

EasyBuild and EESSI

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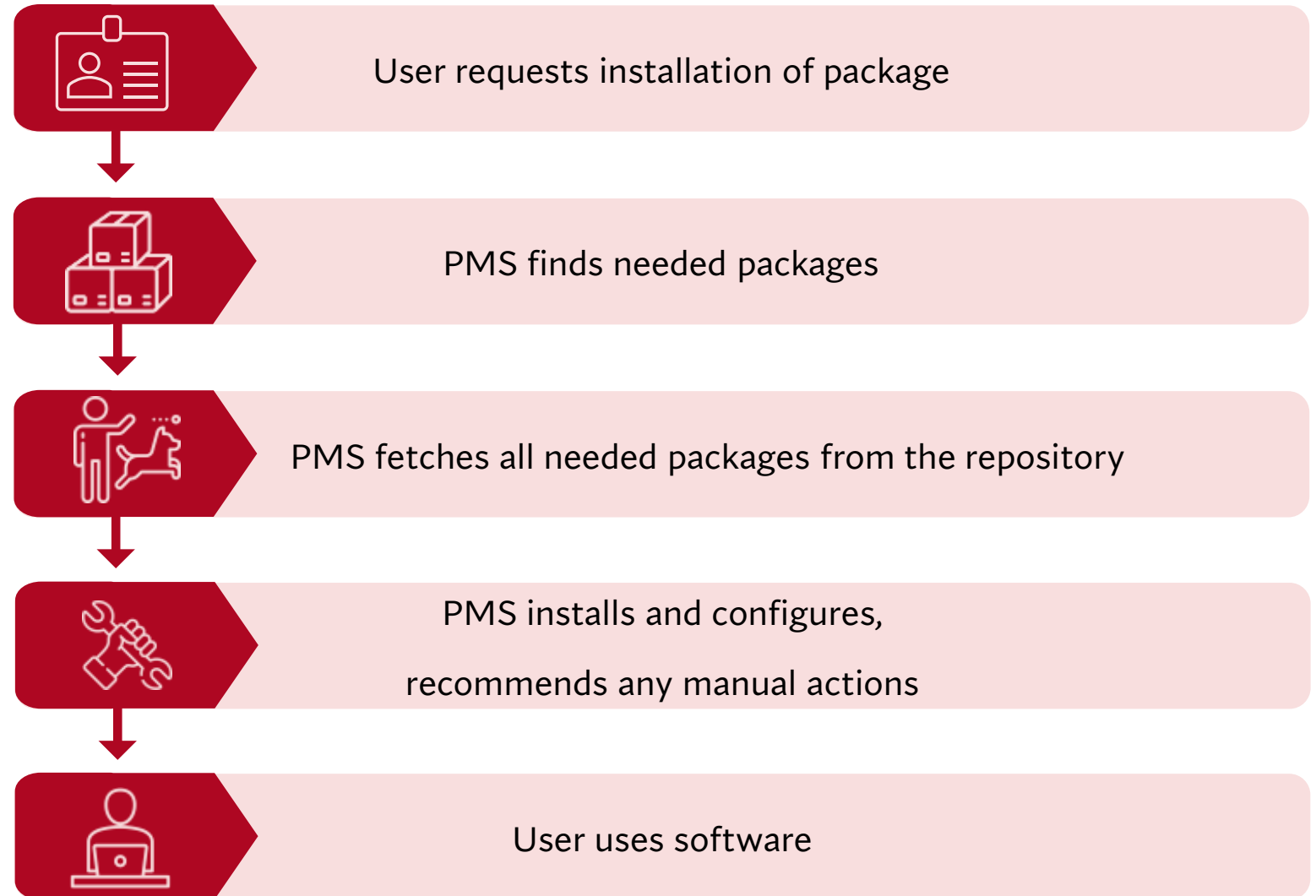


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What is a package manager?

- An HPC environment requires installation of varied software including compilers, MPI, math libraries and more.
- A package manager is a software that allows admins (but users as well) to consistently install software stacks.
- There are several package managers on the market eg Spack, EasyBuild, Conda, Nix (GUI Nix).



