(virtual) HPC Champions meeting (UK)

Tue Dec 15th 2020

EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

Kenneth Hoste (HPC-UGent, Belgium)

kenneth.hoste@ugent.be - @kehoste (Twitter) - @boegel (GitHub)

whoami

kenneth.hoste@ugent.be

@kehoste @boegel

- Computer scientist from Belgium
- Masters & PhD from Ghent University
- **HPC system administrator at UGent since 2010**
- User support & training, **software installations** (RSE?)
- Big fan of FOSS, family, loud music, (good) beer, dad jokes, stickers, ...
- Doesn't like C++, CMake, SCons, Bazel, TensorFlow, OpenFOAM, ...

GHENT UNIVERSITY

Vlaanderen is computing

EESSI

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- **Who** is involved in EESSI?
- **What** is the project about?
- **Why** did we start it?
- **How** are we tackling the problem?
- What are the **challenges**?
- Which **FOSS projects** do we use?
- What is the **current status**?
- **Live demo(s)!**

EESSI in a nutshell

EESSI

- **European Environment for Scientific Software Installations** (EESSI, pronounced as "easy")
- Collaboration between different partners in HPC community
- Goal: **building a common performant scientific software stack** for HPC systems & beyond (cloud, workstations, ...)
- Grass roots project

https://eessi-hpc.org

https://github.com/EESSI

https://eessi.github.io/docs/pilot

@eessi_hpc

Project partners

There's a storm coming... or are we in it already?

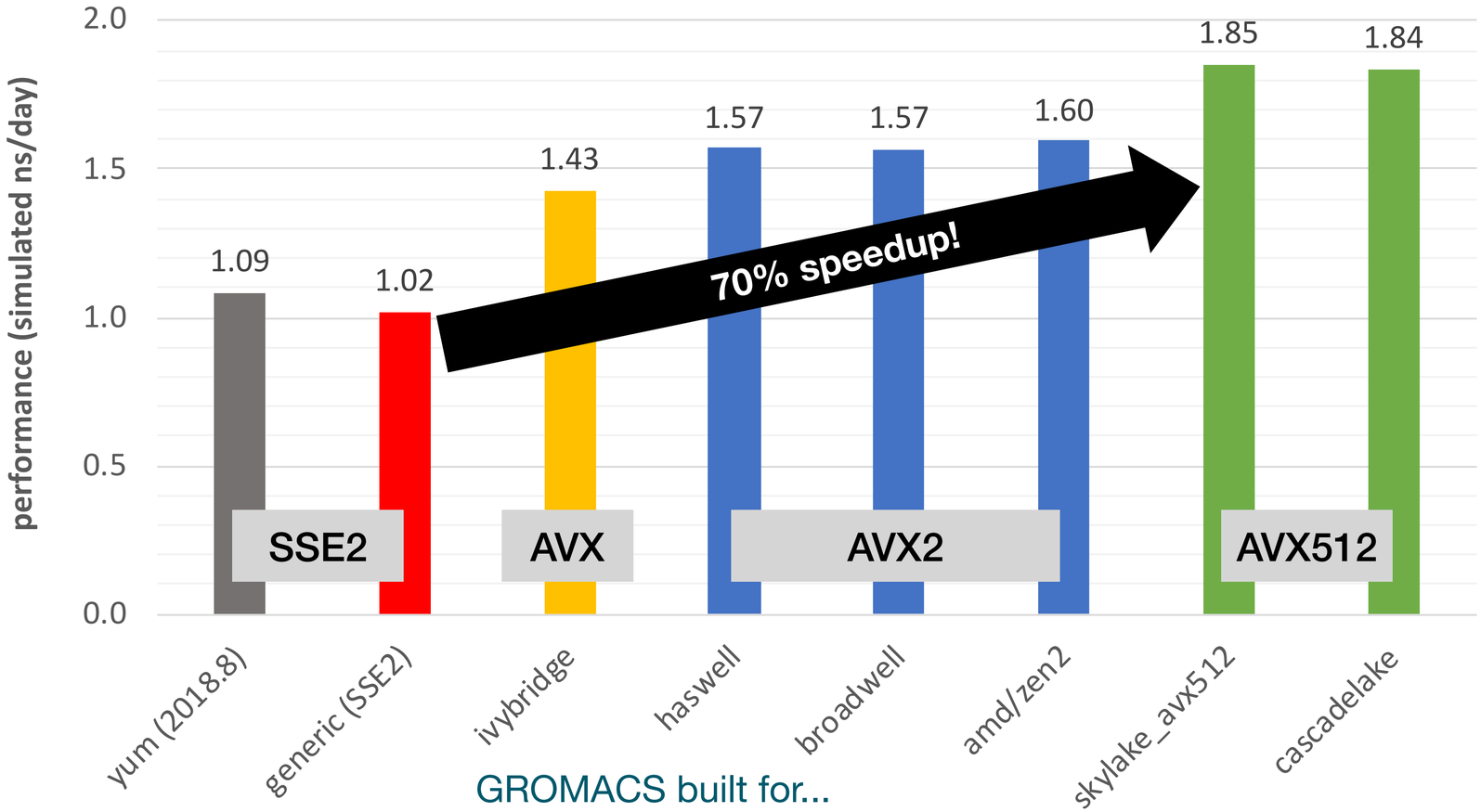
- Explosion of open source scientific software in recent years
- Increasing variety in CPUs: Intel, AMD, Arm, POWER, RISC-V
- Various types of accelerators: NVIDIA & AMD GPUs, Intel Xe, ...
- Rise of the cloud: Amazon EC2, Microsoft Azure, Google, Oracle, ...
- In stark contrast: available manpower in HPC support teams...

Keeping the P in HPC

(HPC: High-Performance Computing)

- **Software should be optimised for the system it will run on**
- Impact on performance is often significant for scientific software

- Example: GROMACS 2020.1
  (PRACE benchmark, Test Case B)
- Metric: (simulated) ns/day,
  higher is better
- Test system: dual-socket
  Intel Xeon Gold 6420
  (Cascade Lake, 2x18 cores)

