KubeCon | CloudNativeCon

Europe 2022

WELCOME TO VALENCIA

KubeCon CloudNativeCon
Europe 2022

Unlimited Data Science Libraries, One Container Image, No Installation!

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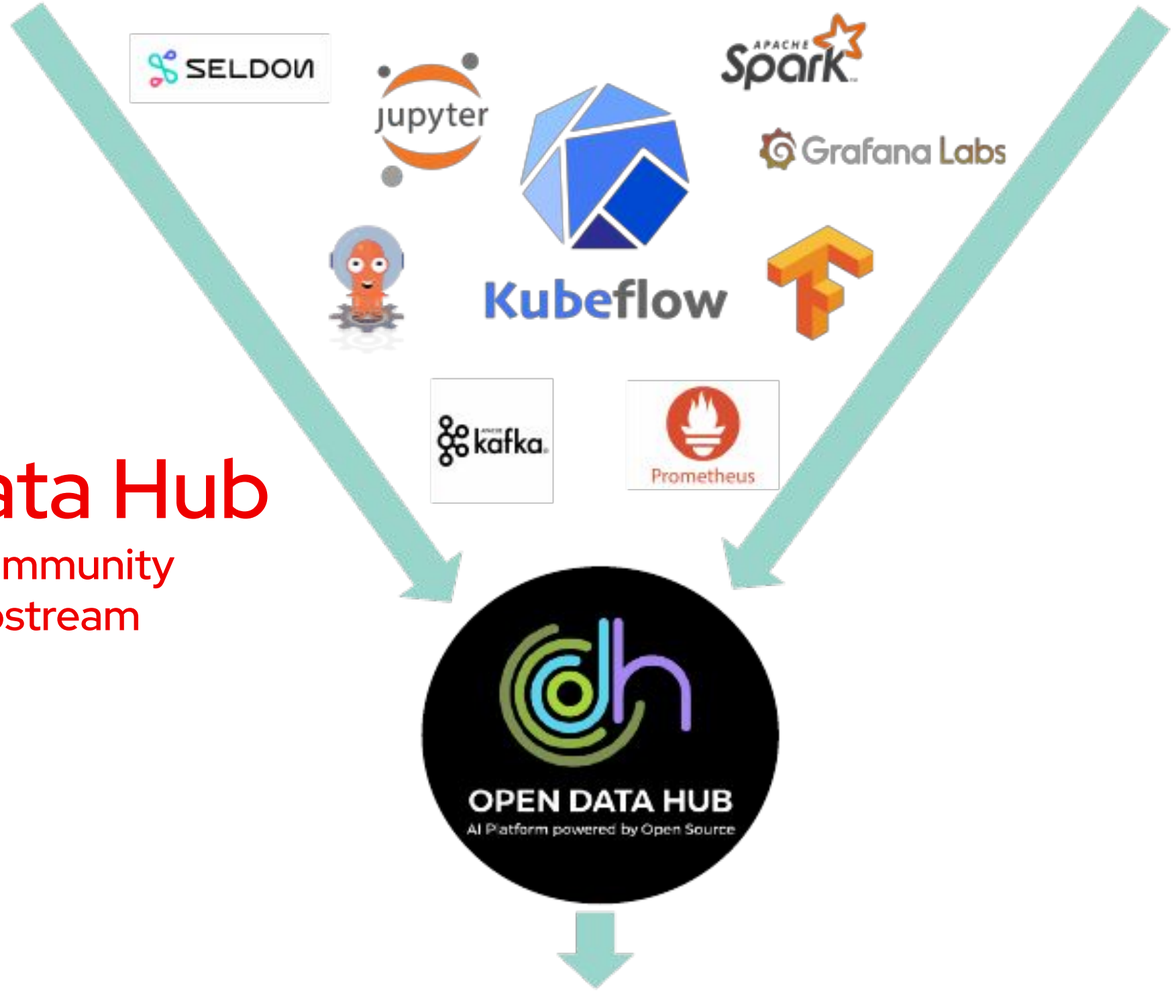
What we'll discuss today...

- Context and Background
- The problem
- The solution
- Demo
- How to...

