FLAGSHIPS

Human Brain Project

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Which tools and services do the HPAC Platform (and Fenix) offer?

1st HPAC Platform Training, 11-12 Dec 2018

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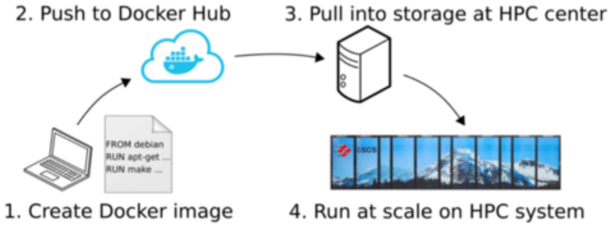
Alberto Madonna (CSCS)

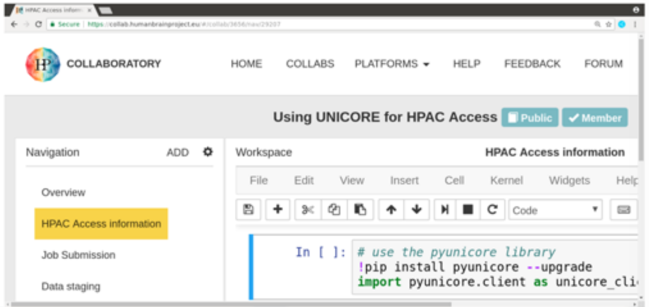
Overview of Services

Fenix/ICEI provides the Base Infrastructure for HPAC

- Support of user workflows
- Job Submission
- Data access
- Site-to-site Data Transfer
- Single sign-on to HPC Allocations
- Launch simulations and data analysis tasks from Jupyter notebooks
- Software deployment via Docker Containers

HPAC Infrastructure



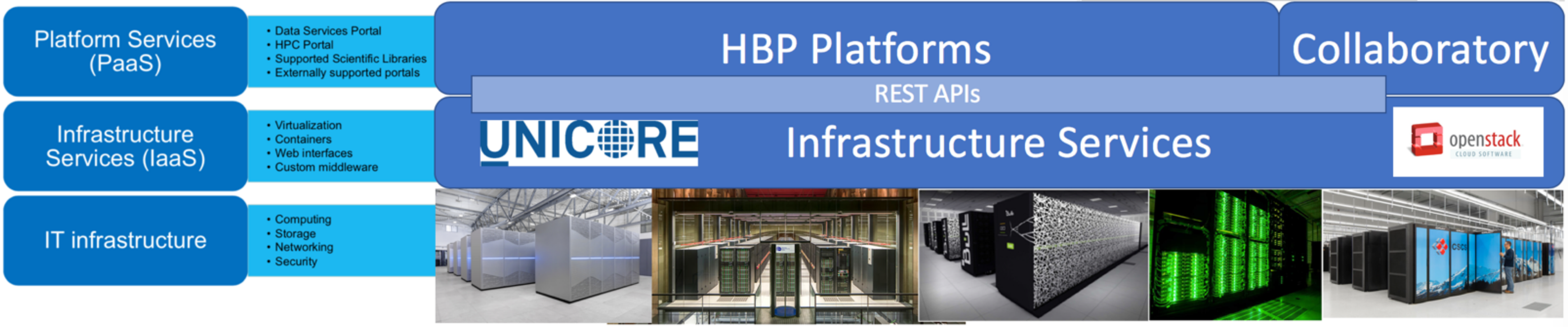


Using UNICORE for HPAC Access

HPAC Access information

- Overview
- HPAC Access information
- Job Submission
- Data staging

```
In [ ]: # use the pyunicore library
        !pip install pyunicore --upgrade
        import pyunicore.client as unicore_cli
```



Platform Services (PaaS)
- Data Services Portal
- HPC Portal
- Supported Scientific Libraries
- Externally supported portals

Infrastructure Services (IaaS)
- Virtualization
- Containers
- Web interfaces
- Custom middleware