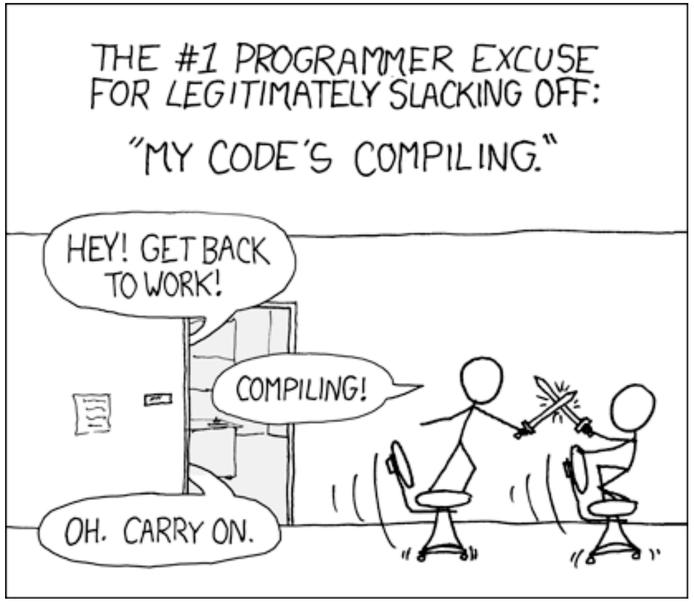


Getting Scientific Software Installed

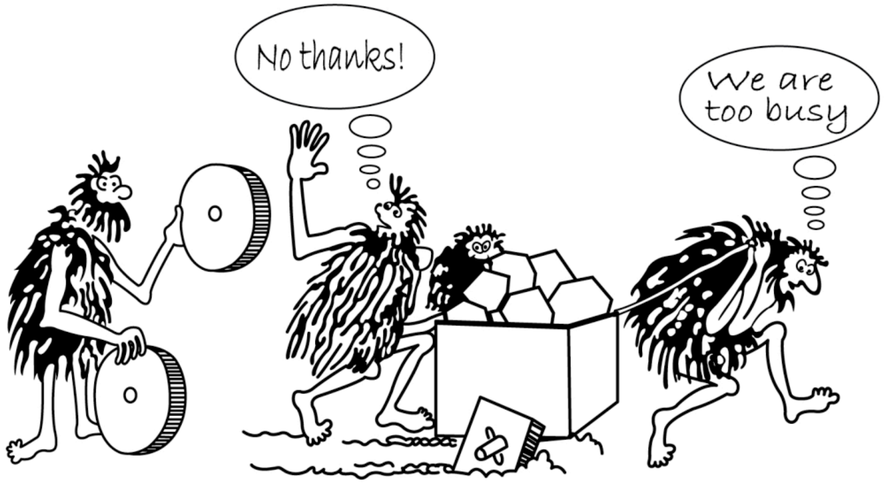
INSTALL.SH

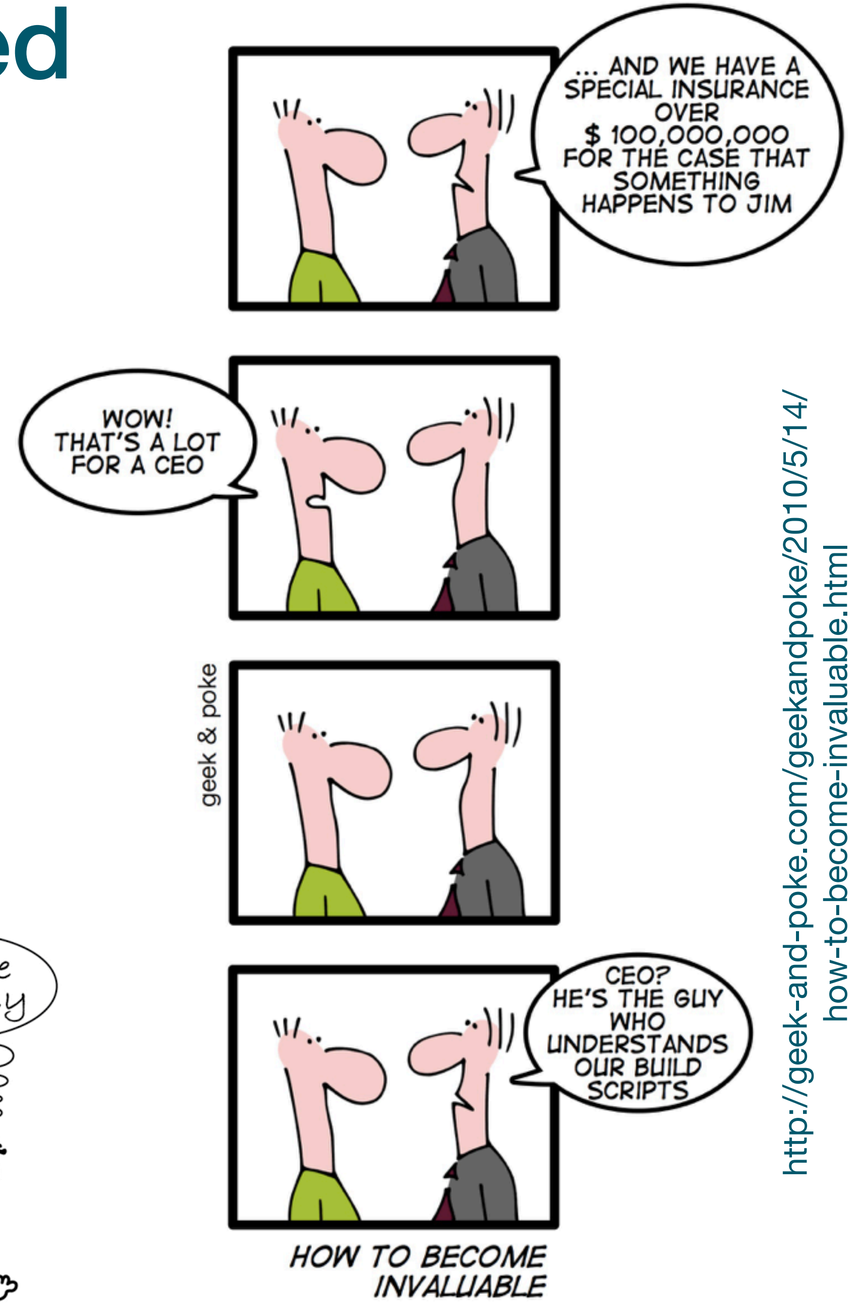
```
#!/bin/bash

pip install "$1" &
easy_install "$1" &
brew install "$1" &
npm install "$1" &
yum install "$1" & dnf install "$1" &
docker run "$1" &
pkg install "$1" &
apt-get install "$1" &
sudo apt-get install "$1" &
steamcmd +app_update "$1" validate &
git clone https://github.com/"$1"/"$1" &
cd "$1";./configure;make;make install &
curl "$1" | bash &
```

https://xkcd.com/303



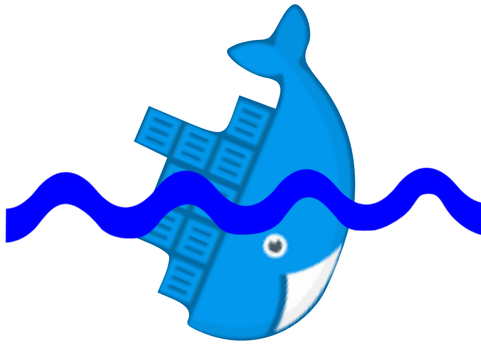
https://xkcd.com/1654





http://geek-and-poke.com/geekandpoke/2010/5/14/how-to-become-invaluable.html

What about... containers?



- Containers are (still) problematic in an HPC context
  - Integration with system resources & services is not a solved problem (MPI, GPUs, ...)
- "Native performance" really means "very little overhead"
  - That's very good, and a *requirement* for HPC, but not sufficient...
- Someone (you trust) has to build (and maintain) the container images you need!
  - Including the software you want to use, for your CPU architecture (x86_64, aarch64, ...)
  - Ideally, the image is properly optimised for the *specific* hardware you'll be using it on (performance vs "mobility of compute")
- **Containers are a symptom, not a cure...**

Scope & goals

EESSI

- **Shared repository of scientific software installations**
- Collaborate, avoid duplicate work across HPC sites
- **Uniform way of providing software to researchers**
- Offer broad platform support (Linux, macOS, Windows via WSL)
- **Targets: laptops, personal workstations, HPC clusters, and the cloud**
- Support for different CPUs, interconnects, GPUs, etc.
- Focus on **performance**, automation, testing, tuning

http://www.thecomicstrips.com/subject/The-Collaboration-Comic-Strips.php

Pick a live demo! (software)

EESSI

1

GROMACS

version 2020.1

Molecular dynamics simulation

PRACE benchmark (MPI)

2

TensorFlow

version 2.3.1

Machine learning

Beginner tutorial with MNIST (single node)

3

OpenFOAM

version 8 (openfoam.org)

Computational Fluid Dynamics (CFD) simulation

motorBike tutorial case (MPI)

4

Bioconductor

version 3.11 (on top of R 4.0)

bioinformatics

Playing with DNA data (single node)

Pick a live demo! (hardware)

A

Raspberry Pi cluster

4x model 3B+

quad-core **Arm** Cortex-A53, 1GB RAM

64-bit Raspberry Pi OS

native CernVM-FS (built from source)

B

Amazon EC2

***heterogeneous* Slurm cluster**

created via Cluster-in-the-Cloud

Intel Xeon, AMD Rome, Gravition2

CentOS 8.3 , native CernVM-FS

C

`Standard_D8s_v3` instance

8-core Intel Xeon (**different CPU generations**)

Ubuntu 18.04

native CernVM-FS, **installed from scratch**

D

Isambard2 cluster (XCI partition)

Cray XC50 @ GW4 / UK Met Office

Marvell Thunder X2 Arm64 CPUs (> 20k cores)

Cray Linux Environment 7 (SLES 15)

CernVM-FS via **Singularity** container

Spoiler demo

GROMACS

Let's run a molecular dynamics simulation on a Raspberry Pi cluster!