Context



Open Data Hub

Open Source Community
Downstream/Upstream

Red Hat Application Services

Red Hat OpenShift

Red Hat OpenShift Data Foundation

Goals

- Provide an end-to-end AI/ML platform on OpenShift
- One stop easy operator deployment for the platform on OCP
- Provide Tools for each stage in the AI/ML platform and for all AI/ML user personas optimized for OpenShift
- Provide monitoring tools for model and services used by DevOps
- Provide development tools for Data Scientists
- Provide ETL tools used by Data Engineers
- AI/ML pipelines and long processing tasks.

https://www.operate-first.cloud/apps/content/odh/README.html

Red Hat OpenShift Data Science

Addressing AI/ML experimentation and integration use cases on a managed platform

Cloud Service

Available on Red Hat OpenShift Dedicated (AWS) and Red Hat OpenShift Service on AWS

Increased capabilities/collaboration

Combines Red Hat components, open source software, and ISV certified software available on Red Hat Marketplace

Core data science workflow

Provides data scientists and intelligent application developers the ability to build, train, and deploy ML models

Rapid experimentation use cases

Model outputs are hosted on the Red Hat OpenShift managed service or exported for integration into an intelligent application

Background

High-Performance Computing (HPC)
a.k.a. supercomputing

- **Large-scale compute** infrastructure, incl. shared filesystem(s), **fast network**, GPUs, …
- **Multi-tenant**: typically 100s to 1000s of users per system
- Used across **wide range of scientific domains**
- Used for **variety of workloads**: simulations, data science, ML, AI, …
- Strong focus on **performance**, scaling, …
- Basically **100% GNU/Linux** nowadays!
- *Should* be easy to use by scientists …
- Beyond classic HPC ⇒ scientific computing

HPC infrastructure @ Ghent University (BE)

Background

HPC since the 80's

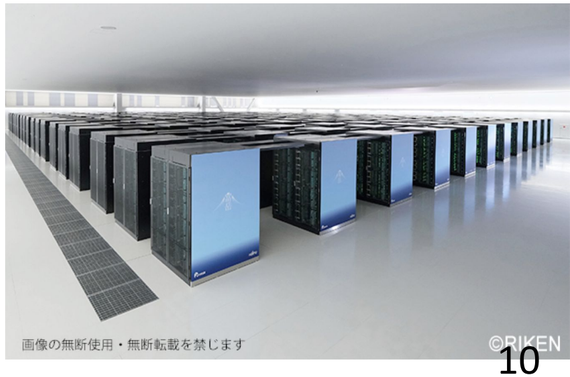
- **1,000x** increase in computing power **every ~12 years** since 1985
- Now in (or close to) **exascale era**: > 10^{18} floating-point operations per sec. (FLOPS)
- Traditional workloads: **simulation** (physics, weather, …)
- Modern workloads are **more diverse:** bioinformatics, AI, data science, …
- Significant part of compute time is still consumed by software written in **Fortran**!


Cray-2 (1985)


ASCI Red (1997)

Jaguar (2009)


Mare Nostrum 4 (2017)



Fugaku (2020)

Background

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The HPC user experience

- Typical usage: **SSH** to login nodes, submit scripts to job scheduler (Slurm), results on disk
- Interaction mostly via **Linux shell command line interface**
- Modern interfaces are gaining traction: Open OnDemand web portal

```
▶ ssh vsc40023@login.hpc.ugent.be
Last login: Tue Jan  8 19:29:07 2019 from gligarha01.gastly.os

STEVIN HPC-UGent infrastructure status on Tue, 08 Jan 2019 19:20:01

   cluster - full - free -  part - total - running - queued
             nodes  nodes   free   nodes    jobs      jobs
-----------------------------------------------------------------
    golett     71      0    128     200      N/A       N/A
    phanpy     15      1      0      16      N/A       N/A
    swalot     46      0     42     128      N/A       N/A
    skitty     63      0      1      72      N/A       N/A
   victini     57      0     32      96      N/A       N/A

For a full view of the current loads and queues see:
 http://hpc.ugent.be/clusterstate/
Updates on maintenance and unscheduled downtime can be found on
 https://www.vscentrum.be/en/user-portal/system-status

-bash-4.2$ hostname
gligar05.gastly.os
-bash-4.2$
```

Background

Using containers on HPC infrastructure remains challenging …

- Leveraging **special-purpose hardware** (GPUs, interconnect, …)
- **Avoid sacrificing performance for mobility-of-compute**
- Growing **diversity** in hardware resources (Intel, AMD, Arm, NVIDIA, …)
- Large **variety** of workloads and user profiles
- Someone needs to (re)build the container image(s) you need!