IT infrastructure
- Computing
- Storage
- Networking
- Security

HBP Platforms

Collaboratory

REST APIs

UNICORE

Infrastructure Services

openstack CLOUD SOFTWARE

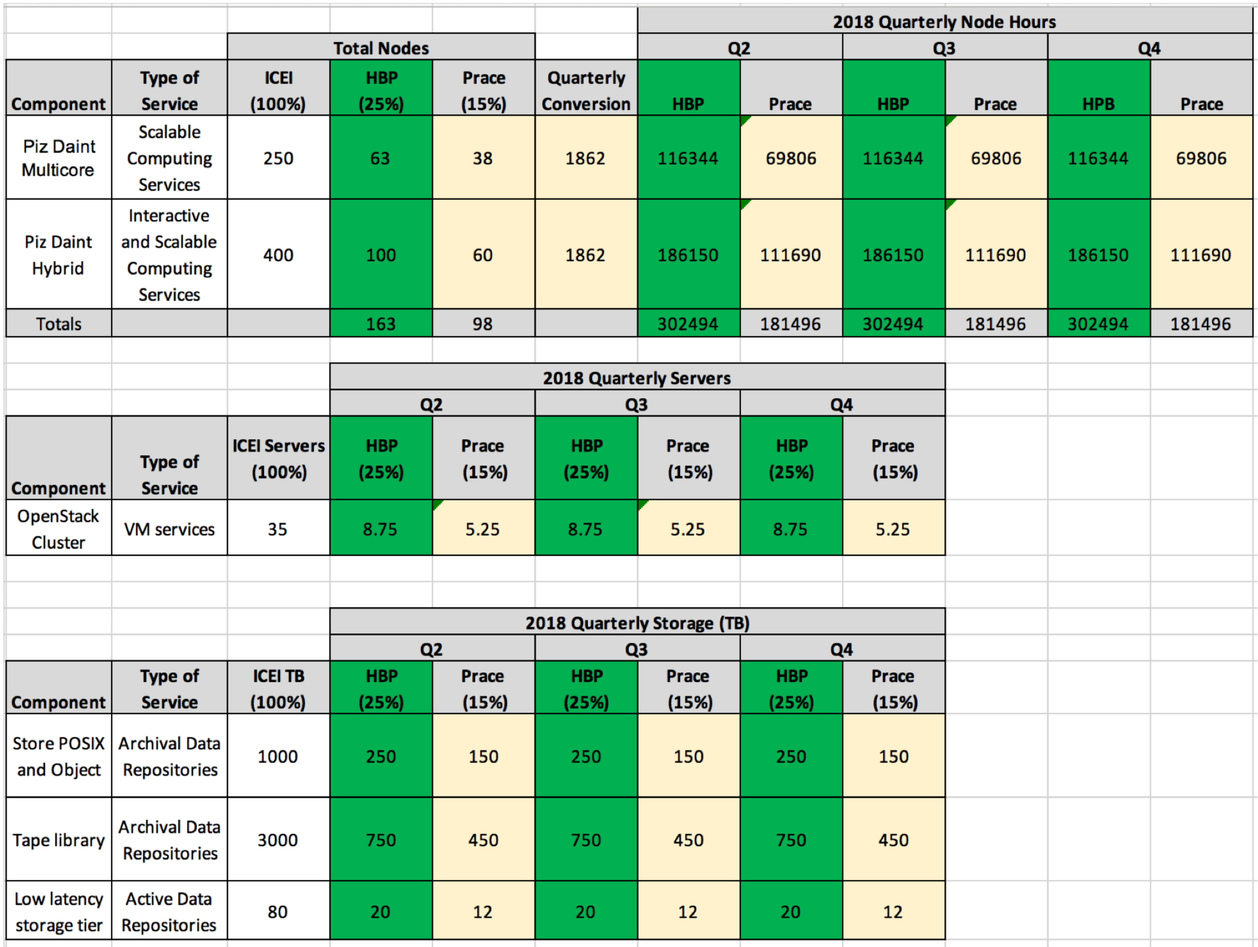
FENIX RESEARCH INFRASTRUCTURE · JÜLICH Forschungszentrum · Barcelona Supercomputing Center Centro Nacional de Supercomputación · cea · CINECA · CSCS Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre · ETHzürich

What Services does Fenix/ICEI provide?

- End-user Services
  - Scalable Compute Services
  - Interactive Compute Services
  - SWIFT Object Storage
  - Data Storage Services
  - (Data Transfer Service) ← HPAC
  - (Continuous Integration Services) ← HPAC
  - (Software Packaging and Deployment Services) ← HPAC
  - {Visualisation Services) ← HPAC
- Platform Services
  - Infrastructure Services (middleware access to HPC resources via RestAPIs)
  - Infrastructure as a Service (e.g. OpenStack) for Virtual Machine Services
  - Data Management Services
  - User and Resource Management Services
  - Service Accounts (currently not available at all sites)

ICEI Resources for HBP

- ICEI resources have already been made available to the HBP (highlighted in green) and PRACE by CSCS
- There are currently 8 HBP projects with compute allocations at CSCS
  - More are in the approval stages
- More resources are available than are being consumed so HBP users are encouraged to apply for a compute allocation
  - More on this in the next session



