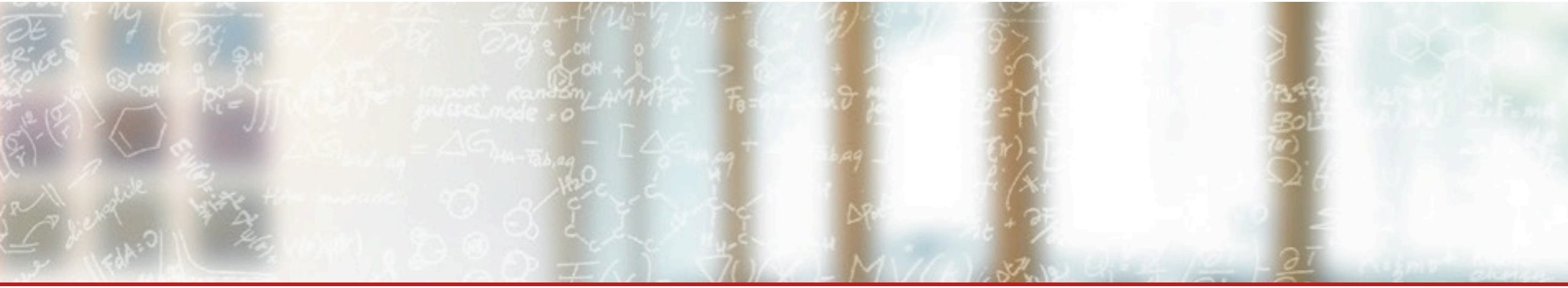
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich