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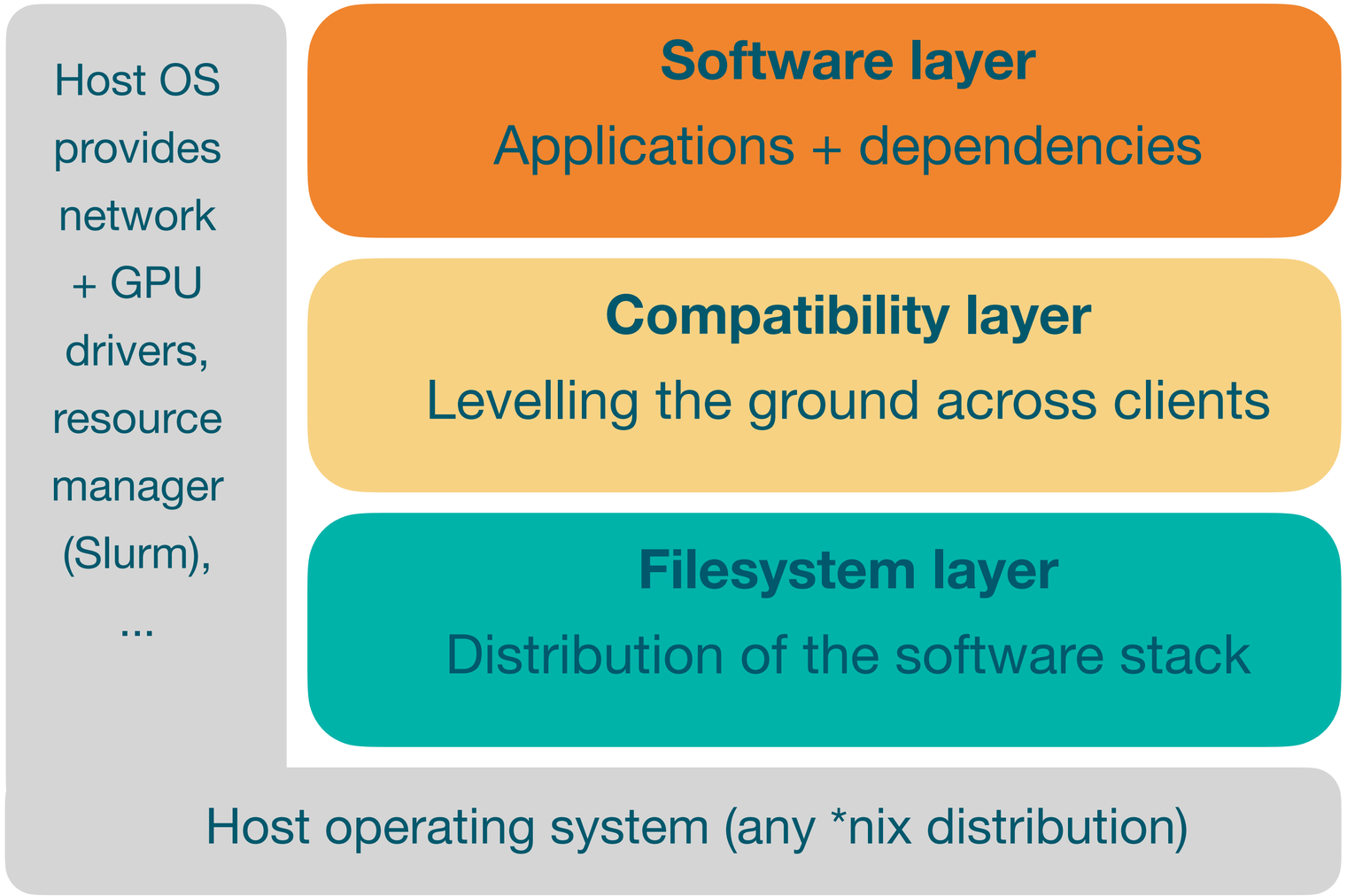
High-level overview of EESSI project



EESSI is powered by FOSS

EESSI

easybuild

- Installation tool for scientific software
- Optimises for build host (by default)
- Supports over 2,000 software pkgs

https://easybuilders.github.io/easybuild

arch spec

- Python library
- Detect processor type
- Check compatibility with host CPU

https://github.com/archspec

Lmod

- Environment modules tool (written in Lua)
- Intuitive access to software installations
- Multiple software versions side-by-side

https://lmod.readthedocs.io

gentoo

https://wiki.gentoo.org/wiki/Project:Prefix

- Linux distribution, installs from source
- Prefix project: install packages in <prefix>
- Supports x86_64, Arm64, POWER, ... & Linux, macOS

ReFrame

- Regression testing framework for HPC
- Verify correctness
- Check performance
- Tests are implemented in Python

https://reframe-hpc.rtfd.io

CernVM-FS

- Software distribution service
- Scalable, read-only, globally distributed filesystem
- Mount filesystem over HTTP

https://cernvm.cern.ch/fs

ANSIBLE

- Automation
- Configuration mgmt

Singularity

- Build isolation
- Easy access for clients

HashiCorp Terraform

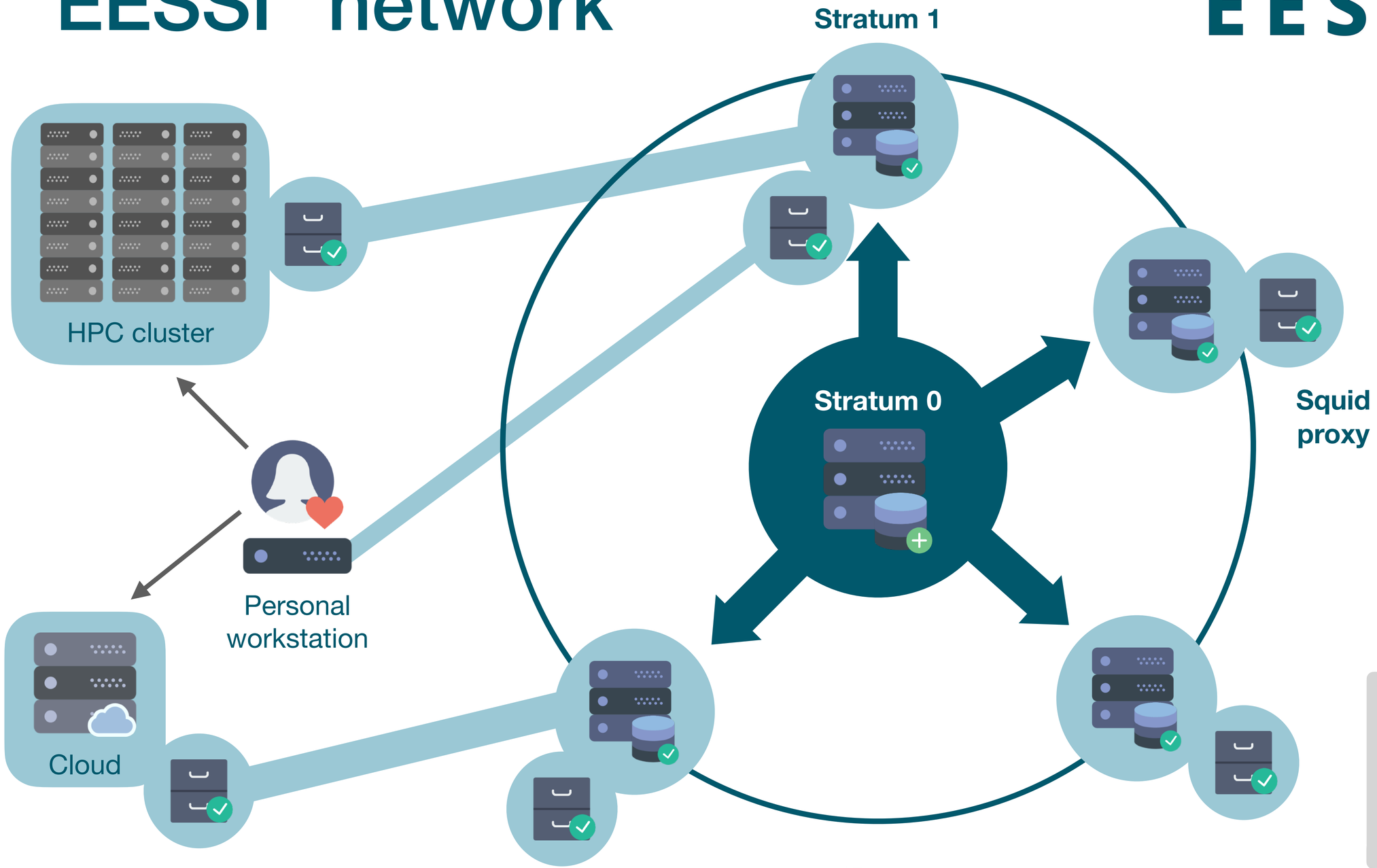
- Creating cloud instances on demand

Inspiration for EESSI

- EESSI concept is **heavily** inspired by Compute Canada software stack
- Shared across 5 major national systems in Canada + a bunch of smaller ones
- 3 layers: CernVM-FS / ~~Nix~~ Gentoo Prefix / EasyBuild + Lmod
- See paper by Maxime Boissonneault & co at PEARC'19 (PDF available here)
  "Providing a Unified Software Environment for Canada's National Advanced Computing Centers"
- See also Maxime's talk at 5th EasyBuild User Meeting (slides - recorded talk)
  and the Compute Canada documentation

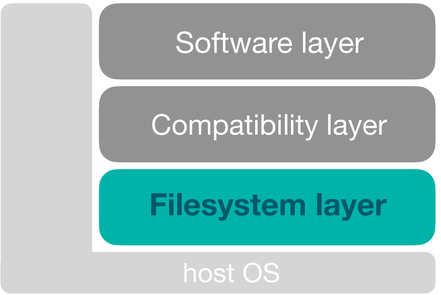
EESSI "network"