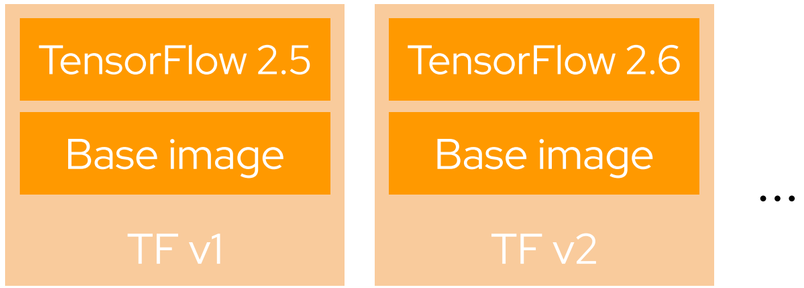
The on-demand notebook example

The “base” container image includes:

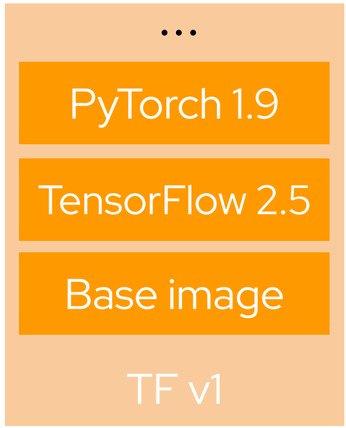
- Python at a specific version
- Some useful libraries and applications
- Jupyter with pre-defined extensions

The problem

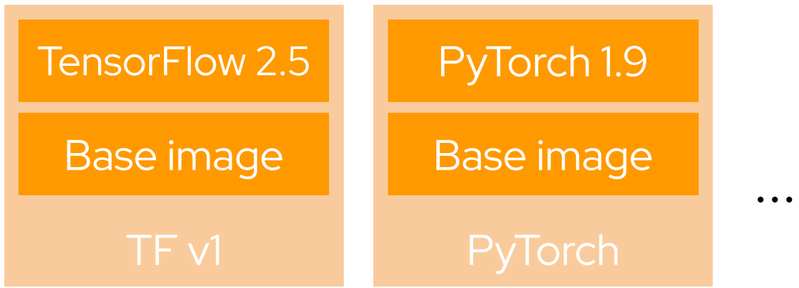
Users want more, what to do?



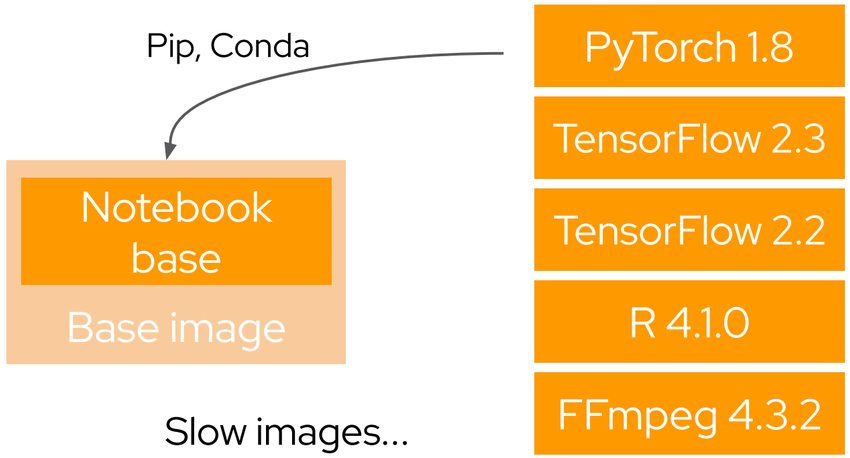
Multiple versions => Multiple images



Overweight images...



Multiple tools => Multiple images



Slow images...

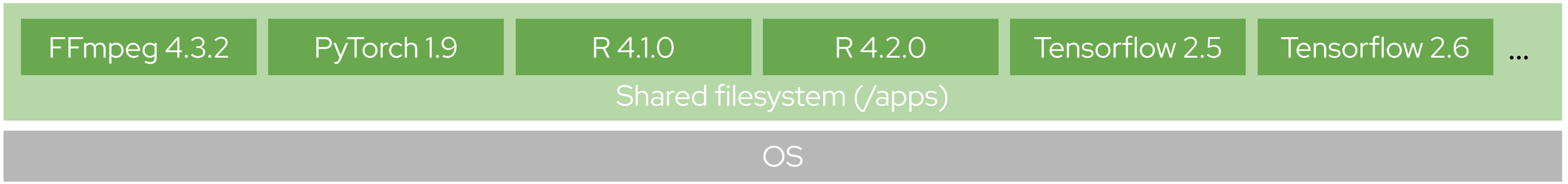
The problem

Users want more, what to do?