		Total Nodes				2018 Quarterly Node Hours					
						Q2		Q3		Q4	
Component	Type of Service	ICEI (100%)	HBP (25%)	Prace (15%)	Quarterly Conversion	HBP	Prace	HBP	Prace	HPB	Prace
Piz Daint Multicore	Scalable Computing Services	250	63	38	1862	116344	69806	116344	69806	116344	69806
Piz Daint Hybrid	Interactive and Scalable Computing Services	400	100	60	1862	186150	111690	186150	111690	186150	111690
Totals			163	98		302494	181496	302494	181496	302494	181496

			2018 Quarterly Servers					
			Q2		Q3		Q4	
Component	Type of Service	ICEI Servers (100%)	HBP (25%)	Prace (15%)	HBP (25%)	Prace (15%)	HBP (25%)	Prace (15%)
OpenStack Cluster	VM services	35	8.75	5.25	8.75	5.25	8.75	5.25

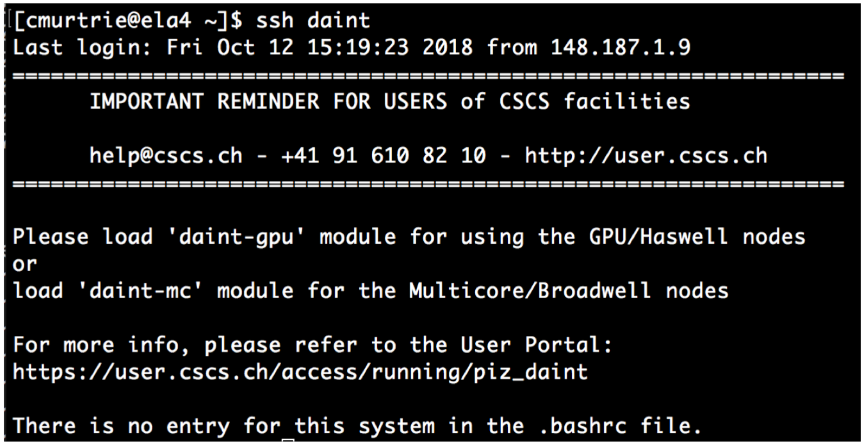
			2018 Quarterly Storage (TB)					
			Q2		Q3		Q4	
Component	Type of Service	ICEI TB (100%)	HBP (25%)	Prace (15%)	HBP (25%)	Prace (15%)	HBP (25%)	Prace (15%)
Store POSIX and Object	Archival Data Repositories	1000	250	150	250	150	250	150
Tape library	Archival Data Repositories	3000	750	450	750	450	750	450
Low latency storage tier	Active Data Repositories	80	20	12	20	12	20	12

How do I use ICEI Resources? (1)

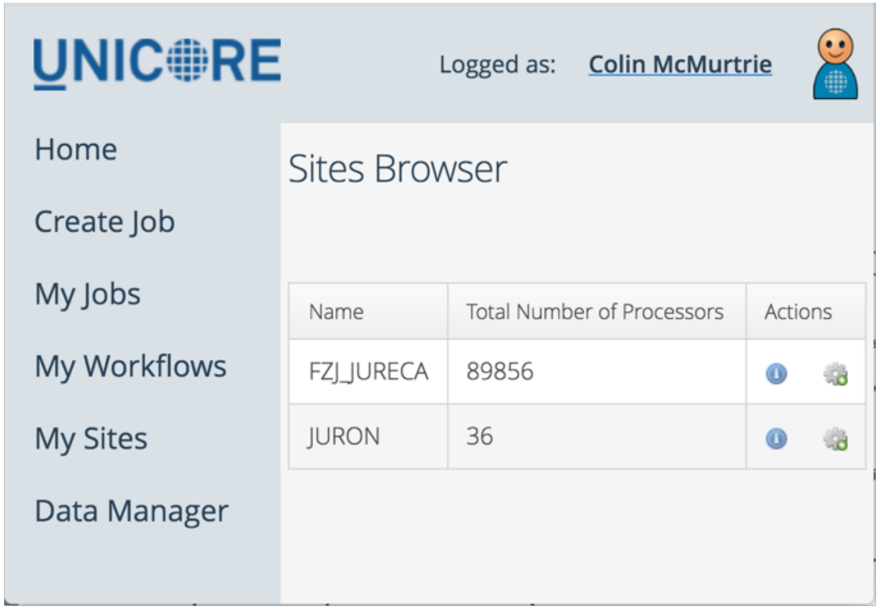
Scalable Compute Resources:

The *Piz Daint* system is available as a state-of-the-art scalable compute resource for use by HBP users

- Accessible globally via Command-line Interface
- Via the Unicore GUI
- Via the RESTful API offered via UNICORE for platforms
  - Use of Service Accounts for Platforms is also acceptable at some sites (e.g. CSCS)
  - See next slide for some more details