Escha/Kesch EasyBuild setup

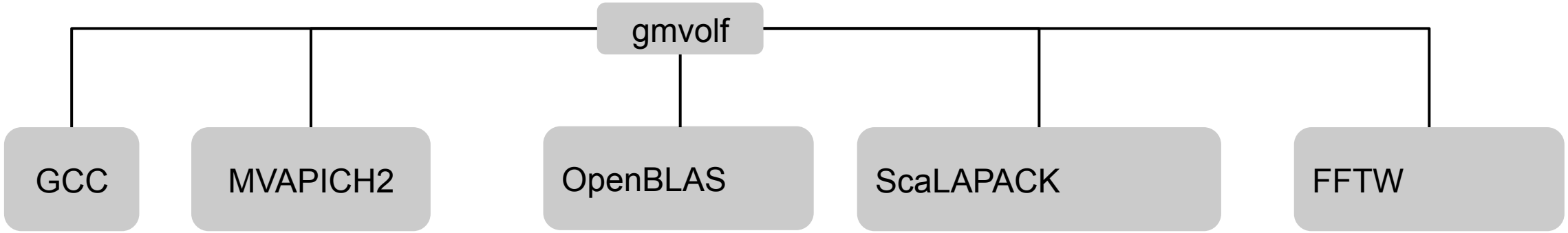
GPP, CSCS

August, 2015

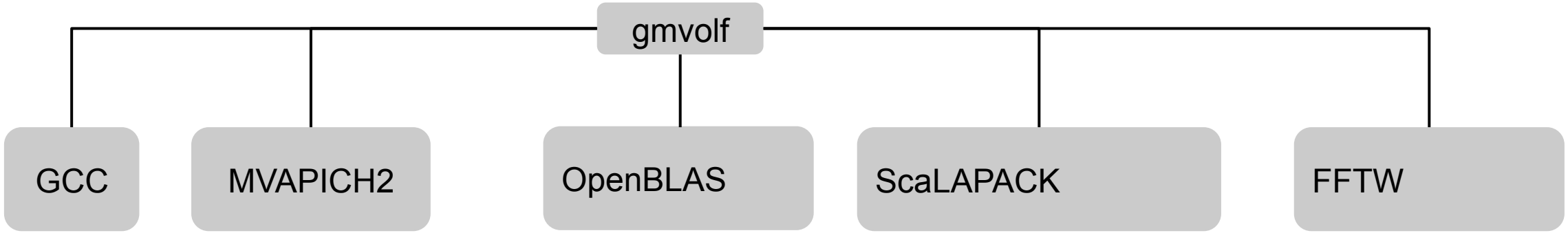
Overview of PE on Escha/Kesch

- PrgEnv-cray
  - cce/8.3.10 (soon 8.3.13)
  - MVAPICH 2.0.1
- GNU
  - GCC 4.8.2
  - MVAPICH 2.0.1
  - MVAPICH 2.1rc2 GDR
- Intel
  - ics-14.0.2.144
  - impi-4.1.3.048
- PGI
  - Not yet available(?)
- Cuda
  - 6.5.14

GNU - gmvolf: BLACS, FFTW, GCC, MVAPICH2, OpenBLAS, ScaLAPACK



GNU - gmvolf: BLACS, FFTW, GCC, MVAPICH2, OpenBLAS, ScaLAPACK



Problem if we want to use system modules:

- Module names do not match with toolchain definition

Possible solutions:

1. Redefine the toolchain
   Need to write a couple of python files

2. **Write modules wrappers to match with system**

GNU - gmvolf: EasyBuild toolchain definition

```
easyblock = "Toolchain"

name = 'gmvolf'
version = '2015a'

# toolchain used to build gmvolf dependencies
comp_mpi_tc_name = 'gmvapich2'
comp_mpi_tc_ver = "%s" % version
comp_mpi_tc = (comp_mpi_tc_name, comp_mpi_tc_ver)

# compiler toolchain depencies
# we need GCC and MVAPICH2 as explicit dependencies instead of gmvapivh2 toolchain
# because of toolchain preperation functions
dependencies = [
    ('GCC', '4.8.2'),
    ('MVAPICH2', '2.0.1_gnu48'),
    (blaslib, blasver, blassuff, comp),
    ('FFTW', '3.3.4', '', comp_mpi_tc),
    ('ScaLAPACK', '2.0.2', '-%s%s' % (blas, blassuff), comp_mpi_tc),
]
```

GNU - gmvolf: Module wrappers for system GCC and MVAPICH

GCC/4.8.2

```
#%Module

module load gcc/4.8.2

setenv      EBROOTGCC /opt/gcc/4.8.2/snos
setenv      EBVERSIONGCC 4.8.2
```

MVAPICH2/2.0.1_gnu48

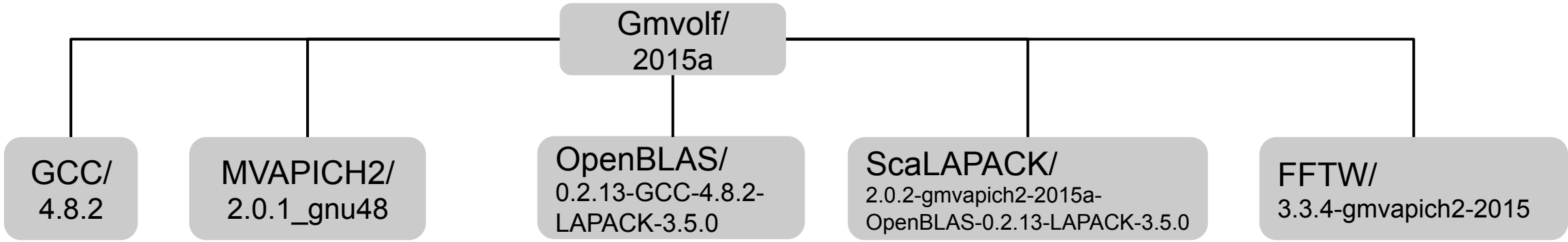
```
#%Module
#

module load mvapich2_gnu/2.0.1_gnu48

setenv      EBROOTMVAPICH2 /opt/cray/mvapich2_gnu/2.0.1/GNU/48/
setenv      EBVERSIONMVAPICH2 2.0.1_gnu48

module load cudatoolkit/6.5.14
```

GNU – gmvolf/2015a (GCC 4.8.2 + MVAPICH 2.0.1)