The solution

HPC systems usually provide a **central software stack**

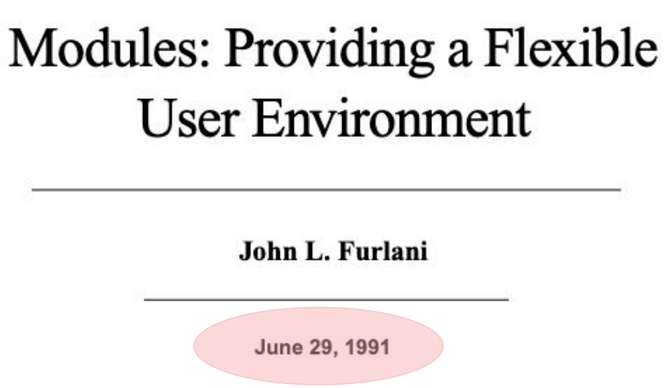
- Software installed in a **non-standard location** on a shared filesystem (like `/apps`)
- Collection of **100's-1000's of installations** (diff. software, versions, compilers)
- **Separate directory** for each software installation (different applications/versions/...)
- Provided software is **optimized for system architecture**
- Software is **built from source** where possible (to ensure good performance)
- **Additional installations are added** on-demand, or as new versions are released



The solution

Easy access to central software stack using **environment modules**

- Traditional way to **let users** of HPC systems **manage their environment**
- Shell-agnostic **module files** specify what to change in shell environment
- **`module` command** to check for available modules, (un)load modules, …
- Two main implementations:



http://modules.sourceforge.net/docs/Modules-Paper.pdf

ENVIRONMENT MODULES

- Evolution of original implementation in Tcl
- Module files written in Tcl
- Actively developed & maintained
- Less popular, but default in RHEL-based OSs
- http://modules.sourceforge.net

Lmod

- Modern implementation in Lua
- Module files written in Lua or Tcl
- Actively developed & maintained
- Developed for hierarchical modules
- Most popular (>85% of systems)
- https://lmod.readthedocs.io

The solution

Environment modules: example

ssh example@supercomputer

```
$ example --version
-bash: example: command not found

$ module use /apps/modules

$ module avail example
----- /apps/modules -----
example/1.2.3

$ module load example/1.2.3

$ example --version
1.2.3
```

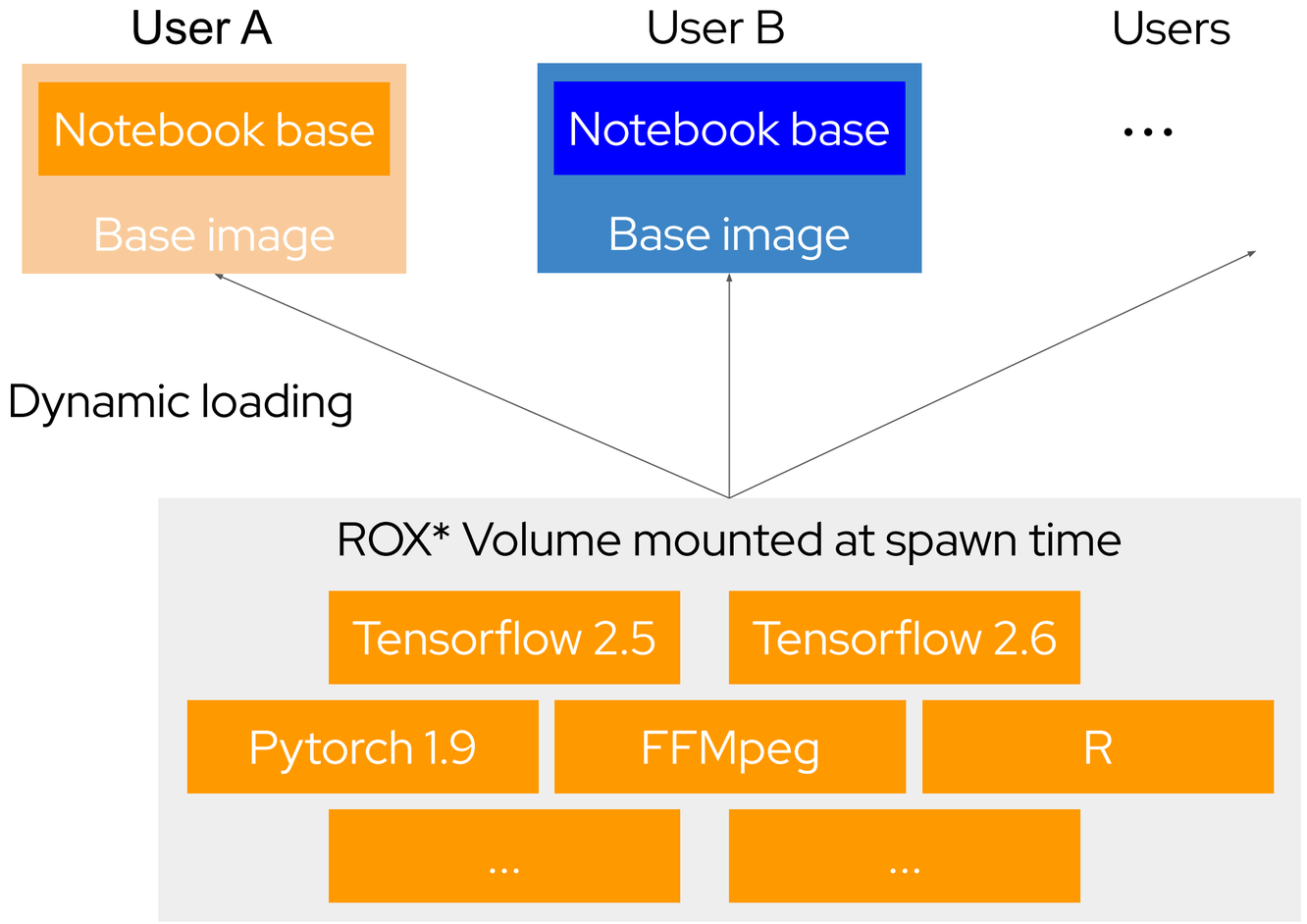
Contents of `/apps/modules/example/1.2.3.lua`:

```
local root = "/apps/software/example/1.2.3"
prepend_path("PATH", pathJoin(root, "bin"))
prepend_path("LD_LIBRARY_PATH", pathJoin(root, "lib"))
prepend_path("LIBRARY_PATH", pathJoin(root, lib"))
prepend_path("PYTHONPATH", pathJoin(root, "lib/python3.9/site-packages"))
setenv("EXAMPLE_ROOT", root)
setenv("EXAMPLE_VERSION", "1.2.3")
setenv("EXAMPLE_ENABLE_DEBUG_OUTPUT", "1")
```