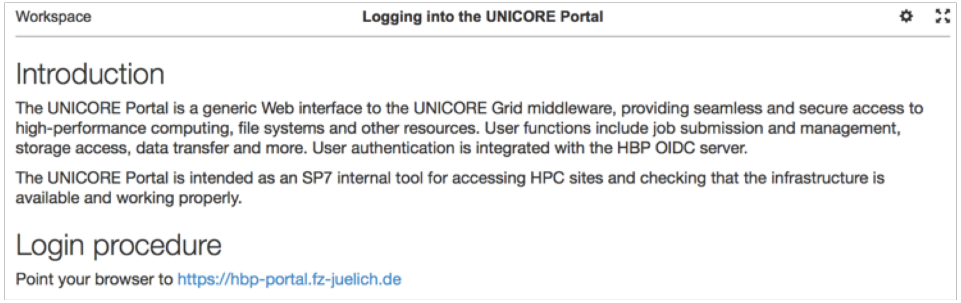
```
[cmurtrie@ela4 ~]$ ssh daint
Last login: Fri Oct 12 15:19:23 2018 from 148.187.1.9
==================================================================
      IMPORTANT REMINDER FOR USERS of CSCS facilities

      help@cscs.ch - +41 91 610 82 10 - http://user.cscs.ch
==================================================================

Please load 'daint-gpu' module for using the GPU/Haswell nodes
or
load 'daint-mc' module for the Multicore/Broadwell nodes

For more info, please refer to the User Portal:
https://user.cscs.ch/access/running/piz_daint

There is no entry for this system in the .bashrc file.
```



Logged as: Colin McMurtrie

Sites Browser

Name	Total Number of Processors	Actions
FZJ_JURECA	89856	ⓘ ⚙
JURON	36	ⓘ ⚙



Logging into the UNICORE Portal

Introduction

The UNICORE Portal is a generic Web interface to the UNICORE Grid middleware, providing seamless and secure access to high-performance computing, file systems and other resources. User functions include job submission and management, storage access, data transfer and more. User authentication is integrated with the HBP OIDC server.

The UNICORE Portal is intended as an SP7 internal tool for accessing HPC sites and checking that the infrastructure is available and working properly.

Login procedure

Point your browser to https://hbp-portal.fz-juelich.de

How do I use ICEI Resources? (2)

Interactive Compute Resources:

The *Piz Daint* system supports the use of Jupyter Notebooks for interactive supercomputing, powered by JupyterHub

- This is a multi-user Hub that spawns, manages and proxies multiple instances of the single-user Jupyter notebook server
  - More details below
- Sessions later in the day will demonstrate the use of this environment

Piz Daint and other HPAC HPC systems are also accessible from the Jupyter Notebooks service of the *Collaboratory*

- This relies on the RESTful API offered via UNICORE for platforms
- The session later this morning will go into the details of how to do this

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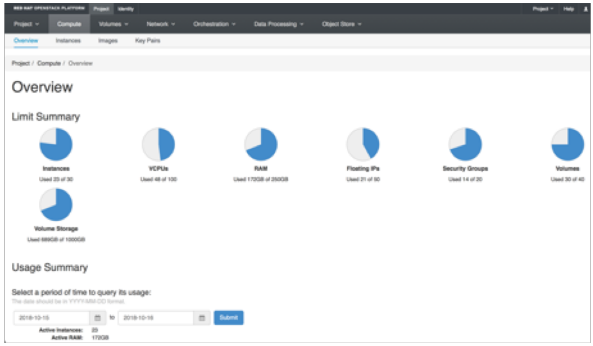
How do I use ICEI Resources? (4)

***Pollux* OpenStack IaaS:**

The *Pollux* OpenStack IaaS is available to host your platform VMs:

- Accessible globally via the Horizon GUI interface
- RESTful API can be used for automation



Overview

Limit Summary

Instances	VCPUs	RAM	Floating IPs	Security Groups	Volumes	Volume Storage
Used 23 of 30	Used 48 of 100	Used 172GB of 250GB	Used 21 of 50	Used 14 of 20	Used 30 of 40	Used 689GB of 1000GB

Usage Summary

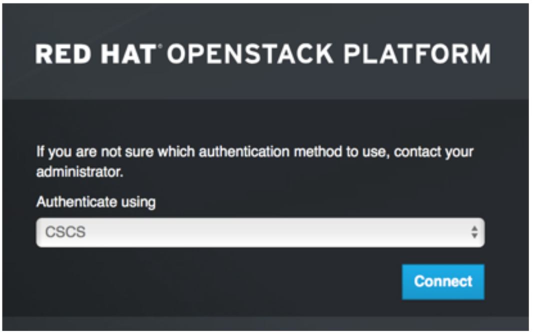
Select a period of time to query its usage:

The date should be in YYYY-MM-DD format.