GNU – gmvolf/2015a – New software stack (built with EasyBuild)

Boost/1.49.0
CDO/1.6.9
CMake/3.2.2
Cube/4.3.2
ddt/5.0(default)
ddt/5.1
gmvapich2/2015a
GSL/1.16
HDF/4.2.8
HDF5/1.8.15
Java/1.7.0_80
matplotlib/1.4.3
NCO/4.5.1
ncurses/5.9
ncview/2.1.5
netCDF/4.3.3.1
netcdf-python/1.1.8
OPARI2/1.1.4
OTF2/1.5.1
Python/2
R/3.1.3
R/3.2.0-bare
Ruby/2.2.2
Scalasca/2.2.2

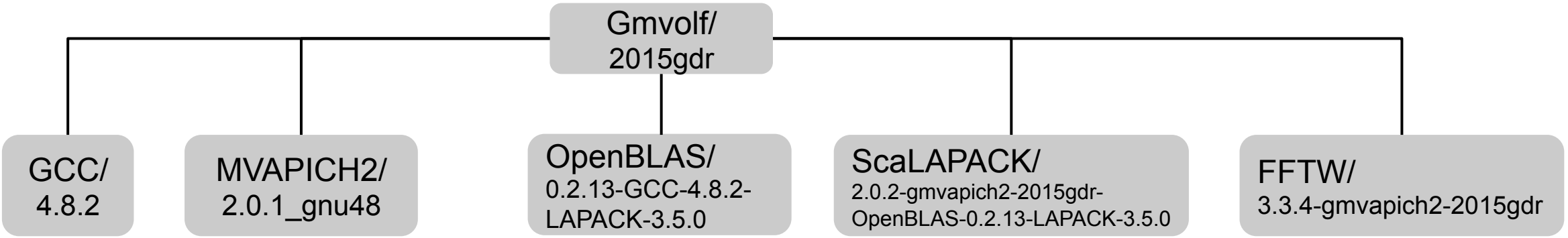
Toolchain

gmvolf/2015a
FFTW/3.3.4-gmvapich2-2015a
GCC/4.8.2
MVAPICH2/2.0.1_gnu48
OpenBLAS/0.2.13-GCC-4.8.2-LAPACK-3.5.0
ScaLAPACK/2.0.2-gmvapich2-2015a-…

