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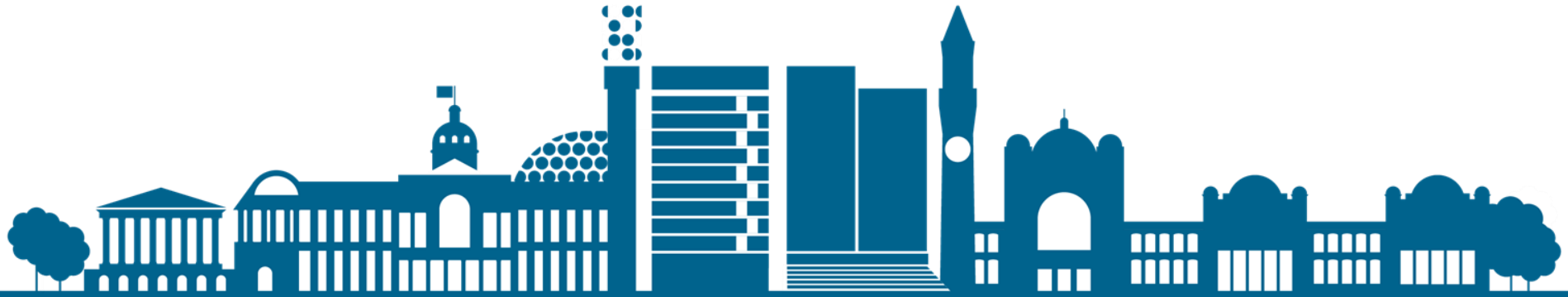
easybuild

EasyBuild and HPC



EasyBuild

"a software build and installation framework that allows you to manage (scientific) software on High Performance Computing (HPC) systems in an efficient way"

http://easybuild.readthedocs.io/en/latest/

EasyBuild Components

- Github repos (https://github.com/hpcugent):
  - EasyConfig: a text file for each specific version of an application (extensible)
  - EasyBlock: a python module defining how to install an application.
  - EasyFramework: the EasyBuild code itself

