Python for HPC

Andrea Zonca - SDSC

Jupyter Notebook

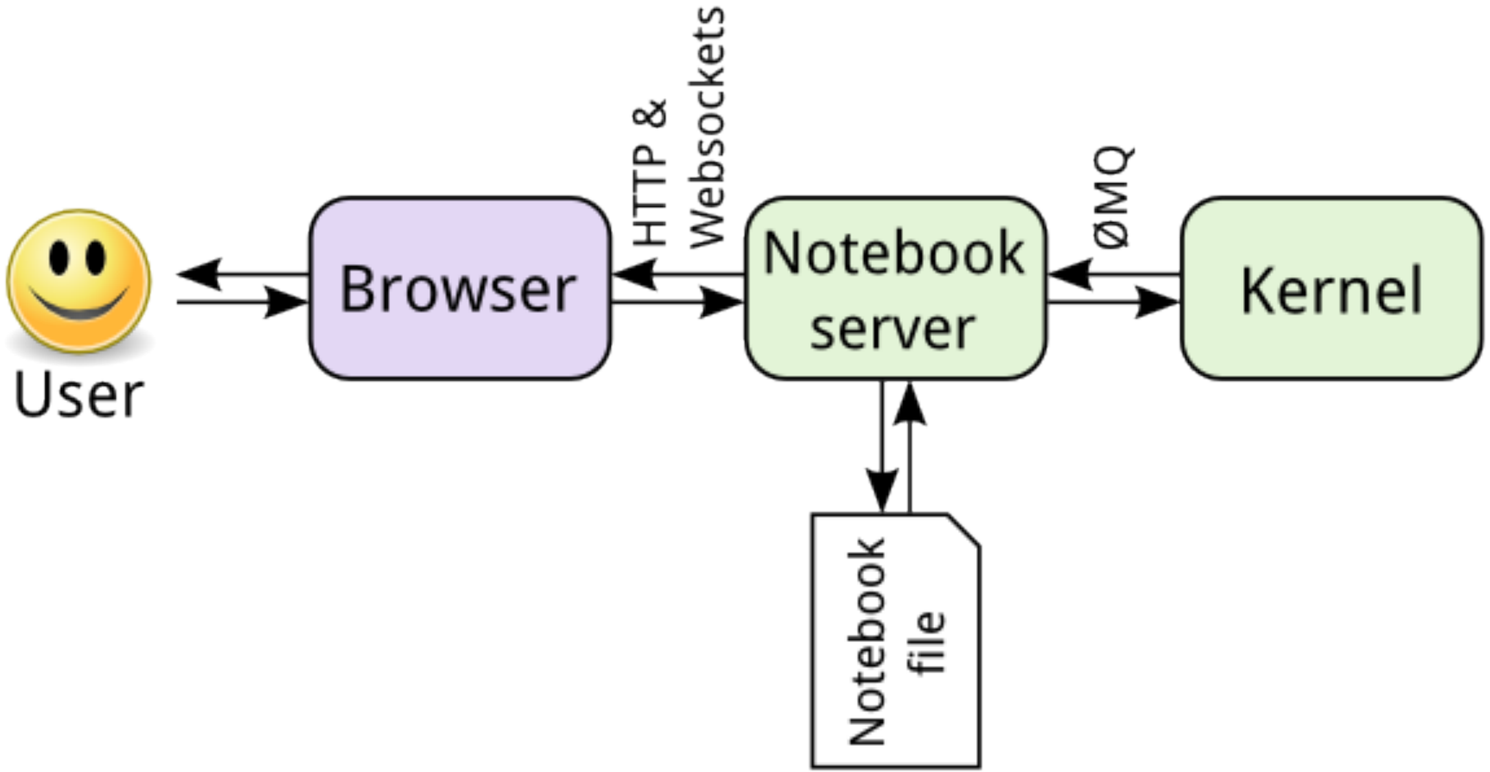
Data exploration in your browser

What is the notebook?