The solution

So let's use environment modules!

ODH Highlander



**ROX: Read-Only Many, a volume that can be mounted simultaneously into many containers*

The solution

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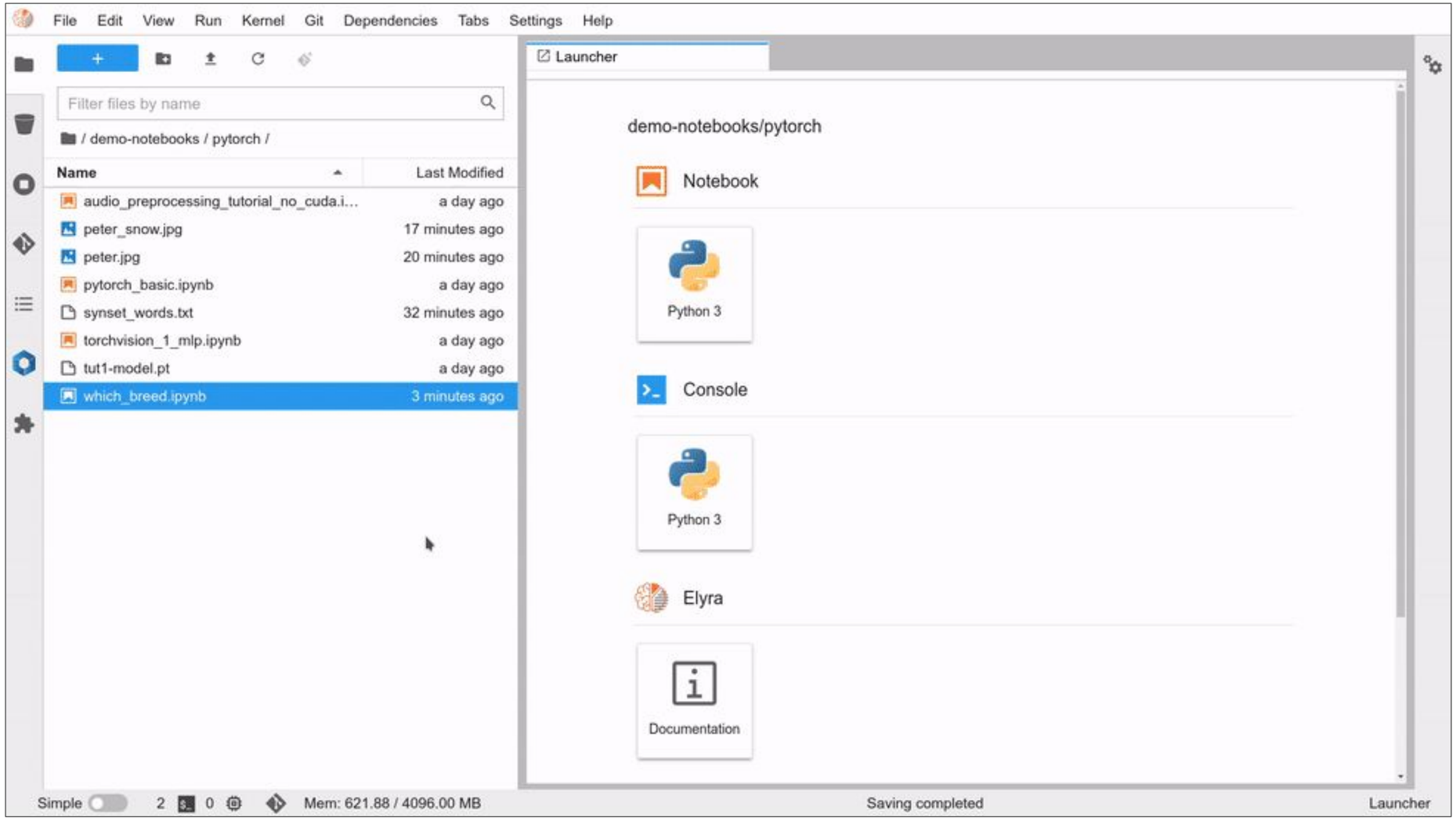
DEMO