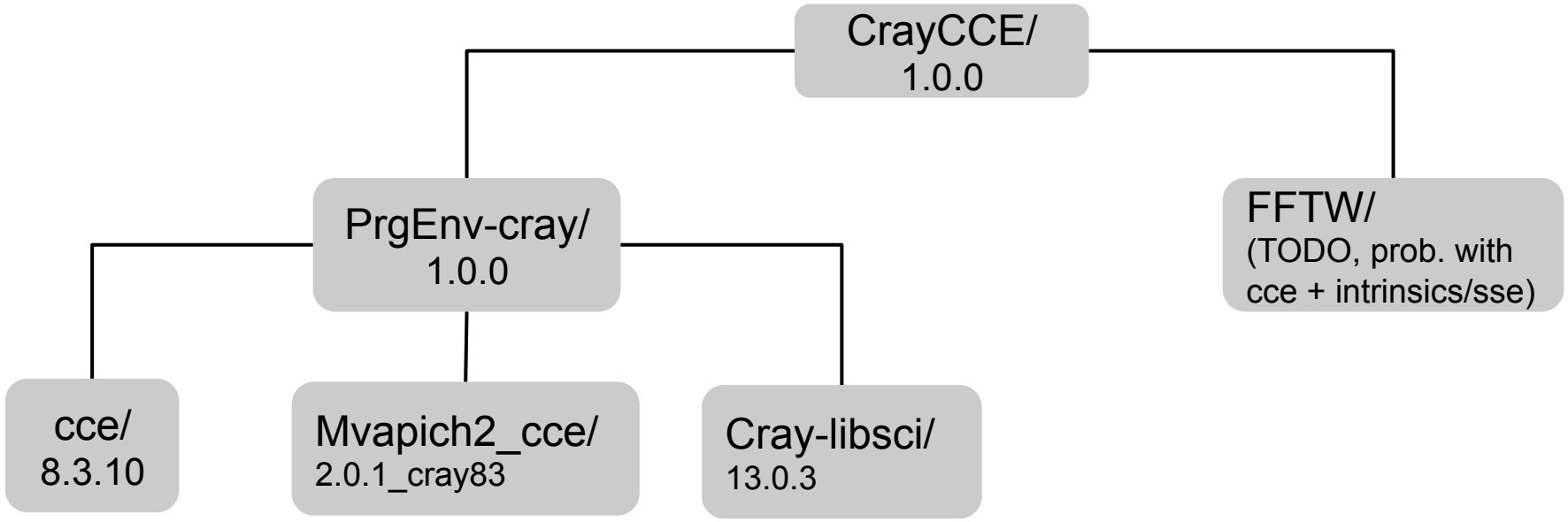
Dependencies

binutils/2.25
Bison/3.0.3
bzip2/1.0.6
cURL/7.40.0
Doxygen/1.8.9.1
flex/2.5.39
freetype/2.5.5
gettext/0.18.2
GLib/2.34.3
JasPer/1.900.1
libffi/3.0.13
libjpeg-turbo/1.4.0
libpng/1.6.16
libreadline/6.2
libreadline/6.3
libxml2/2.9.1
M4/1.4.17
NASM/2.11.06
Szip/2.1
SQLite/3.8.8.1
Tcl/8.6.3
UDUNITS/2.1.24
zlib/1.2.8

GNU – gmvolf/2015gdr (GCC 4.8.2 + MVAPICH 2.1 rc2 GDR) - WIP



CrayCCE/1.0.0 (PrgEnv-cray + Libsci) – WIP

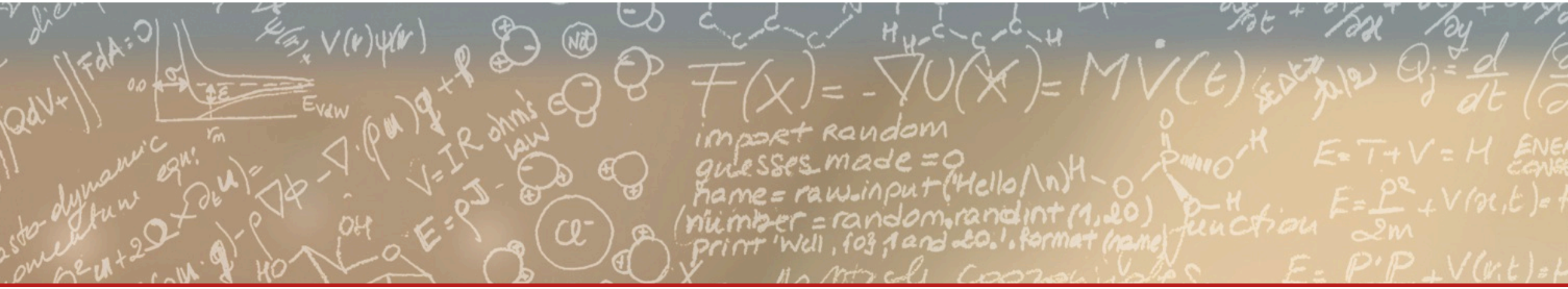


Current/upcoming activities + Issues

- Test apps built with gmvolf/2015a
- Fix/build toolchain gmvolf/2015gdr
  - Problem with libpmi linking
- Fix/build toolchain CrayCCE/1.0.0
  - Problem compiling fftw with cce
- Define EB toolchain for Intel
- Overview of PE status as of 05.08.2015 (by jgp)

MPI	C	C++	F90
CCE	ok	ok	ok
GNU	ok	ok	ok
GNUgdr	pmi	pmi	pmi

MPICUDA	C
CCE	stdc++
GNU	stdc++
GNUgdr	stdc++



Thank you for your attention.