- Browser based interactive console
- Supports multiple sessions in browser tabs
- Each session has a Kernel executing computation
- Saved in JSON format

Notebooks on Nature

http://www.nature.com/news/interactive-notebooks-sharing-the-code-1.16261



How the notebook works

Modules on Comet

- module load python
- module load scipy
- add them to .bashrc

Setup on Comet

- ssh to Comet
- salloc --nodes=1 --tasks-per-node=24 -t 04:00:00 --partition=gpu
- ssh comet-xx-xx
- ipython notebook --no-browser --ip="*" # better setup config file

ssh-tunneling setup

ssh etrainXX@comet.sdsc.edu -R 8888:comet-xx-xx:8888 -f -N

Open browser on your laptop and connect to localhost:PORT

New -> Notebook

!hostname

IPython notebook demo

- Python code
- Formatted text
- Equations
- Plots
- Cells execution, cells order
- Clear output

Why the notebook?

- Literate programming: code and explanation together
- Reproducible science: document easily every step
- Easy to share computations: send one single notebook instead of scripts/plots/.doc

ipynb documents

- JSON format
- includes plots in binary format
- easy to convert to .html/.pdf for sharing
- http://nbviewer.ipython.org
- Recently rendered automatically on Github

HPC: interactive notebooks

- Analyze large amount of data
- In-situ visualization
- Centralized Python stack
- Check long-running computations
- Prepare and submit batch jobs

Notebooks as scripts

- demo of runipy
  - open and execute fit_line.ipynb
  - uncomment cell with (os.environ)
  - white_noise_scale=1000 runipy fit_line.ipynb fit_line_1000.ipynb
  - open fit_line_1000.ipynb, what happened?
- demo of batch submission of SLURM serial runipy jobs using pipes

Hands-on

- Open the notebook interactively
- Add saving the plot with plt.savefig ("figurename.png") in the same cell
- Test with runipy on the interactive node
- Rerun the jobs through the queue

IPython parallel

Parallel computing the easy way

IPython parallel

- High-level API for distributed computing with Python
- Engines (Python worker processes) connected to Controller with ZeroMQ
- Client, i.e. user's IPython session, connects to the Controller

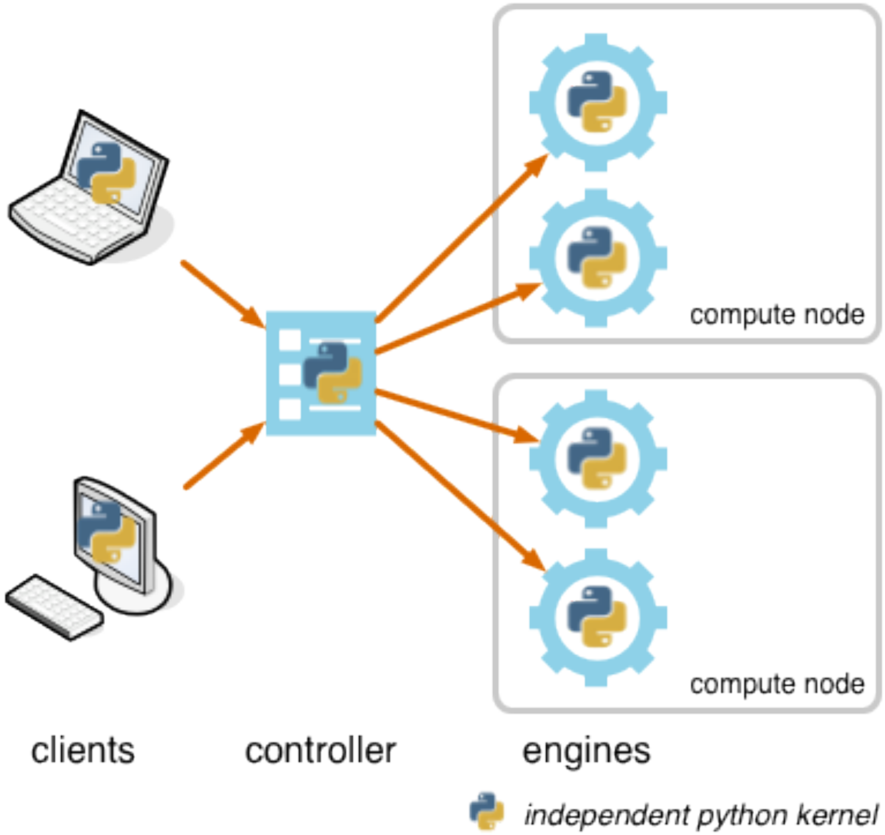


Image by Continuum Analytics

IPython parallel architecture

Functionalities

- Load balanced queue for trivially parallel jobs
- Supports job dependencies
- Direct interface to Engines
- Supports MPI applications, Python or C/C++/Fortran