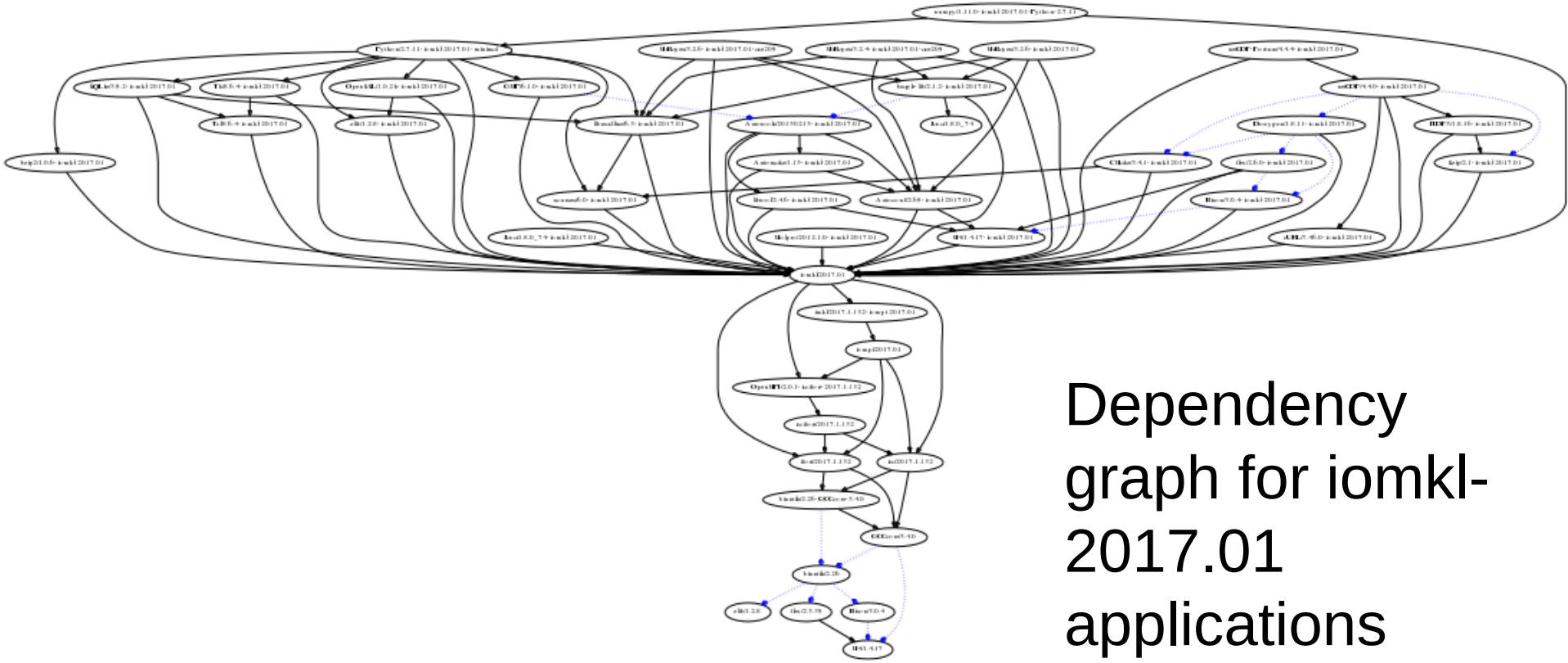
BEAR

- BEAR (Birmingham Environment for Academic Research)
  - BlueBEAR
    - Old(er) HPC cluster: EL6
    - New water-cooled HPC cluster: EL7
  - BEAR Cloud
    - Virtual Machines: EL7, Ubuntu 16.04, ...

EasyBuild and BEAR

- Local clones of EasyConfigs and EasyBlocks
  - More applications added
  - Local customisations and conventions
  - Changes pushed upstream on occasion
  - Stored in GPFS and accessible from all nodes and Vms
  - E.g. “module load apps/openfoam/v1606+” works on all platforms

EasyBuild and BEAR



Dependency graph for iomkl-2017.01 applications

EasyBuild and BEAR

- To date, built by EasyBuild on BEAR:
  - 94 packages (e.g. OpenFOAM)
  - 271 user-facing modules (e.g. OpenFOAM v1606+)
  - 564 total modules (including binutils, Automake, ...)
- Upstream supports
  - ~ 1,300 packages
  - > 8,000 EasyConfigs (≈ modules)

Example EasyConfig

```
name = 'Amber'
version = '16'
ambertools_ver = '16'
cudaver = '8.0.44'
patchlevels = (5, 14)  # (AmberTools, Amber)
versionsuffix = '-AmberTools-%s-patchlevel-%s-%s-CUDA-%s' %(ambertools_ver, patchlevels[0], patchlevels[1],
cudaver)

homepage = 'http://ambermd.org/amber.html'
description = "Amber (originally Assisted Model Building with Energy Refinement) is software for performing
molecular dynamics and structure prediction."

toolchain = {'name': 'iomkl', 'version': '2016.09'}
toolchainopts = {'usempi': True}

sources = [
    'Amber%(version)s.tar.bz2',
    'AmberTools%s.tar.bz2' % ambertools_ver,
]

dependencies = [
    ('CUDA', cudaver, '', True),
    ('netCDF', '4.4.0'),
    ('netCDF-Fortran', '4.4.4'),
    ('Python', '2.7.11', '-minimal'),
    ('numpy', '1.11.0', '-Python-2.7.11'),
]

patches = ['Amber-16_fix-hardcoding.patch',
           'Amber-16_test_cuda.patch']

moduleclass = 'chem'
```

Example:
Amber 16 with CUDA 8 and OpenMPI 1.10.2 support

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