EESSI

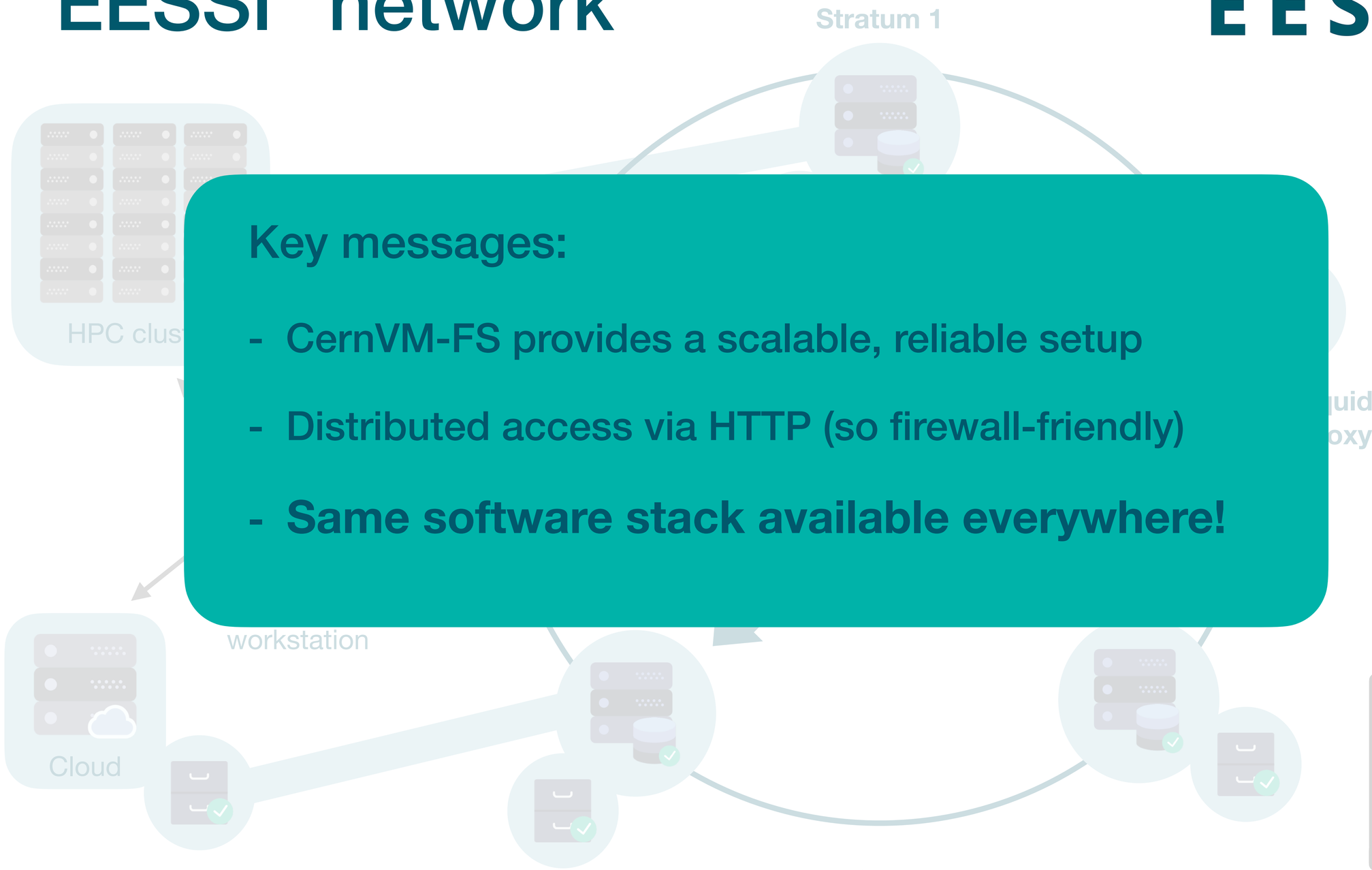


powered by

CernVM-FS



EESSI "network"

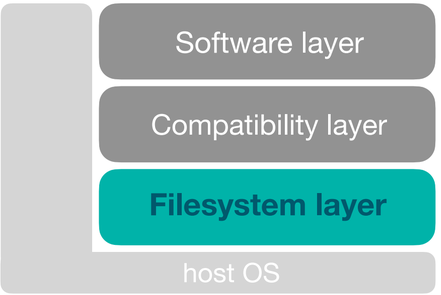


Key messages:

- CernVM-FS provides a scalable, reliable setup
- Distributed access via HTTP (so firewall-friendly)
- **Same software stack available everywhere!**

powered by

CernVM-FS



Compatibility layer

- Set of tools & libraries installed in non-standard location
- Using Gentoo's package manager Portage
- Limited to low-level stuff, incl. glibc
- Only targets a supported processor **family** (x86_64, Arm64)
- **Levels the ground for different client operating systems** (Linux distros, macOS)
- Currently in pilot repository:

```
/cvmfs/pilot.eessi-hpc/2020.12/compat/linux/aarch64
/cvmfs/pilot.eessi-hpc/2020.12/compat/linux/x86_64
```

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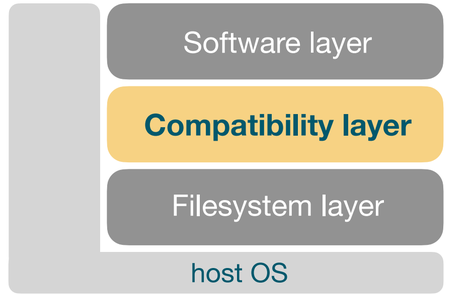


Software layer

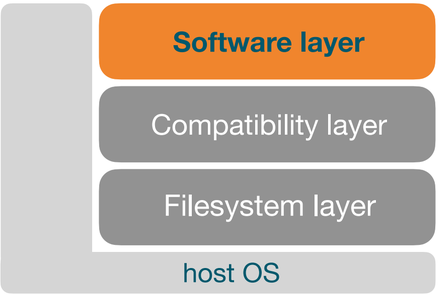
- Provides scientific software applications, libraries, and dependencies
- **Optimised for specific CPU microarchitectures** (Intel Haswell, ...)
- **Leverages libraries from compatibility layer** (not from host OS)
- Installed with EasyBuild, incl. environment module files
- Lmod environment modules tool is used to access installations
- Different subdirectories: one per target CPU microarchitecture
- **Best subdirectory for host is picked automatically** via archspec

EESSI

powered by

easybuild

Lmod



Current status: pilot repository

- Ansible playbooks, scripts, docs at `https://github.com/eessi`
- Stratum 0 @ Univ. of Groningen + two Stratum 1 servers
- Compatibility layer for both `x86_64` and `aarch64` (only Linux clients, for now)
- Software (CPU-only): Bioconductor, GROMACS, OpenFOAM, TensorFlow
- Hardware targets:
  - `x86_64/generic`, `intel/haswell`, `intel/skylake_avx512`, `amd/zen2`
  - `aarch64/generic`, `aarch64/graviton2`, **`aarch64/thunderx2`**

NOT FOR PRODUCTION USE!

Try it yourself: https://eessi.github.io/docs/pilot

From zero to science in 3 steps

Step 1: Access the (pilot) EESSI CernVM-FS repository

Option 1: Native CernVM-FS installation (requires admin privileges)

- Install CernVM-FS, see https://cernvm.cern.ch/fs
- Also install configuration files for EESSI repositories, available at https://github.com/EESSI/filesystem-layer/releases
- Run "`cvmfs_config setup`"

Option 2: Use a Singularity container (no admin rights needed!)