2018-10-15 to 2018-10-16 Submit

Active Instances: 23

Active RAM: 172GB

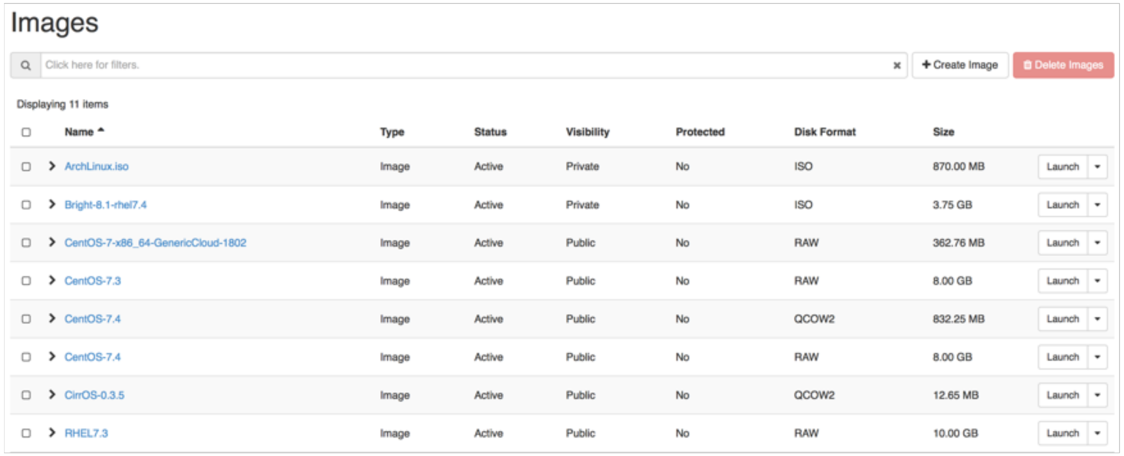


RED HAT OPENSTACK PLATFORM

If you are not sure which authentication method to use, contact your administrator.

Authenticate using: CSCS

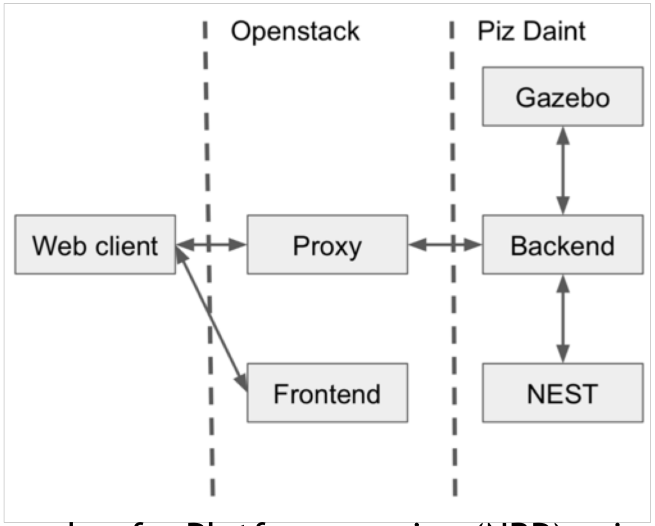
Connect



Images

Displaying 11 items

□	Name	Type	Status	Visibility	Protected	Disk Format	Size	
□	ArchLinux.iso	Image	Active	Private	No	ISO	870.00 MB	Launch
□	Bright-8.1-rhel7.4	Image	Active	Private	No	ISO	3.75 GB	Launch
□	CentOS-7-x86_64-GenericCloud-1802	Image	Active	Public	No	RAW	362.76 MB	Launch
□	CentOS-7.3	Image	Active	Public	No	RAW	8.00 GB	Launch
□	CentOS-7.4	Image	Active	Public	No	QCOW2	832.25 MB	Launch
□	CentOS-7.4	Image	Active	Public	No	RAW	8.00 GB	Launch
□	CirrOS-0.3.5	Image	Active	Public	No	QCOW2	12.65 MB	Launch
□	RHEL7.3	Image	Active	Public	No	RAW	10.00 GB	Launch



Example of a Platform service (NRP) using VMs AND HPC resources.