Installing and using EasyBuild

Installing and using EasyBuild steps:

1. Specify Temporary directory
2. Install EasyBuild Python module to TEMP
3. Tell Python where the module is
4. Use the temporary eb to install EasyBuild as an env module to specified path
5. Load EasyBuild module

How to:

System Python

```
export  
EB_TMPDIR=/tmp/$USER/eb_tmp
```

```
pip install --prefix $EB_TMPDIR easybuild
```

```
eb --install-latest-eb-release --  
installpath=$PATH
```

```
export :  
PATH=$EB_TMPDIR/bin:$PATH  
PYTHONPATH=$EB_TMPDIR/proper  
path:$PYTHONPATH
```

module load EasyBuild



Using EasyBuild (browse and install packages)

Searching and installing packages

- Search packages

```
eb -S package (Not case sensitive!)
```

- Check Dependencies:

```
eb package.eb -Dr (total list)
```

```
eb package.eb -M (missing ones)
```

- Installing Packages:

```
eb package.eb -r (by default 16 CPUs used or number of cores in machine if less. Change with --parallel=N )
```

- Troubleshoot: (from EasyBuild 5.x.x)

```
cmd.sh (allows you to get the interactive shell to debug)
```



EasyBuild code has two main concepts: Easyblocks and EasyConfigs

EasyBlocks:

Python modules (sections of code) that provide a set of linux commands like:

`./configure`

`make`

`make install`

Without any specifics

EasyConfigs:

Add-ons in the form of text files (Python dictionaries)

Follows up by “fine tuning” on the “general” EasyBlock set of instructions

eg

`configure` using a particular file

do not use `make install`

choose the version of compiler, library, etc



Easyconfigs (the input files of EasyBuild):

Mandatory easyconfig parameters

A handful of easyconfig parameters are mandatory:

- **name, version:** specify what software (version) to build
- **homepage, description:** metadata (used for module help)
- **toolchain:** specifies name and version of compiler toolchain to use

Example of program CPMD

Input file =

```
easyblock = 'ConfigureMake'  
name = 'CPMD'  
version = '4.3'
```

```
homepage = 'https://github.com/CPMD-code'  
description="""The CPMD code is a plane wave /  
pseudopotential implementation of DFT, /  
particularly designed for ab-initio molecular dynamics."""
```

```
toolchain = {'name': 'foss', 'version': '2022a'}
```

```
source_urls = ['https://github.com/CPMD-code/CPMD/archive/refs/tags/']  
sources = ['%(version)s.tar.gz']  
patches = ['myfile.patch', 'configure.patch']
```

Download
and prepare files

```
configure_cmd = "cd CPMD-4.3; chmod u+x configure.sh ; "  
configure_cmd += "./configure.sh -omp LINUX-X86_64-GFORTRAN-MPI"
```