- CernVM-FS repositories can be mounted via Singularity's `--fusemount` option
- See detailed walkthrough at https://eessi.github.io/docs/pilot

From zero to science in 3 steps

Step 1: Access the (pilot) EESSI CernVM-FS repository

Option 1 (example): native CernVM-FS installation on fresh (x86_64) RHEL 8.2 system


```
# install CernVM-FS (see https://cernvm.cern.ch/fs/)
sudo yum install -y https://ecsft.cern.ch/dist/cvmfs/cvmfs-release/cvmfs-release-latest.noarch.rpm
sudo yum install -y cvmfs

# install CernVM-FS configuration files for EESSI repositories (see https://github.com/EESSI/filesystem-layer)
wget https://github.com/EESSI/filesystem-layer/releases/download/v0.2.3/cvmfs-config-eessi-0.2.3-1.noarch.rpm
sudo yum install -y cvmfs-config-eessi-0.2.3-1.noarch.rpm

# create local CernVM-FS configuration file (direct access, no proxy; 10GB for CernVM-FS cache)
sudo bash -c "echo 'CVMFS_HTTP_PROXY=DIRECT' > /etc/cvmfs/default.local"
sudo bash -c "echo 'CVMFS_QUOTA_LIMIT=10000' >> /etc/cvmfs/default.local"

# set up CernVM-FS
sudo cvmfs_config setup

# access EESSI pilot repository
ls /cvmfs/pilot.eessi-hpc.org/2020.10
```

From zero to science in 3 steps

Step 1: Access the (pilot) EESSI CernVM-FS repository

Option 2 (example): use Singularity to run Docker container to access EESSI

```
# configure Singularity (bind mounts + home directory)
mkdir -p /tmp/$USER/{var-lib-cvmfs,var-run-cvmfs,home}
export SINGULARITY_BIND="/tmp/$USER/var-run-cvmfs:/var/run/cvmfs,/tmp/$USER/var-lib-cvmfs:/var/lib/cvmfs"
export SINGULARITY_HOME="/tmp/$USER/home:/home/$USER"

# values to pass to --fusemount (EESSI config + pilot repositories)
export EESSI_CONFIG="container:cvmfs2 cvmfs-config.eessi-hpc.org /cvmfs/cvmfs-config.eessi-hpc.org"
export EESSI_PILOT="container:cvmfs2 pilot.eessi-hpc.org /cvmfs/pilot.eessi-hpc.org"

# minimal Docker container from Docker Hub (includes CernVM-FS + EESSI configuration files)
export DOCKER_IMAGE="docker://eessi/client-pilot:centos7-$(uname -m)-2020.10"

# start shell in Singularity container (ignore the scary looking 'setxattr' warnings, they're harmless)
singularity shell --fusemount "$EESSI_CONFIG" --fusemount "$EESSI_PILOT" $DOCKER_IMAGE

# access EESSI pilot repository
ls /cvmfs/pilot.eessi-hpc.org/2020.10
```

From zero to science in 3 steps

Step 2: Set up your environment by sourcing the EESSI `init` script

```
# source the EESSI init script to set up your environment
$ source /cvmfs/pilot.eessi-hpc.org/2020.10/init/bash
Found EESSI pilot repo @ /cvmfs/pilot.eessi-hpc.org/2020.10!
Using x86_64/intel/haswell as software subdirectory.
Initializing Lmod...
Prepending /cvmfs/pilot.eessi-hpc.org/2020.10/software/x86_64/intel/haswell/modules/all to $MODULEPATH...

Environment set up to use EESSI pilot software stack, have fun!

[EESSI pilot 2020.10] $ echo $EESSI_PREFIX
/cvmfs/pilot.eessi-hpc.org/2020.10

[EESSI pilot 2020.10] $ echo $EESSI_SOFTWARE_SUBDIR
x86_64/intel/haswell
```

From zero to science in 3 steps

Step 3: Load the modules for the software you want to use, and go!

```
# check which modules are available
[EESSI pilot 2020.10] $ module avail gromacs

---------- /cvmfs/pilot.eessi-hpc.org/2020.10/software/x86_64/intel/haswell/modules/all ----------
   GROMACS/2020.1-foss-2020a-Python-3.8.2

# load the module(s) for the software you want to use
[EESSI pilot 2020.10] $ module load GROMACS

# ready to compute!
[EESSI pilot 2020.10] $ gmx mdrun -s ion_channel.tpr -maxh 0.50 -resethway -noconfout -nsteps 1000
```

Demo time!

https://github.com/EESSI/eessi-demo

Red Hat Enterprise Linux

debian

ubuntu

CentOS

Raspberry Pi cluster

Bioconductor

aws

GROMACS

CLUSTER IN THE CLOUD

OpenFOAM

Microsoft Azure

TensorFlow

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Isambard (XCI)

intel

AMD

ARM

Future work

- Further improve pilot EESSI repository (~ monthly revisions)
- Identify problems, and fix them...
- **Automate** deployment of different EESSI layers (Ansible, Terraform, ...)
- **Testing** (with ReFrame) + continuous integration in GitHub Actions
- Let developers of scientific software validate the installation of *their* software
- Also support macOS / POWER / GPUs, add more software
- Solicit more manpower, get project funded to make it sustainable
- Work towards production setup...

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Kenneth Hoste
kenneth.hoste@ugent.be
@kehoste (Twitter)

Website: https://www.eessi-hpc.org

Join our mailing list & Slack channel

https://www.eessi-hpc.org/join

Documentation: https://eessi.github.io/docs

GitHub: https://github.com/eessi

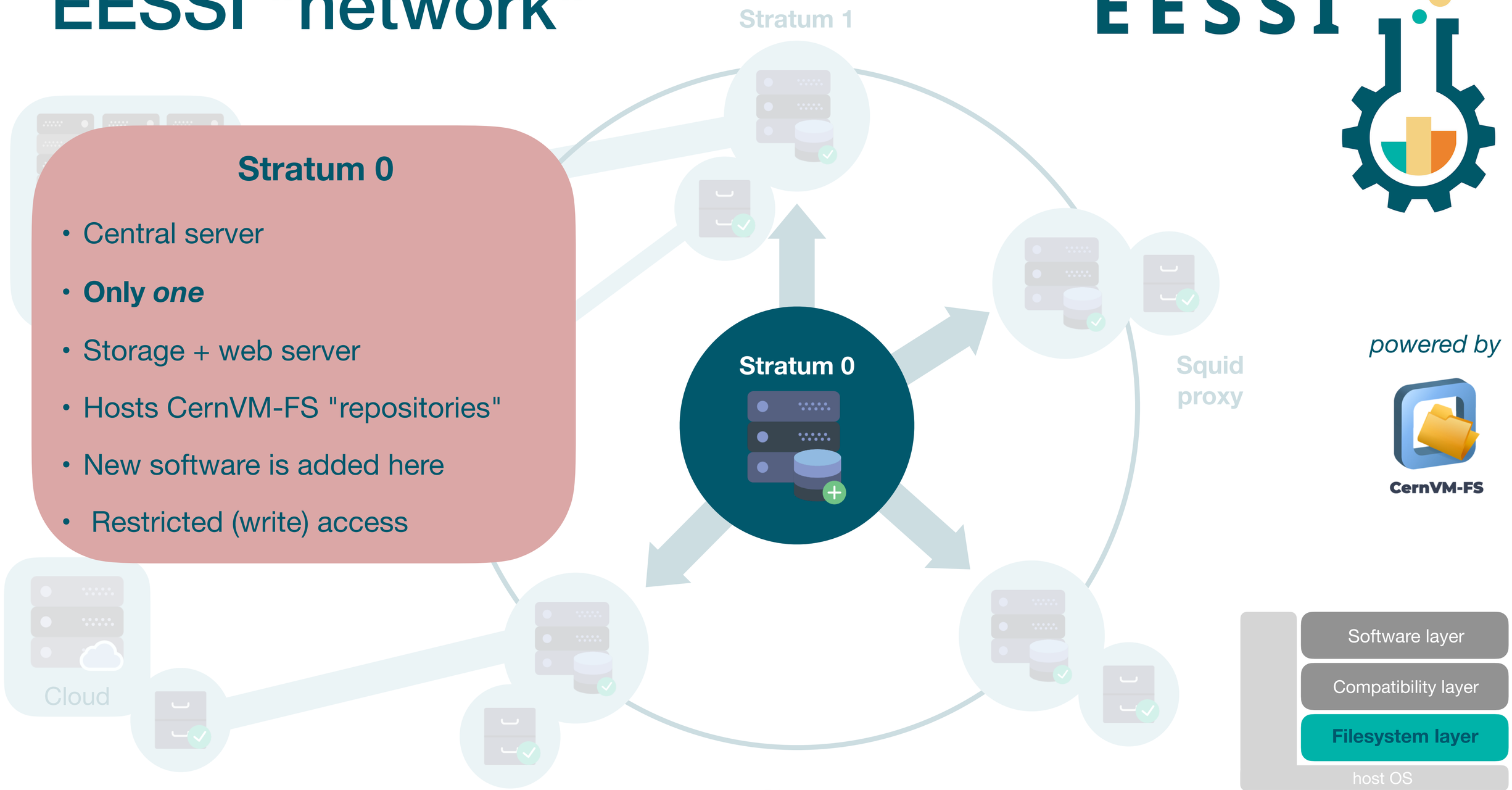
Twitter: @eessi_hpc

Monthly online meetings (first Thursday, 2pm CET)

(BACKUP SLIDES)

EESSI "network"

