LearnIT 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: Mills HPC Cluster
LEARNIT EXPRESS

in a Nutshell
• Most programs have preferences that tailor their behavior

• Word, Matlab, Mathematica: all rely on preference files

• The BASH shell (and many other programs) use the environment to customize their behavior

  • A set of named values; variable name = value

  • e.g. PATH = ”/bin:/usr/bin”
IMPORTANT ENVIRONMENT VARIABLES

- PATH: Where does the shell look for commands?
- LD_LIBRARY_PATH: Where does the OS look for libraries?
- MANPATH: Where does man look for manual pages?
- INFOPATH: Where does info look for manual pages?
What’s the Connection?

- HPC systems have many software packages, usually with multiple versions/variants

- Each software package has its own directories containing:
  - executable programs (\texttt{bin}) $\rightarrow$ PATH
  - shared libraries (\texttt{lib}) $\rightarrow$ LD_LIBRARY_PATH
  - manual pages (\texttt{man, share/info}) $\rightarrow$ MANPATH, INFOPATH
What's the Connection?

- Example: Open MPI 1.4.4, GCC variant

```
$ cd /opt/shared/openmpi/1.4.4-gcc
$ ls -l
bin
etc
include
lib
share

$ ls -1d bin/mpicc
bin/mpicc

$ ls -ld lib/libmpi.so
lib/libmpi.so

$ ls -l share/man
man1
man3
man7
```
Many software packages suggest you edit your .bashrc or .bash_profile to make them available in your environment.

- YOU must know *how* to make the changes.
- YOU must know *what* to add to PATH, etc.
- YOU must re-edit whenever you use a different version of the package.
- YOU must debug any problems that arise.
LET THE COMPUTER DO IT!

• That’s a lot of work for YOU to be doing — none of which equates directly to “research”

• VALET Automates Linux Environment Tasks
  • On-demand alteration of PATH, LD_LIBRARY_PATH, etc.
  • Easily change which version of a package you’re using
  • Add your own package definitions
• Displays a list of packages

• Shows the package identifiers

• Packages are defined in XML files
  • /opt/shared/valet/etc
  • your own directories

$ vpkg_list
Available packages:
  acml
  cmake
  fftw
  gaussian
  gcc
  gromacs
  gsl
  hdf4
  hdf5
  imsl
  intel

$
For a given package, displays what versions of that package are available.

An * indicates the default version of the package.

Listed by version identifier and a description.
VALET IDENTIFIERS

versioned package identifier = package identifier / version identifier

<table>
<thead>
<tr>
<th>identifier</th>
<th>meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>gaussian</td>
<td>The Gaussian package (default version)</td>
</tr>
<tr>
<td>gaussian/g09a02</td>
<td>Gaussian ’09, revision A02</td>
</tr>
<tr>
<td>gaussian/g03e01</td>
<td>Gaussian ’03, revision E01</td>
</tr>
</tbody>
</table>
• Show what VALET knows about a package or versioned package

• Using a package identifier alone shows info for all versions

• Using a versioned package identifier shows info for that specific version
What Info is Shown?

- The *prefix* is the directory in which the software package is installed.
- The *dependencies* indicates what other packages are required by this one.
- Under *directories*, the directories containing executables, libraries, manual pages are shown.
• For more “exotic” situations, the environment changes can be scripted

• That script will be called by VALET

```bash
$ vpkg_info gaussian/g09a02
Versioned package information for `gaussian/g09a02`:
Gaussian - Quantum Chemistry
http://www.gaussian.com/
[g09a02] {
  '09, Revision A02
  prefix: /opt/shared/Gaussian/g09a02
  affect dev env: yes
  scripts: {
    sh = {
      g09.sh
    }
  }
  dependencies: {
    pgi/11
  }
  directories: {
    bin: {
    }
    lib: {
      }
  }
}
• Add a versioned package to your current environment

• Any dependencies will be satisfied first (e.g. pgi/11)

• Re-adding the same package has no effect

• Adding one version on top of another is forbidden

$ vpkg_require gaussian/g09a02
Adding dependency `pgi/11` to your environment
Adding package `gaussian/g09a02` to your environment

$ which g09
/opt/shared/Gaussian/g09a02/g09/g09

$ vpkg_require gaussian/g09a02

$ vpkg_require gaussian/g03e01
ERROR: unable to add versioned package: gaussian/g03e01 conflicts with version: gaussian/g09a02
vpkg_rollback

• Remove the environment changes introduced by the last vpkg_require command

• Include the word all to remove the effects of every vpkg_require command issued in the current shell

