Research Express is on its way!

- The demonstration will start at 12:30 pm.
- To use the Live Chat:
  - Maximize your browser window so you can see the postings.
  - If you refresh the browser page, you'll need to log in again.
  - After the demonstration, staff will remain available in the chat for a few minutes to answer additional questions.

Today's topic: Python
Python (NumPy, SciPy and mpi4py) on Mills
Objectives

- Use VALET to automate your environment-setup for Python (Numpy, SciPy and mpi4py)
- Modify queue submission scripts to work with Grid Engine on Mills

Python (Cornell Virtual Workshop) at [http://www.udel.edu/001278](http://www.udel.edu/001278)
NumPy Tutorial (SciPy.org) at [http://www.udel.edu/001279](http://www.udel.edu/001279)
Python packages on Mills

- vpkg_list | grep py
  - mpi4py
  - numpy
  - python
  - python-nose
  - scipy
Python versions on Mills

- **vpkg_versions python**

  Available versions in package (* = default version):
  
  python  
  - 3.2  Version 3.2
  - * 3   Version 3
  - 2.7  Version 2.7
  - 2    Version 2

- **module list python**
NumPy versions on Mills

- `vpkg_versions numpy`

Available versions in package (* = default version):

- `numpy` Python NumPy
  - *1.6.1-2.7.2* Version 1.6.1 for Python 2.7.2
SciPy versions on Mills

- **vpkg_versions scipy**

  Available versions in package (* = default version):
  
  scipy  Python SciPy - Scientific Tools for Python
  * 0.10.0-2.7.2  Version 1.6.1 for Python 2.7.2
mpi4py versions on Mills

vpkg_versions mpi4py

Available versions in package (* = default version):

mpi4py       mpi4py - MPI for Python
* 1.3-2.7.2  Version 1.3 for Python 2.7.2
  1.3-3.2.2  Version 1.3 for Python 3.2.2
Using Python on Mills

- `vpkg_require python`
  
  Adding package `python/3` to your environment

- `module add python` ☒

- `vpkg_rollback all`

- `vpkg_require python/2.7`
  
  Adding dependency `mkl/10.3.8-64bit` to your environment

  Adding package `python/2.7` to your environment
NumPy, SciPy and mpi4py

- NumPy and SciPy: Python 2.7.2
  mpi4py: Python 2.7.2 and 3.2.2

- Important to use the built in dependencies by VALET

- An incorrect version of Python added will generate a conflict when we try to add a library

ERROR: unable to add versioned package: python/2.7 conflicts with version: python/3

vpkg_rollback all
NumPy

- vpkg_require numpy

  Adding dependency `mkl/10.3.8-64bit` to your environment
  Adding dependency `python/2.7` to your environment
  Adding dependency `python-nose/1.1.2-2.7.2` to your environment
  Adding package `numpy/1.6.1-2.7.2` to your environment
SciPy

- vpkg_require scipy

Adding dependency `mkl/10.3.8-64bit` to your environment
Adding dependency `python/2.7` to your environment
Adding dependency `python-nose/1.1.2-2.7.2` to your environment
Adding dependency `numpy/1.6.1-2.7.2` to your environment
Adding package `scipy/0.10.0-2.7.2` to your environment
mpi4py

- `vpkg_require mpi4py`

  Adding dependency `openmpi/1.4.4-gcc` to your environment
  Adding dependency `mkl/10.3.8-64bit` to your environment
  Adding dependency `python/2.7` to your environment
  Adding package `mpi4py/1.3-2.7.2` to your environment

- `vpkg_require mpi4py/1.3-3.2.2`

  Adding dependency `openmpi/1.4.4-gcc` to your environment
  Adding dependency `python/3` to your environment
  Adding package `mpi4py/1.3-3.2.2` to your environment
mpi4py and NumPy

- `vpkg_require mpi4py numpy`

  Adding dependency `openmpi/1.4.4-gcc` to your environment
  Adding dependency `mkl/10.3.8-64bit` to your environment
  Adding dependency `python/2.7` to your environment
  Adding package `mpi4py/1.3-2.7.2` to your environment
  Adding dependency `python-nose/1.1.2-2.7.2` to your environment
  Adding package `numpy/1.6.1-2.7.2` to your environment
mpi4py and SciPy