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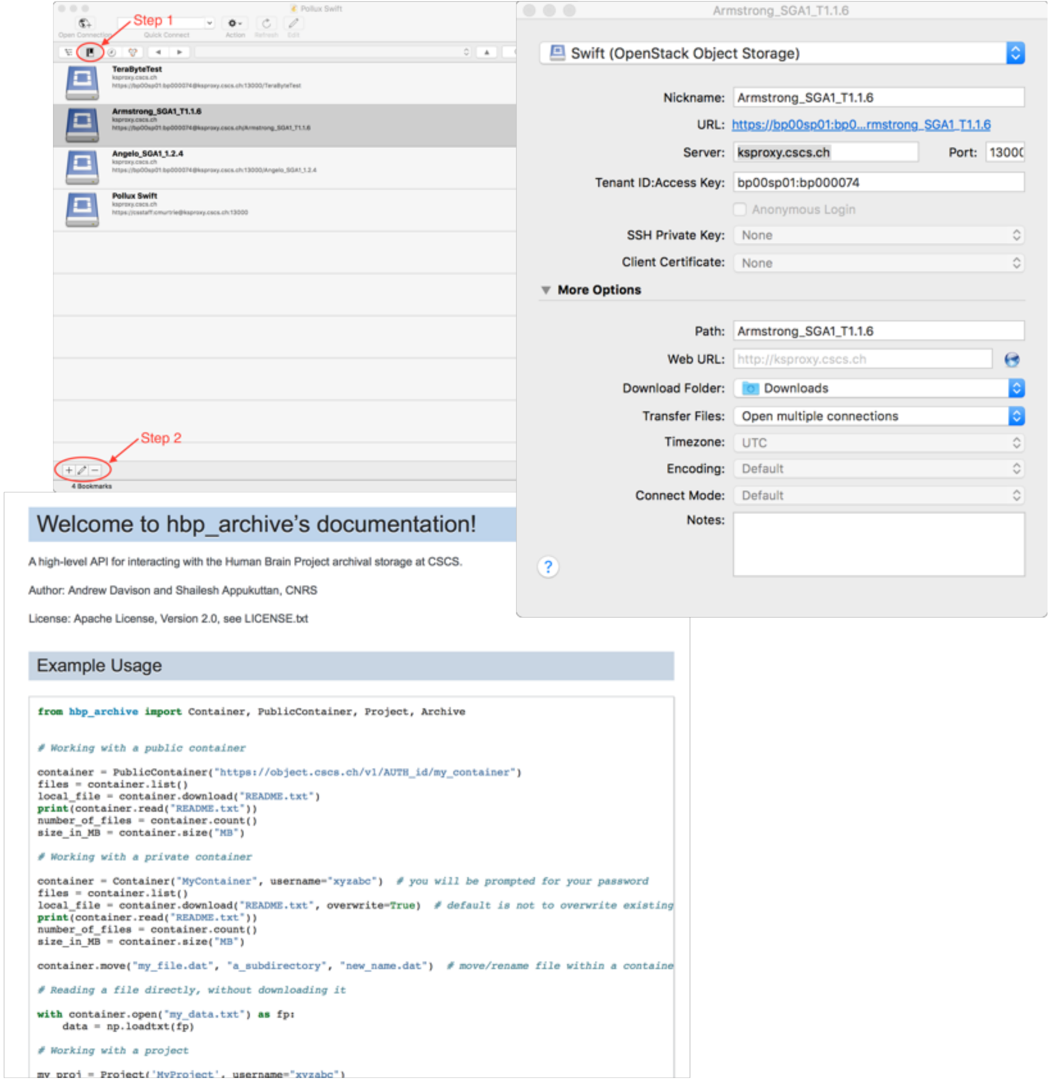
How do I use ICEI Resources? (3)

Swift Object Storage:
SWIFT OS can be accessed directly from your personal computer

- GUI clients e.g. CyberDuck
- SP5 Python Library
  - Better for mgmt. of the ACLs and Object Buckets
  - https://hbp-archive.readthedocs.io/en/latest/

Reachable from inside the *Collaboratory*

- Get/Put from Jupyter Notebooks
- More capabilities coming soon



TeraByteTest
ksproxy.cscs.ch
https://bp00sp01:bp000074@ksproxy.cscs.ch:13000/TeraByteTest

Armstrong_SGA1_T1.1.6
ksproxy.cscs.ch
https://bp00sp01:bp000074@ksproxy.cscs.ch/Armstrong_SGA1_T1.1.6

Angelo_SGA1_1.2.4
ksproxy.cscs.ch
https://bp00sp01:bp000074@ksproxy.cscs.ch:13000/Angelo_SGA1_1.2.4

Pollux Swift
ksproxy.cscs.ch
https://csstaff:cmurtrie@ksproxy.cscs.ch:13000

Armstrong_SGA1_T1.1.6

Swift (OpenStack Object Storage)

Nickname: Armstrong_SGA1_T1.1.6
URL: https://bp00sp01:bp0...rmstrong_SGA1_T1.1.6
Server: ksproxy.cscs.ch Port: 13000
Tenant ID:Access Key: bp00sp01:bp000074
□ Anonymous Login
SSH Private Key: None
Client Certificate: None

▼ More Options

Path: Armstrong_SGA1_T1.1.6
Web URL: http://ksproxy.cscs.ch
Download Folder: Downloads
Transfer Files: Open multiple connections
Timezone: UTC
Encoding: Default
Connect Mode: Default
Notes:

Welcome to hbp_archive's documentation!

