

# **Immediate Goals and Wish-list**

G. Tsouloupas, The Cyprus Institute  
F. Georgatos, Univ. of Luxembourg

# EasyBuild has been a blessing, really!

- Within days of being introduced to it (many thanks to Fotis) we delivered a sizeable collection of software to our users.
- Really came into use during a GPU workshop in December.
- Strong Commitment from Cyl...
- Potential for environment uniformity in LinkSCEEM (Integration of resources).

# CUDA Integration

- CUDA is a Library? CUDA is a toolchain?
- Multiple Versions of CUDA
- GPU-enabled **application components**
- GPU-enabled **libraries**
- `--with-cuda` in OpenMPI

# **PGI toolchain, fresh ictce**

- New PGI toolchain, high on the wishlist
- FlexNet License manager
- OpenACC

# OFED and -no-OFED

- Currently:
  - Set up EB by copying and modifying all \*-no-OFED.eb files
- 1 line in OpenMPI  
"--with-openib --with-udapl" # why udapl???  
is reflected in the filename of 230 packages
- The OFED / -no-OFED should be an initialization config?

# User environment

- Mechanisms to easily allow users to expand the EB software tree. I need a replacement for this:

```
export EBVER='eb'  
export PYTHONPATH=$PYTHONPATH:$HOME/$EBVER/lib/python2.4/site-packages  
export PATH=$PATH:$HOME/$EBVER/bin/:/gpfs/apps/Modules/3.2.9/bin/  
export EASYBUILDINSTALLPATH=$HOME/$EBVER  
export EASYBUILDPREFIX=$HOME/$EBVER
```

```
echo $MODULEPATH | grep /gpfs/$EBVER/modules/all > /dev/null || export  
MODULEPATH=$MODULEPATH:/gpfs/$EBVER/modules/all  
echo $MODULEPATH | grep $HOME/$EBVER/modules/all > /dev/null || export  
MODULEPATH=$MODULEPATH:$HOME/$EBVER/modules/all
```

- Differently configured builds in user homes
- Sticky version suffixes?

# FFTW single and double precision

- Currently in another .eb with "-FLOAT" versionsuffix
  - FFT default is Double Prec.
  - -FLOAT builds the Single Prec. version.
- Naming in Single Prec. and Double Prec. library files is different (ie. different filenames) so they could be the result of a single EB.
- Why not support --enable-avx by default?

# Local Climate Group requirements

netcdf	( <a href="http://www.unidata.ucar.edu/software/netcdf/">http://www.unidata.ucar.edu/software/netcdf/</a> )	OK
ferret	( <a href="http://ferret.pmel.noaa.gov/Ferret/downloads">http://ferret.pmel.noaa.gov/Ferret/downloads</a> )	
pyferret	( <a href="http://ferret.pmel.noaa.gov/Ferret/downloads">http://ferret.pmel.noaa.gov/Ferret/downloads</a> )	
ncl	( <a href="http://www.ncl.ucar.edu/">http://www.ncl.ucar.edu/</a> )	OK (more versions)
nco	( <a href="http://nco.sourceforge.net/">http://nco.sourceforge.net/</a> )	
ncview	( <a href="http://meteora.ucsd.edu/~pierce/ncview_home_page.html">http://meteora.ucsd.edu/~pierce/ncview_home_page.html</a> )	
R	( <a href="http://www.r-project.org/">http://www.r-project.org/</a> )	OK
python	(with pylab, numpy - OK, scipy OK, pandas)	
GNU Octave	( <a href="http://www.gnu.org/software/octave/">http://www.gnu.org/software/octave/</a> )	
GNU parallel	( <a href="http://www.gnu.org/software/parallel/">http://www.gnu.org/software/parallel/</a> )	OK
IDL	( <a href="http://www.exelisvis.com/ProductsServices/IDL.aspx">http://www.exelisvis.com/ProductsServices/IDL.aspx</a> .)	proprietary



# More...

- --download-only
- EB-provided Python
  - goalfp toolchain?
- Managing multiple EB versions
  - We need Guidelines and Best Practices so that we can follow EB versions.
  - What **should** sites customize? What should be left untouched?
- e.g. default use of "/tmp", should be \$HOME/tmp?
- Package explosion (are we being ungrateful here?)

# More...

- goalf or ictce naming schemes; how to adopt for custom use? (should we?)
- Predictable toolchain versioning? (version dispenser is Ken?)
- OpenMPI beyond v1.5
- Let's get GROMACS on top of the above!
- PRACE Common Production Environment
- Totalview LM\_LICENSE\_MANAGER, TVDSVRLAUNCHCMD & custom easyconfigs/modulefiles (and similar issues)