Howto

- Tool to **get scientific software installed** (preferably from source), incl. module files
- Focus on **Linux & HPC** systems, specific attention to **performance**
- Implemented in **Python**, integrates with environment modules tool
- In active development **since 2009**, available as open source software for 10 years
- **GPLv2** license, available via **GitHub** and **PyPI**
- Support for different compiler toolchains + over 2,600 (scientific) software packages (excl. versions, extensions)
- Created by HPC-UGent team, now supported & developed by a **worldwide community**...

Howto

Example: installing TensorFlow (from source) with 

ssh example@supercomputer

```
$ eb TensorFlow-2.6.0-foss-2021a-CUDA-11.3.1.eb
...
== building and installing TensorFlow/2.6.0-foss-2021a-CUDA-11.3.1...
...
== configuring...
== building...
== testing...
== installing...
...
== creating module...
...
== COMPLETED: Installation ended successfully

$ module load TensorFlow/2.6.0-foss-2021a-CUDA-11.3.1
$ python tensorflow_cat_or_dog.py
Tensors are flowing...
```

Howto

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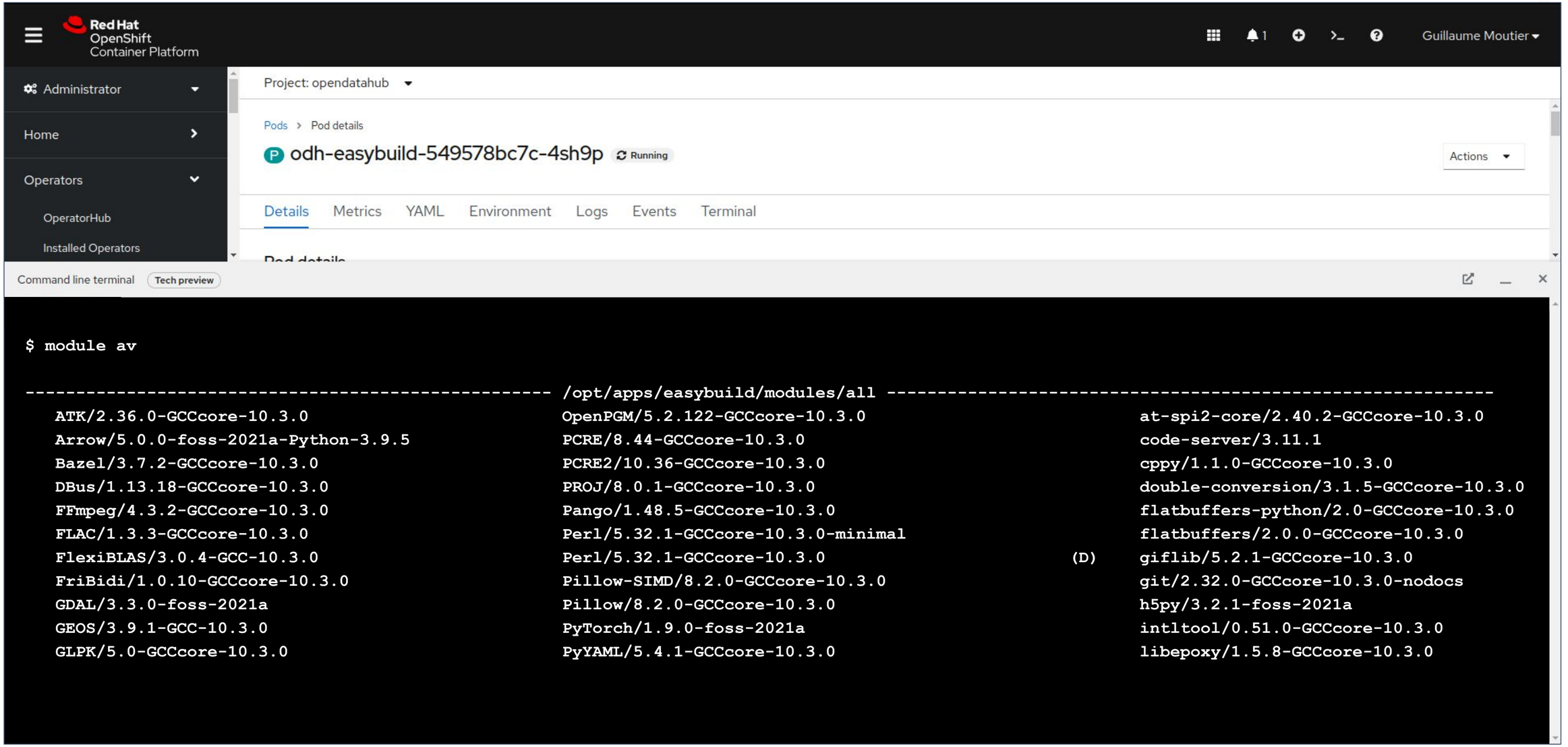
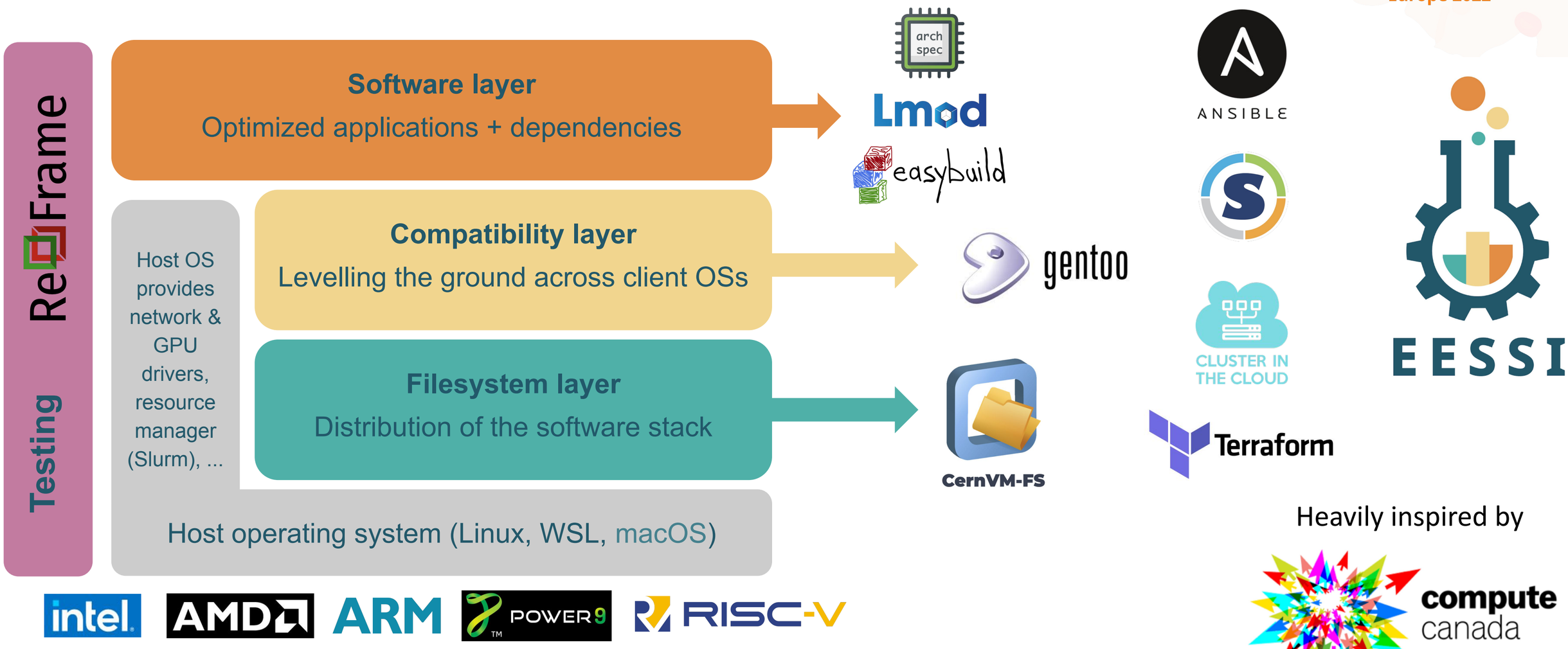
DEMO