Particular
configure options

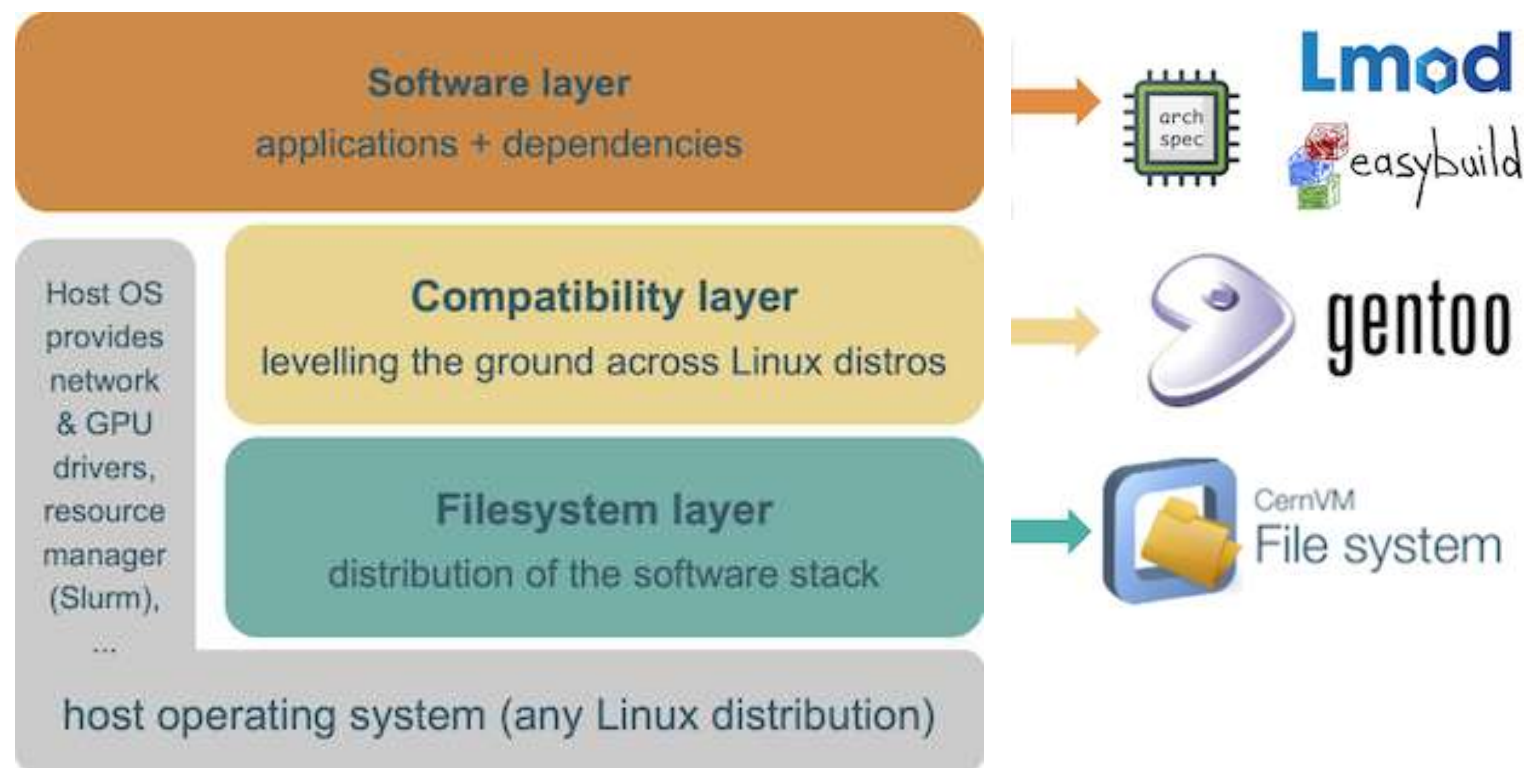
```
installopts = 'PREFIX=$(installdir)s'
```

Install options

```
moduleclass = 'chem'
```



EESSI



Software stack works on:

