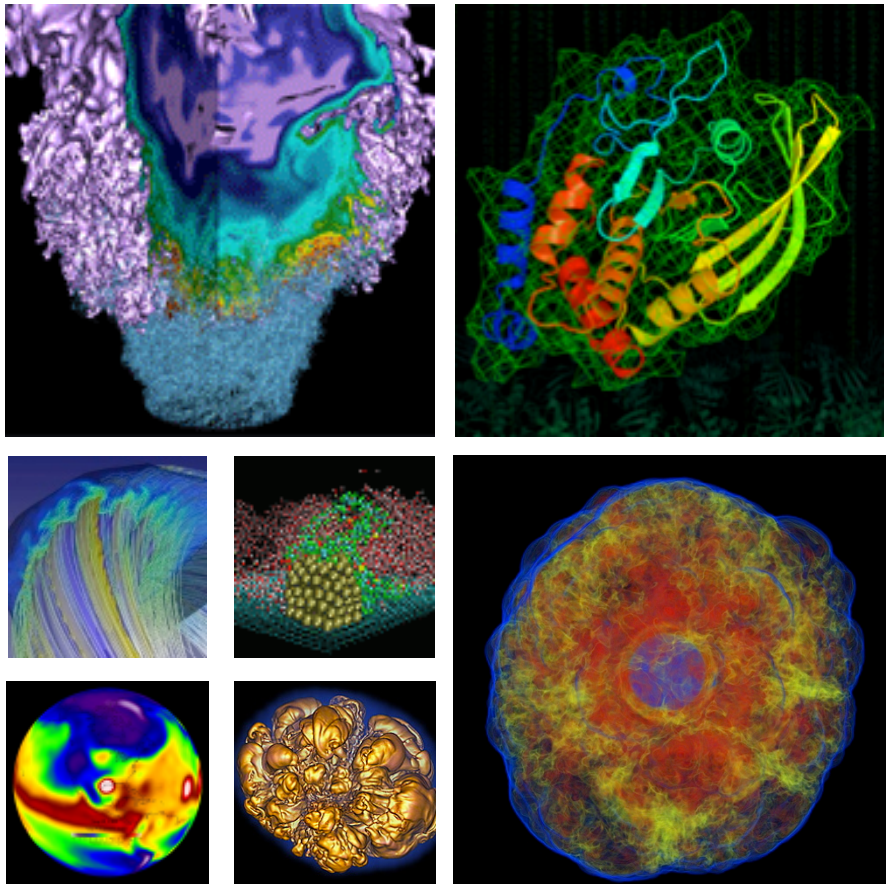
Using Python on Hopper, Carver and Edison



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Python up to 2.7.2

- **All-in-one installation approach for python up to 2.7.2**
- **Single fixed versions of popular packages (numpy, scipy, …) were installed together with core Python, under its site-packages directory**
  - For example, Python/2.7.1 has
    - numpy/1.5.1, scipy/0.9.0b1, ipython/0.10.1, matplotlib/1.0.1, etc.

Different approach from python/2.7.3

- Python base package is installed in /usr/common/usg/python/x.y.z (x.y.z is a version number)
- Other individual packages are installed in their own directories under /usr/common/usg/python/*name*/x.y.z, separately from the core python
- Module files ("module" as in Linux module utility) are provided for individual packages to prepend a search path to PYTHONPATH

Why do we do this?

- Allow multiple versions to exist for each package
- Can always provide users up-to-date versions for a python module
- Users can pick the most suitable version for their work by loading the module for the version
- Easy to maintain packages
- Re-use individualized packages

Module file for new python

- **To maintain consistency in core functionalities with pre-2.7.3 versions, a module file for new python loads**
  - python_base/x.y.z: Python-x.y.z + nose + pycairo + pygobject + pygtk + setuptools
  - numpy
  - scipy
  - matplotlib
  - ipython

```
% module load python
% module list
Currently Loaded Modulefiles:
  1) modules                    5) usg-default-modules/1.0    9) matplotlib/1.1.0
  2) nsg/1.2.0                  6) python_base/2.7.3         10) ipython/0.12.1
  3) pgi/12.9                   7) numpy/1.6.1-nothread      11) python/2.7.3
  4) openmpi/1.4.5              8) scipy/0.10.1
```

- **Version numbers for python and python_base (x.y.z in python/x.y.z and python_base/x.y.z): taken from the distributed python software package version number (Python-x.y.z.tgz)**
- **Default versions for numpy, scipy, matplotlib and ipython are used**

Installed python modules

- **You can use a non-default version by swapping modules**

```
% module load python
% module avail scipy

--------------------------- /usr/common/usg/Modules/modulefiles ----------------------
scipy/0.10.0          scipy/0.10.1(default) scipy/0.11.0          scipy/0.9.0

% module swap scipy scipy/0.11.0
% module list
Currently Loaded Modulefiles:
  1) modules                    5) usg-default-modules/1.0   9) matplotlib/1.1.0
  2) nsg/1.2.0                  6) python_base/2.7.3        10) ipython/0.12.1
  3) pgi/12.9                   7) numpy/1.6.1-nothread     11) python/2.7.3
  4) openmpi/1.4.5              8) scipy/0.11.0
```

Installed python modules

- **Current list of additional python modules**
  - ase, cython, gpaw, h5py, mercurial, mpi4py, mysqlpython, numexpr, pil, pycdf, pyhdf, pytables, virtualenv, and virtualenvwrapper

- **To use a package, load a module file for the package**

```
% module load python
% module load cython

% module list
Currently Loaded Modulefiles:
  1) modules                    5) usg-default-modules/1.0    9) matplotlib/1.1.0
  2) nsg/1.2.0                  6) python_base/2.7.3         10) ipython/0.12.1
  3) pgi/12.9                   7) numpy/1.6.1-nothread      11) python/2.7.3
  4) openmpi/1.4.5              8) scipy/0.10.1              12) cython/0.17.4
```

- **Don't use them with pre-2.7.3 python**

Installing python modules in your home directory

- We will provide and maintain highly used python modules
- Users are asked to install other python modules in their own directory

- To install using the "home" scheme

```
% tar -xvzf foo-1.0.tar.gz
% cd foo-1.0
% module load python
% setenv PYTHONPATH ~/python_modules/hopper/foo/1.0/lib/python:$PYTHONPATH
% python setup.py build
% python setup.py install --home=~/python_modules/hopper/foo/1.0
```

- To use

```
% module load python
% setenv PYTHONPATH ~/python_modules/hopper/foo/1.0/lib/python:$PYTHONPATH
% python
...
>>> import foo
>>>
```

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