A high-level API for interacting with the Human Brain Project archival storage at CSCS.

Author: Andrew Davison and Shailesh Appukuttan, CNRS

License: Apache License, Version 2.0, see LICENSE.txt

Example Usage

```
from hbp_archive import Container, PublicContainer, Project, Archive


# Working with a public container

container = PublicContainer("https://object.cscs.ch/v1/AUTH_id/my_container")
files = container.list()
local_file = container.download("README.txt")
print(container.read("README.txt"))
number_of_files = container.count()
size_in_MB = container.size("MB")

# Working with a private container

container = Container("MyContainer", username="xyzabc")  # you will be prompted for your password
files = container.list()
local_file = container.download("README.txt", overwrite=True)  # default is not to overwrite existing
print(container.read("README.txt"))
number_of_files = container.count()
size_in_MB = container.size("MB")

container.move("my_file.dat", "a_subdirectory", "new_name.dat")  # move/rename file within a containe

# Reading a file directly, without downloading it

with container.open("my_data.txt") as fp:
    data = np.loadtxt(fp)

# Working with a project

my_proj = Project('MyProject', username="xyzabc")
```

How do I use ICEI Resources? (3)

Active Data Repositories:

- Come as part of the with the compute allocation (= $SCRATCH)
- Low-latency storage tier (Cray DataWarp with SSDs) in *Piz Daint* can also be requested

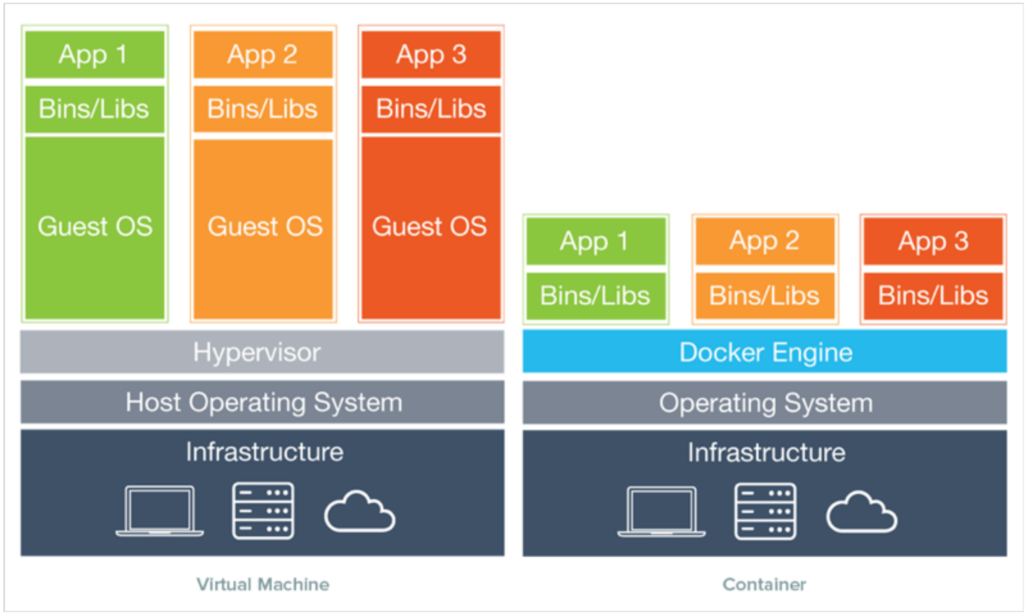
Archival Data Repositories:

- Are available either as part of a computing request (your proposal should state how much you need)
- Separately in a data-storage only use case (in which case a separate proposal is needed)