```bash
$ vpkg_rollback
$ vpkg_rollback
WARNING: no snapshots defined
$ vpkg_rollback all
```
Example: Compilers

- I want to use the Intel compiler; 32-bit version
- Add to my environment
- Compile hello.c
- Use “file” to determine what kind of executable I produced

```bash
$ vpkg_versions intel
intels         Intel Compiler Suite
  2011-32bit  Version 2011 for 32-bit x86
  * 2011-64bit  Version 2011 for x86-64

$ vpkgRequire intel/2011-32bit
Adding package `intel/2011-32bit` to your environment

$ icc -o hello hello.c
$ file hello
hello: ELF 32-bit LSB executable, Intel 80386, version 1 (GNU/Linux), dynamically linked (uses shared libs), for GNU/Linux 2.6.18, not stripped
```
Example: Compilers

- Now, switch to the 64-bit compiler and do the same process
- Rollback to remove the 32-bit compiler first

```bash
$ vpkg_rollback

$ vpkg_require intel
Adding package `intel/2011-64bit` to your environment

$ icc -o hello hello.c
$ file hello
hello: ELF 64-bit LSB executable, x86-64, version 1 (GNU/Linux), dynamically linked (uses shared libs), for GNU/Linux 2.6.18, not stripped
```
YOUR OWN PACKAGES

• You can add your own package definitions on top of the ones that IT provides

• First order of business: learn how to write a package definition file

  • http://beren.engr.udel.edu/doku.php/valet:packagefile
YOUR OWN PACKAGES

• You can add your own package definitions on top of the ones that IT provides

• First order of business: learn how to write a package definition file

• Next, create a directory to house your package definitions

• VALET automatically looks for a directory named “.valet” in your home directory
$ cd ~
$ mkdir .valet
$ cd .valet
:
$ cat dummy.vpkg

<?xml version="1.0" encoding="UTF-8"?>
<package
  xmlns="http://www.udel.edu/xml/valet/1.0"
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:schemaLocation="http://www.udel.edu/xml/valet/1.0
  http://www.udel.edu/xml/valet/1.0/schema.xsd"
  id="dummy">
  <description>Dummy: A Fake Package</description>
  <prefix>/not/a/valid/path</prefix>
  <default-version>0.1a</default-version>
  <version id="0.1a">
    <description>Version 0.1a</description>
  </version>
</package>
$ vpkg_list
Available packages:
    acml
cmake
dummy
    fftw
gaussian
    :

Example
$vpkg_info dummy
[dummy] {
  Dummy: A Fake Package
  prefix: /not/a/valid/path
  affect dev env: yes
  default version: 0.1a
  versions: {
    [0.1a] {
      Version 0.1a
      prefix: /not/a/valid/path/0.1a
      affect dev env: yes
      directories: {
        bin: {
        }
        lib: {
        }
        inc: {
        }
      }:
    }
  }
}
• VALET helps IT provide you with easy access to the many versions of software available on the cluster.

• VALET helps IT to deploy new software and new versions of software without users’ having to change their scripts or login files.

• VALET helps YOU maintain your own software packages that are installed in your home directory or your group’s LUSTRE work directory.
FOR MORE INFORMATION...

- Use the `vpkg_help` command to summarize all of the commands.
- Use `man valet` to view the VALET manual page.

Official VALET documentation:
http://beren.engr.udel.edu/doku.php/valet:start
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