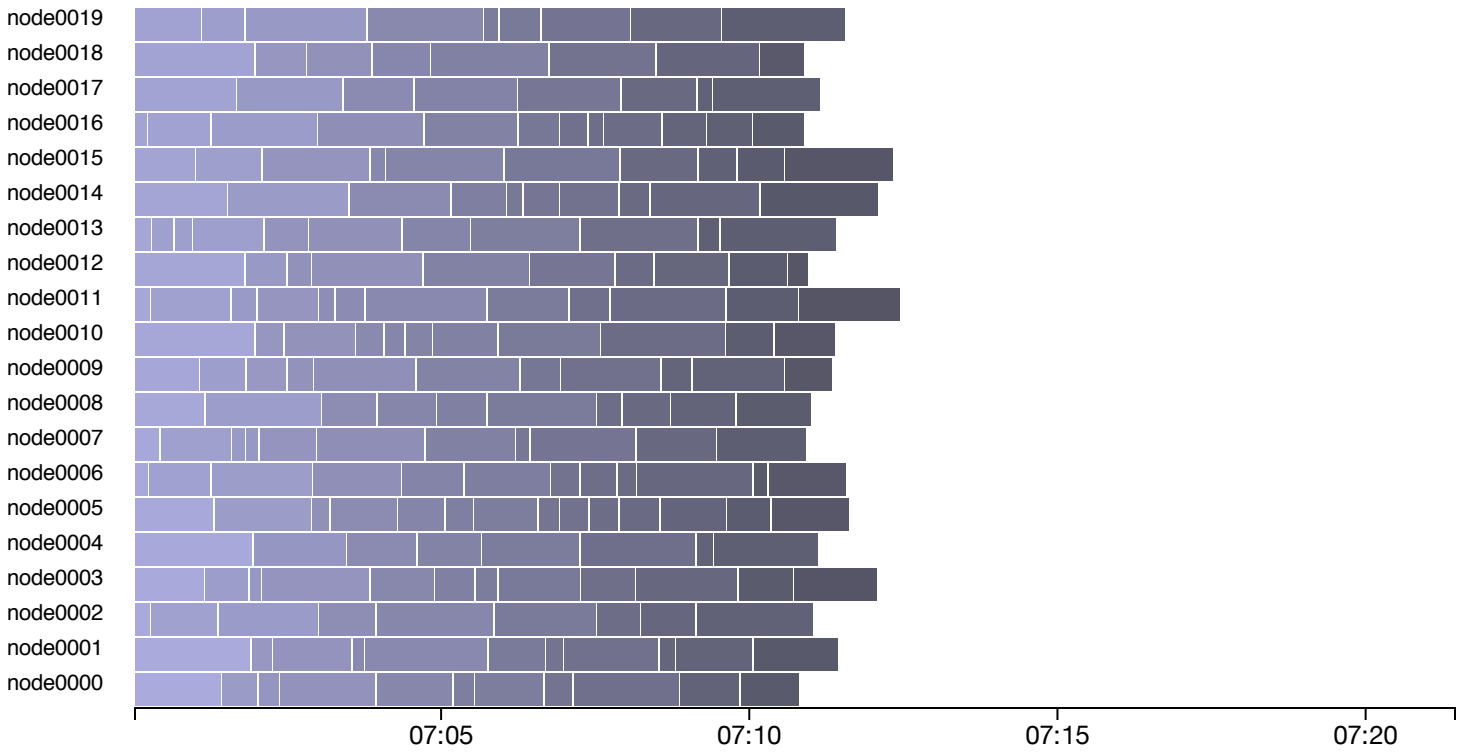
Scheduling: Bash



Scheduling: Static



Scheduling: Dynamic




1949

Tenacious Robustness Test

```
@require('time','socket','random',
'IPython.parallel.error.KernelError')
def simulation(x):

   time.sleep(5)
   if random.random() < 0.3:
      raise KernelError
   return {'task':x,
           'host' :socket.gethostname()}
```

Launch 10 nodes

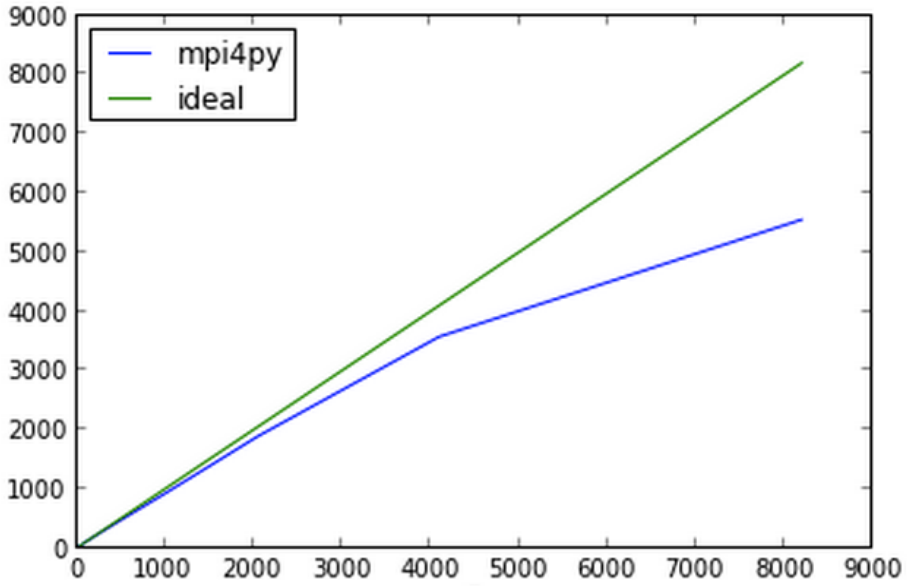
Run **several** tasks

At some point, **kill a node**

mpi4py

```
from mpi4py import MPI

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

if rank == 0:

   data = {'key1' : [7, 2.72, 3.2],
           'key2' : ( 'abc', 'xyz')}
else:
   data = None

data = comm.bcast(data, root=0)
```

mpi4py Scaling



3 second jobs

2048	92
4096	87%
8192	67%

Data Analysis

This webpage is not available

Google Chrome's connection attempt to **127.0.0.1** was rejected. The website may be down, or your network may not be properly configured.

Here are some suggestions:

- Reload this webpage later.
- Check your Internet connection. Restart any router, modem, or other network devices you may be using.
- Add Google Chrome as a permitted program in your firewall's or antivirus software's settings. If it is already a permitted program, try deleting it from the list of permitted programs and adding it again.
- If you use a proxy server, check your proxy settings or contact your network administrator to make sure the proxy server is working. If you don't believe you should be using a proxy server, adjust your proxy settings: Go to **Applications > System Preferences > Network > Advanced > Proxies** and deselect any proxies that have been selected.

Error 102 (net::ERR_CONNECTION_REFUSED): The server refused the connection.

Conclusions

Python makes **supercomputing accessible**

Combine libraries to achieve the task at hand.

- Simulate and analyze
- Share methods in a notebook
- Push your data to a database
- Share it on the web
- In **parallel**

References

- Python Scripting for Computational Science (http://www.springer.com/mathematics/computational+science+%26+eng 3-540-73915-9)
- Python Snakes Its Way Into HPC (http://www.hpcwire.com/hpcwire/2010-11-17/python_snakes_its_way_into_hpc.html)
- Andy Terrel: Getting Started with Python in HPC (http://andy.terrel.us/blog/2012/09/27/starting-with-python/)
- Python Tutorial (http://docs.python.org/2/tutorial/)
- Think Python (http://www.greenteapress.com/thinkpython/)
- Data Analysis with Python