Future work

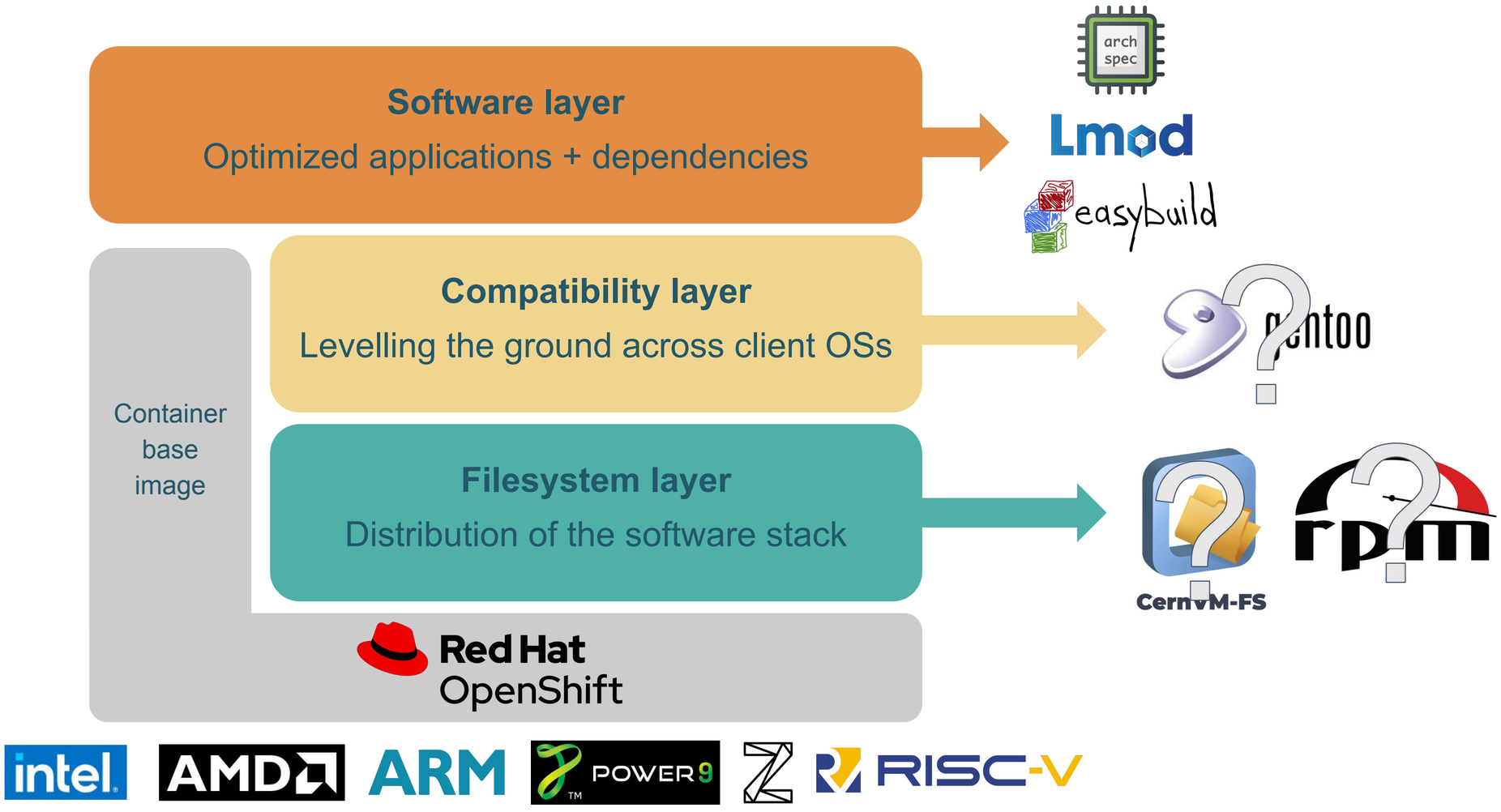
- **European Environment for Scientific Software Installations (EESSI)**
- Collaborative project, by and for the computational science community
- **Shared central stack of (optimized) scientific software installations**
- Uniform way of providing software to users, regardless of system they use
- Should work regardless of OS and system architecture (HPC, cloud, ...)
- Focus on **performance**, **automation**, **testing**, **collaboration**

Future work - EESSI, built with FOSS tools



Proof-of-concept is working, looking for funding to make EESSI a reliable service...

Future work - Open Data Hub Highlander



EESSI

ODH-Highlander Repository of curated pre-compiled modules

References

- Open Data Hub: opendatahub.io
- OpenShift Data Science: red.ht/datascience
- Operate First: operate-first.cloud
- ODH-Highlander: odh-highlander.github.io
- Environment modules: modules.sourceforge.net
- Lmod environment modules tool: lmod.readthedocs.io
- EasyBuild: easybuild.io - dx.doi.org/10.1109/HUST.2014.8
- EESSI project: eessi-hpc.org - eessi.github.io/docs - dx.doi.org/10.1002/spe.3075
- How To Make Package Managers Cry: https://www.youtube.com/watch?v=NSemlYagjlU

Questions are welcome!

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