EESSI



Stratum 0

- Central server
- **Only *one***
- Storage + web server
- Hosts CernVM-FS "repositories"
- New software is added here
- Restricted (write) access

powered by

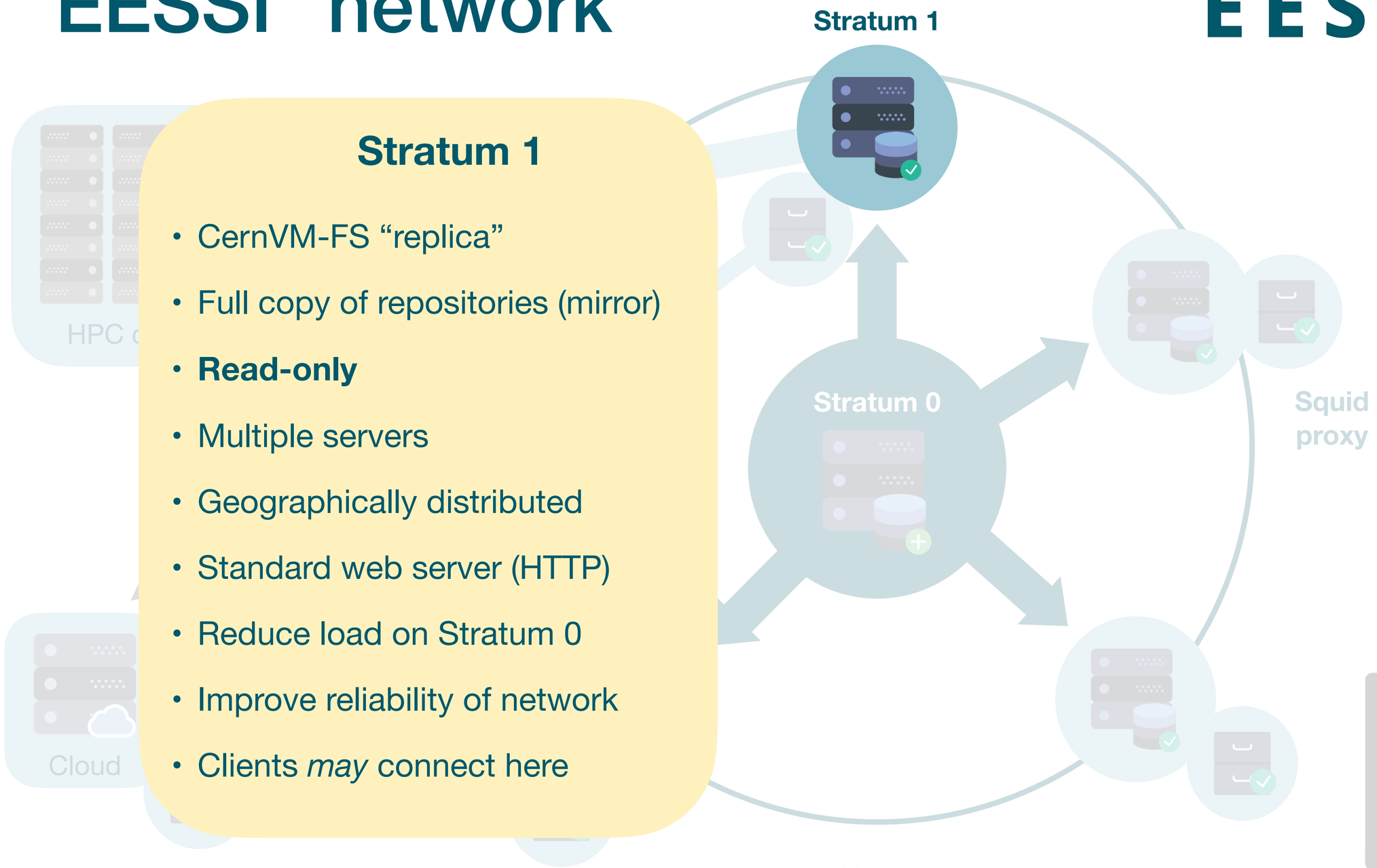
CernVM-FS

EESSI "network"

EESSI

Stratum 1

- CernVM-FS “replica”
- Full copy of repositories (mirror)
- **Read-only**
- Multiple servers
- Geographically distributed
- Standard web server (HTTP)
- Reduce load on Stratum 0
- Improve reliability of network
- Clients *may* connect here



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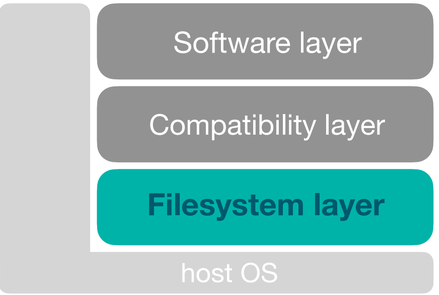
CernVM-FS



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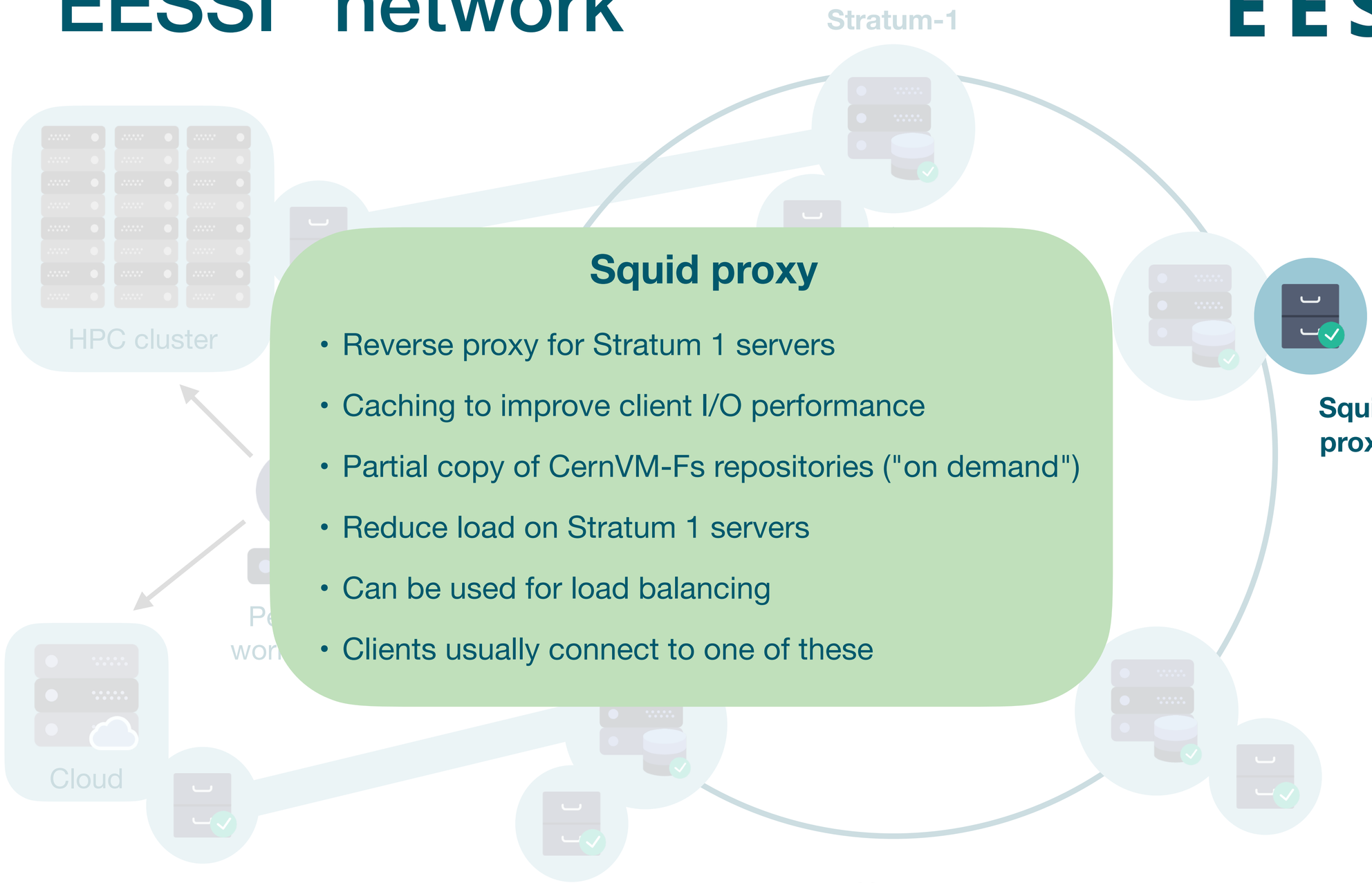

Squid proxy

- Reverse proxy for Stratum 1 servers
- Caching to improve client I/O performance
- Partial copy of CernVM-Fs repositories ("on demand")
- Reduce load on Stratum 1 servers
- Can be used for load balancing
- Clients usually connect to one of these