IPython parallel config

- ipython profile create --parallel
- ipcontroller_config.py: c.HubFactory.ip = u'*'
- ipcluster_config.py:
    - c.IPClusterEngines.engine_launcher_class = 'PBSEngineSetLauncher'
    - c.PBSEngineSetLauncher.batch_template_file = 'slurm.engine.template'
    - c.PBSEngineSetLauncher.submit_command =

IPython parallel Demo

- Launch cluster with 48 engines:
  - ipcluster start --n=48
- Connect with IPython Notebook
- Print ids, hostnames
- Launch demo job and check it runs correctly

Hands-on

- Create a duplicate of fit_line.ipynb
- Reformat fit_line code into a single function
- Send it to engines for execution within the balanced queue
- Print out the results from the notebook

IPython parallel and MPI

```
from mpi4py import MPI
import numpy as np

def psum(a):
    locsum = np.sum(a)
    rcvBuf = np.array(0.0,'d')
    MPI.COMM_WORLD.Allreduce([locsum, MPI.DOUBLE],
        [rcvBuf, MPI.DOUBLE],
        op=MPI.SUM)
    return rcvBuf
```

```
In [1]: from IPython.parallel import Client

In [2]: c = Client()

In [3]: view = c[:]

In [4]: view.activate() # enable magics

# run the contents of the file on each engine:
In [5]: view.run('psum.py')

In [6]: view.scatter('a',np.arange(16,dtype='float'))

In [7]: view['a']
Out[7]: [array([ 0.,  1.,  2.,  3.]),
         array([ 4.,  5.,  6.,  7.]),
         array([  8.,   9.,  10.,  11.]),
         array([ 12.,  13.,  14.,  15.])]

In [7]: %px totalsum = psum(a)
Parallel execution on engines: [0,1,2,3]

In [8]: view['totalsum']
Out[8]: [120.0, 120.0, 120.0, 120.0]
```

Numba

Run code on GPU with Python

JIT compiler for Python

- based on LLVM (compiler infrastructure behind clang, Apple's C++ compiler)
- turns Python code into machine code
- on-the-fly

Numba

export NUMBAPRO_NVVM=/usr/local/cuda-7.0/nvvm/lib64/libnvvm.so

export NUMBAPRO_LIBDEVICE=/usr/local/cuda-7.0/nvvm/libdevice/

Interactive GPU node

salloc --nodes=1 --tasks-per-node=24 --
partition=gpu -t 01:00:00

```python
from numba import jit
from numpy import arange

# jit decorator tells Numba to compile this function.
# The argument types will be inferred by Numba when function is called.
@jit
def sum2d(arr):
    M, N = arr.shape
    result = 0.0
    for i in range(M):
        for j in range(N):
            result += arr[i,j]
    return result

a = arange(9).reshape(3,3)
print(sum2d(a))
```

Numba CPU

run with %timeit

increase size of matrix to see performance improvements

Numba GPU

```
from numba import cuda

@cuda.jit
def matmul(A, B, C):
    """Perform square matrix multiplication of C = A * B
    """
    i, j = cuda.grid(2)
    if i < C.shape[0] and j < C.shape[1]:
        tmp = 0.
        for k in range(A.shape[1]):
            tmp += A[i, k] * B[k, j]
        C[i, j] = tmp
```

```
import numpy as np
shape = (5,5)
a = np.ones(shape)
b = np.ones(shape) * 4
c = np.zeros(shape)
matmul[1,(16,16)](a,b,c)
print(c)
```

Hands-on

- create a loop that runs matmul with different matrix sizes
- compare with np.dot
- range from 20x20 to 10000x10000
- plot timing

Advanced CUDA

Tiled matrix multiplication to exploit GPU fast local memory:

http://numba.pydata.org/numba-doc/0.20.0/cuda/examples.html#cuda-matmul

PyTrilinos

Distributed linear algebra with Python

Distributed linear algebra

Large complete C++ packages with Python support:

- PETSC, petsc4py
- Trilinos, PyTrilinos

Both use C++ for MPI communication and LAPACK/BLAS for local computing

Both subclass numpy arrays

PyTrilinos example

See pytrilinos.ipynb