- `vpkg_require mpi4py scipy`

Adding dependency `openmpi/1.4.4-gcc` to your environment
Adding dependency `mkl/10.3.8-64bit` to your environment
Adding dependency `python/2.7` to your environment
Adding package `mpi4py/1.3-2.7.2` to your environment
Adding dependency `python-nose/1.1.2-2.7.2` to your environment
Adding dependency `numpy/1.6.1-2.7.2` to your environment
Adding package `scipy/0.10.0-2.7.2` to your environment
mpi4py, NumPy and SciPy

- `vpkg_require mpi4py numpy`
  - Adding dependency `openmpi/1.4.4-gcc` to your environment
  - Adding dependency `mkl/10.3.8-64bit` to your environment
  - Adding dependency `python/2.7` to your environment
  - Adding package `mpi4py/1.3-2.7.2` to your environment
  - Adding dependency `python-nose/1.1.2-2.7.2` to your environment
  - Adding package `numpy/1.6.1-2.7.2` to your environment

- `vpkg_require scipy`
  - Adding package `scipy/0.10.0-2.7.2` to your environment
Interactive example

$ vpkg_require numpy mpi4py
Adding dependency `mkl/10.3.8-64bit` to your environment
Adding dependency `python/2.7` to your environment
Adding dependency `python-nose/1.1.2-2.7.2` to your environment
Adding package `numpy/1.6.1-2.7.2` to your environment
Adding dependency `openmpi/1.4.4-gcc` to your environment
Adding package `mpi4py/1.3-2.7.2` to your environment

$ python
Python 2.7.2 (default, Dec 27 2011, 15:05:10)
[GCC 4.4.5 20110214 (Red Hat 4.4.5-6)] on linux2
Type "help", "copyright", "credits" or "license" for more information.

>>> from numpy import *
>>> a = arange(10).reshape(2,5)
>>> a
array([[0, 1, 2, 3, 4],
       [5, 6, 7, 8, 9]])
>>> a.shape
(2, 5)
>>> a.ndim
2
>>> a.dtype.name
'int64'
>>> a.itemsize
8
>>>
Interactive example

```python
>>> from scipy import *
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ImportError: No module named scipy

>>> $ vpkg_require scipy
Adding package `scipy/0.10.0-2.7.2' to your environment

>>> $ python
Python 2.7.2 (default, Dec 27 2011, 15:05:10)
[GCC 4.4.5 20110214 (Red Hat 4.4.5-6)] on linux2
Type "help", "copyright", "credits" or "license" for more information.

>>> from scipy import *
>>> x = r_-2:3
>>> x
array([-2, -1,  0,  1,  2])
>>> select([x > 3, x >= 0],[0,x+2])
array([0, 0, 2, 3, 4])
>>> r_[3,[0]*5,-1:1:10j]
array([ 3.        ,  0.        ,  0.        ,  0.        ,  0.        ,
        0.        , -1.        , -0.77777778, -0.55555556, -0.33333333,
        -0.11111111,  0.11111111,  0.33333333,  0.55555556,  0.77777778,  1.])
```
#!/bin/bash
#$ -q development
#$ -A TG-STA060015N
#$ -V
#$ -cwd
#$ -N mpi4py-demo
#$ -j y
#$ -o $JOB_NAME.o$JOB_ID
#$ -pe 12way 12
#$ -l h_rt=00:05:00
#$ -M 6075920299@vtext.com
#$ -m be

# Prohibit writing core files on error.
ulimit -c 0

set -x

python receiver.py&

ibrun python sample.py --loghost `hostname` --level debug

pkill python
#$ -N mpi4py-demo
#$ -o $JOB_NAME.o$JOB_ID
#$ -pe openmpi 12
#$ -l h_rt=00:05:00
#$ -M traine@udel.edu
#$ -m be

#
source /opt/shared/valet/docs/valet.sh
vpkg_require mpi4py numpy

# Prohibit writing core files on error.
ulimit -c 0

set -x

python receiver.py&

mpirun python sample.py --loghost `hostname` --level debug

pkill python
Summary

- Take advantage of the power of VALET to do the work for you to automate your environment-setup.

- Use the Mills User Guide to help with modifications of Grid Engine scripts that may be different from other HPC sites.
Upcoming Python Training

HPC Python Training Webcast in 011 Smith Hall on Mon, Apr 23 10am-5pm

Register at:
http://webapps.css.udel.edu/calendar/detail.php?classid=3711
More information

- IT Research Computing
  http://www.it.udel.edu/research-computing
Contact the IT Support Center

- **Email**: consult@udel.edu
  If you make the first line of the e-mail message
  Type=Cluster-Mills
  your question will be routed more quickly.

- **Phone**: (302) 831-6000

- **Text**: (302) 722-6820