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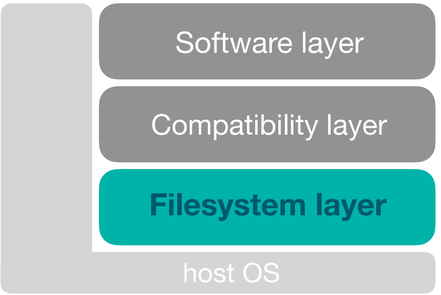
CernVM-FS



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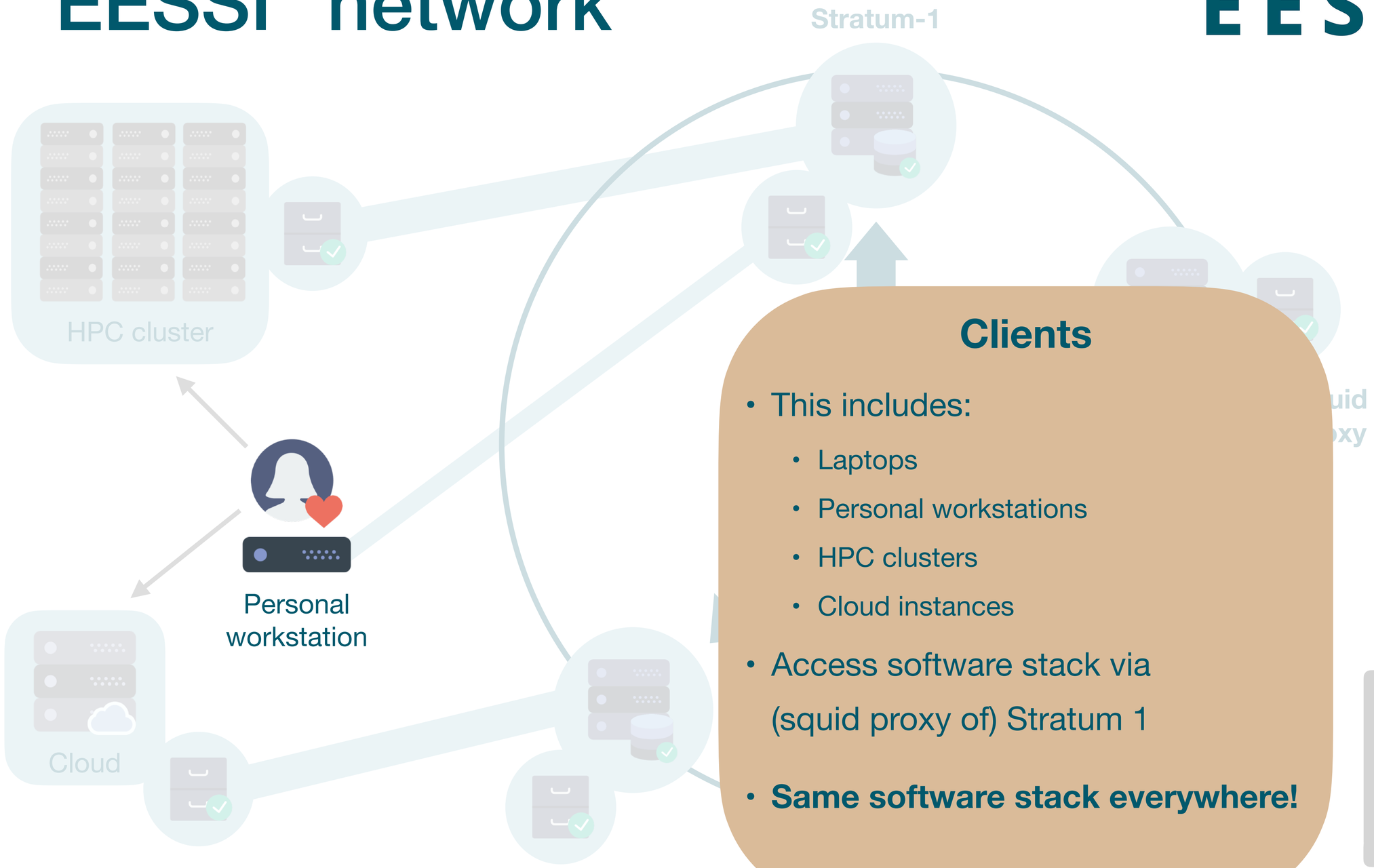
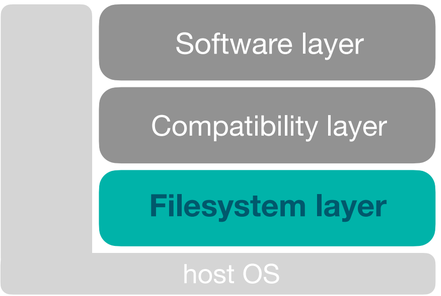


Clients

- This includes:
  - Laptops
  - Personal workstations
  - HPC clusters
  - Cloud instances
- Access software stack via (squid proxy of) Stratum 1
- **Same software stack everywhere!**

powered by

CernVM-FS



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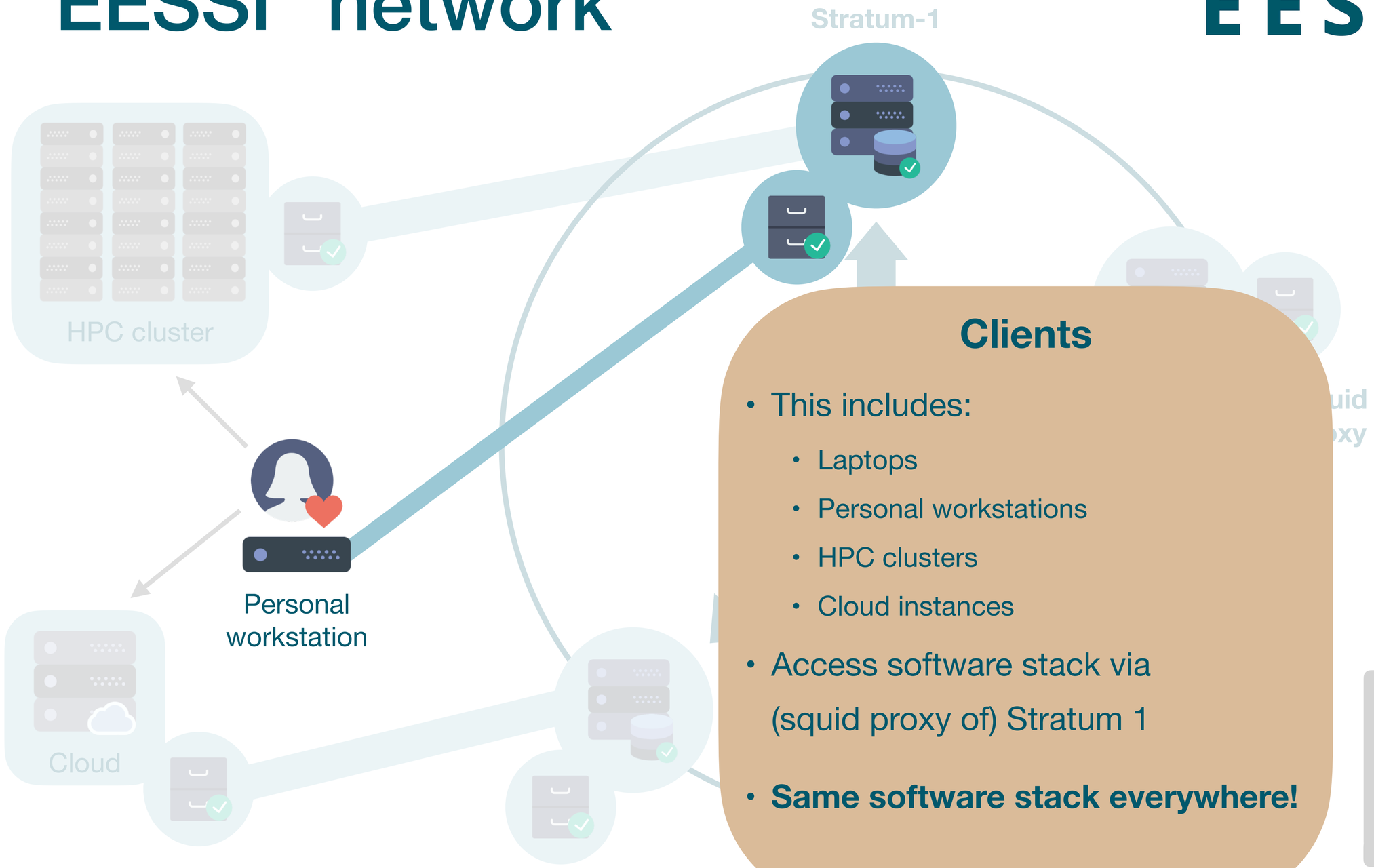