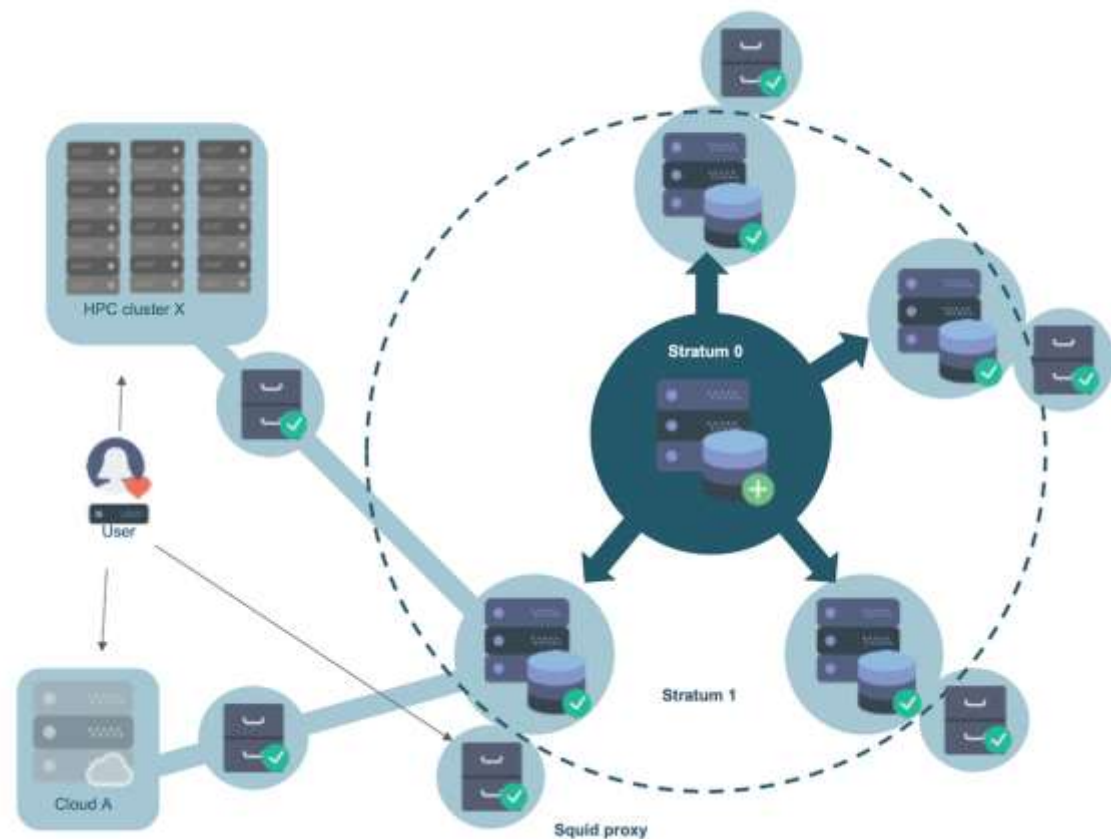
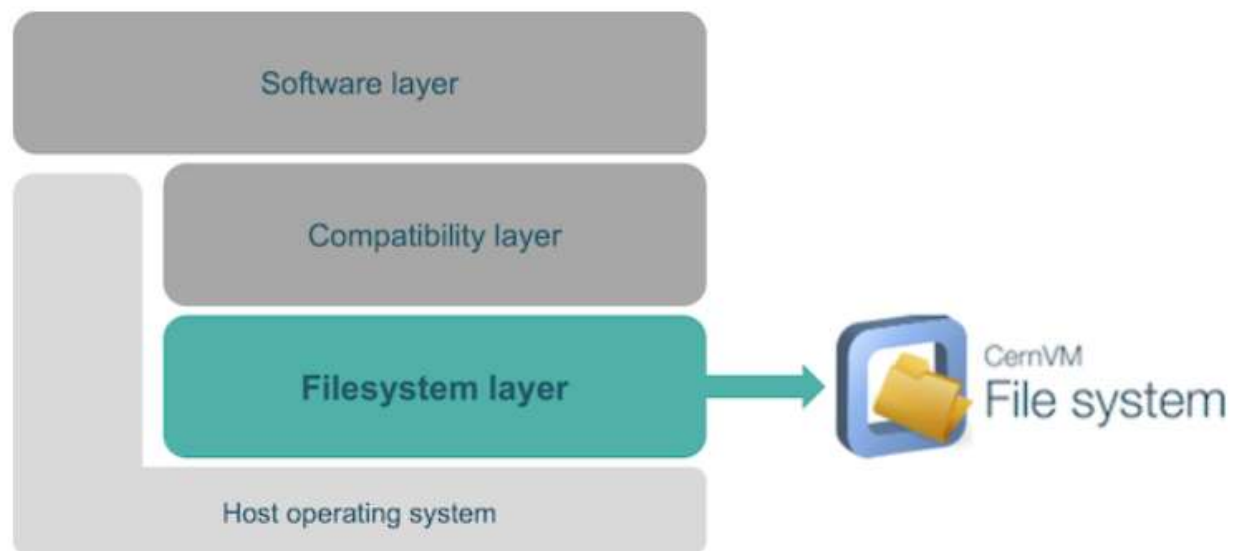
- Laptops
- Personal workstations
- HPC, Cloud

Support for:

- Different CPUs
- Intel, AMD, ARM, POWER, RISC-V
- Networks
- GPUs



Filesystem layer



CernVM File System (CernVM-FS)