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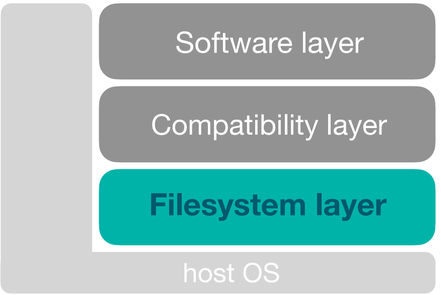

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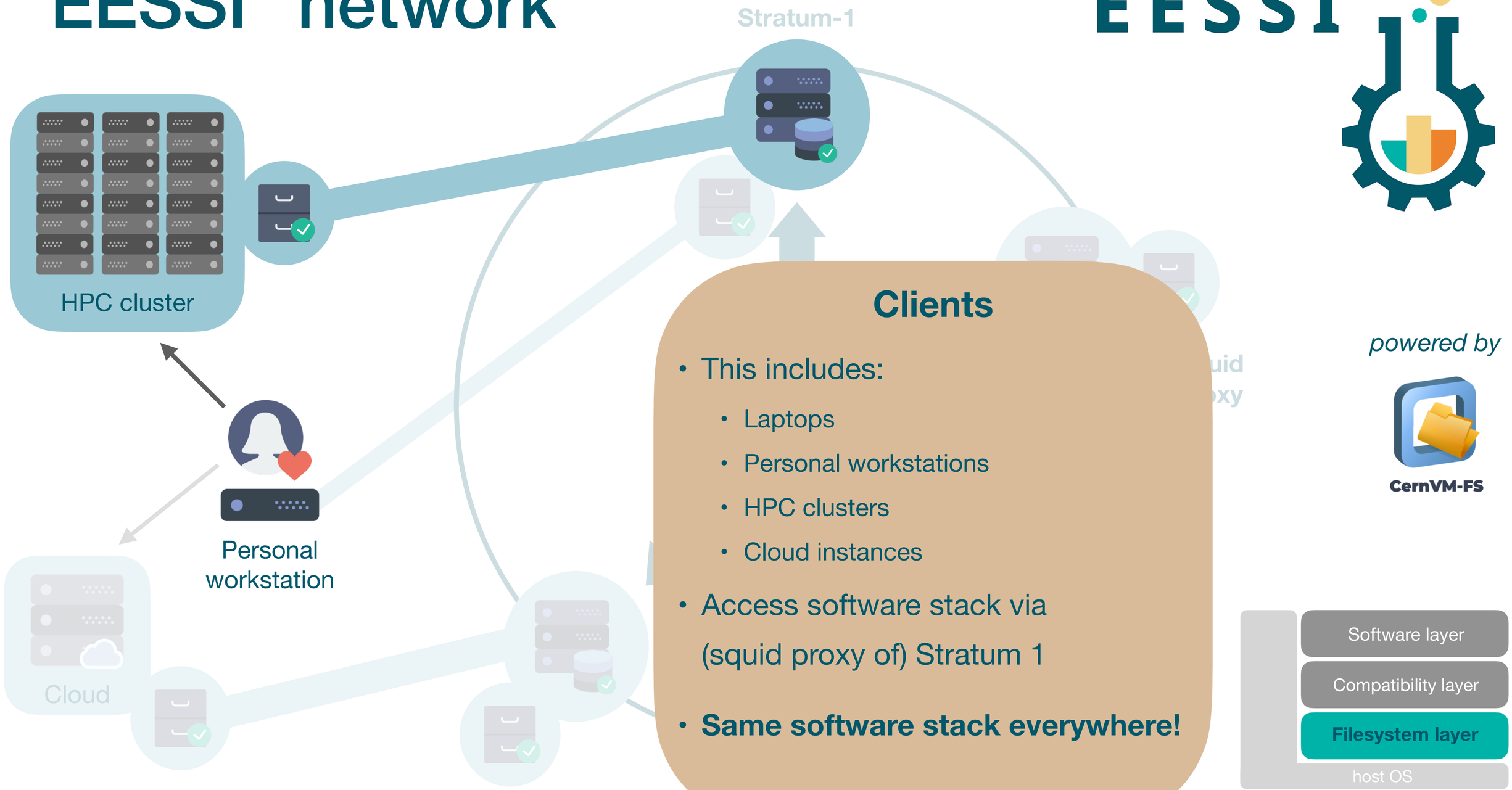

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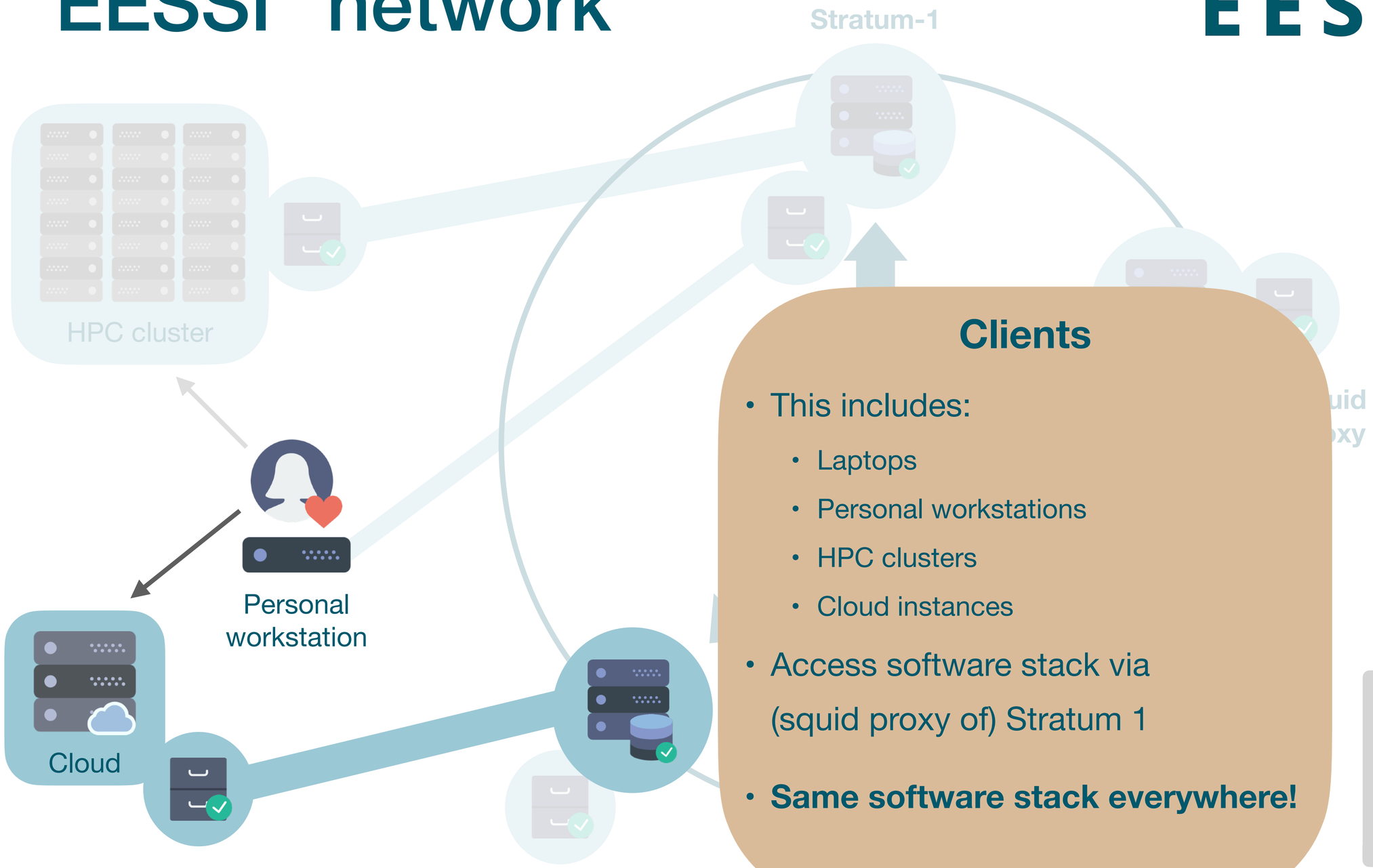
EESSI "network"

EESSI



Clients

- This includes:
  - Laptops
  - Personal workstations
  - HPC clusters
  - Cloud instances
- Access software stack via (squid proxy of) Stratum 1
- **Same software stack everywhere!**

powered by

CernVM-FS