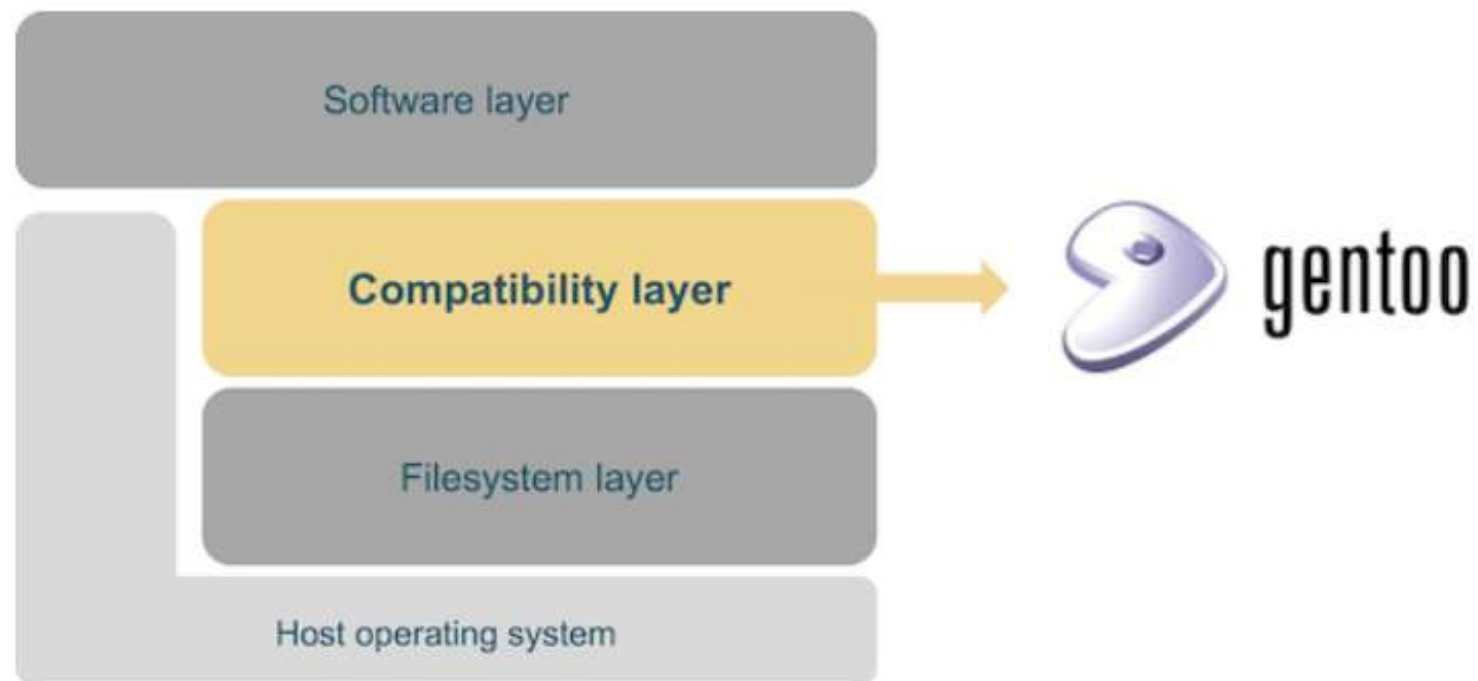
github.com/EESSI/filesystem-layer

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Compatibility layer



Using EESSI

EESSI available?

Try checking the contents of the `/cvmfs/software.eessi.io` directory with the `ls` command:

```
$ ls /cvmfs/software.eessi.io
README.eessi  host_injections  versions
```

Initialise shell environment

```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
Found EESSI repo @ /cvmfs/software.eessi.io/versions/2023.06!
archdetect says x86_64/amd/zen2
Using x86_64/amd/zen2 as software subdirectory.
Using /cvmfs/software.eessi.io/versions/2023.06/software/linux/
Found Lmod configuration file at /cvmfs/software.eessi.io/versi
Initializing Lmod...
Prepending /cvmfs/software.eessi.io/versions/2023.06/software/l
Environment set up to use EESSI (2023.06), have fun!
```

Load module(s)

```
$ module avail tensorflow

----- /cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/amd/zen2/modi

TensorFlow/2.13.0-foss-2023a
```