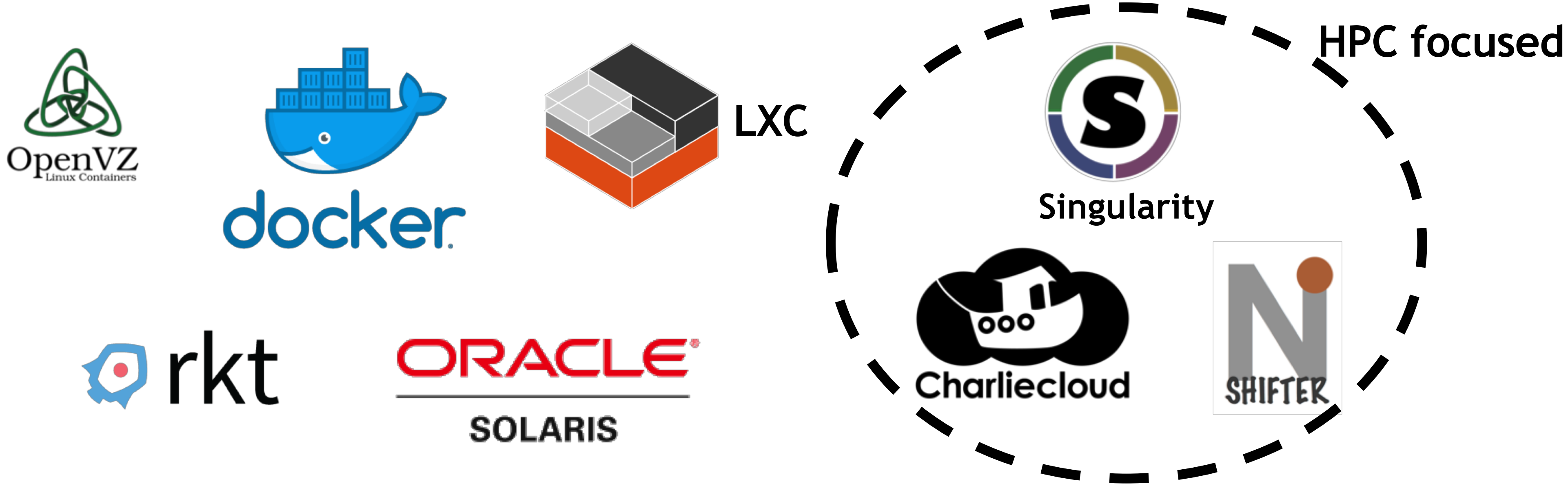
Service Detail: Software Packaging and Deployment

Containers

- Lightweight, isolated environments to run applications/services
- Already include all software dependencies
- Interest from HPC: a way to provide user-defined software stacks



Container implementations



Docker

- Extremely popular container implementation

- Easy to use authoring tools
  - Container images are created from recipe-like files
  - Images can be named, tagged and built on top of other images

- Cloud-based image distribution strategy
  - Several remote registries available (e.g. Docker Hub)
  - Client includes facilities to authenticate, push and pull images

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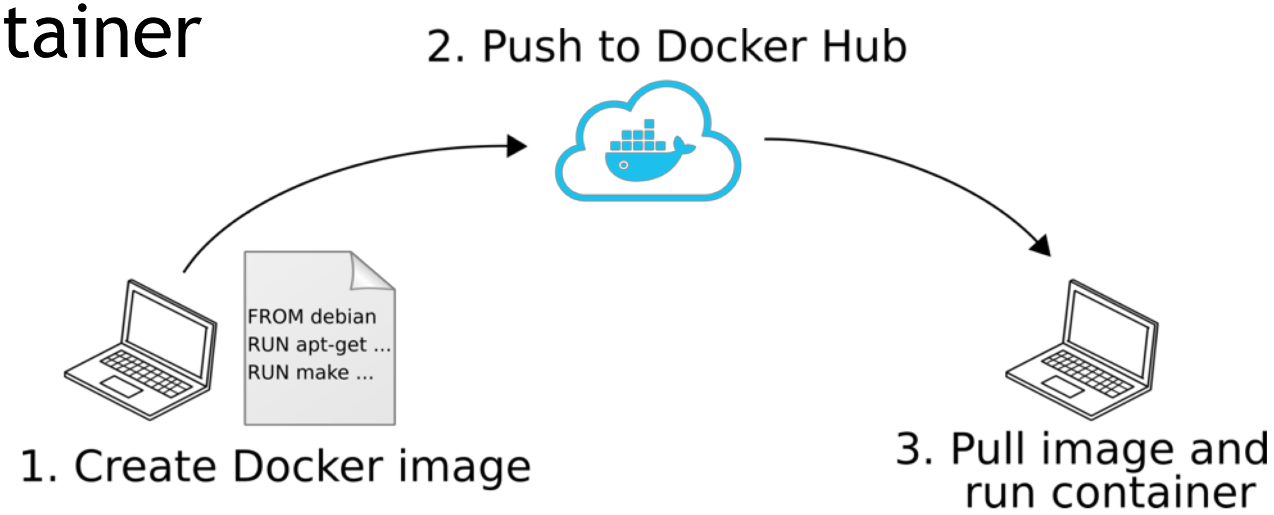
Docker workflow

1. An image is created locally from a *Dockerfile*
2. Push (i.e. upload) the image to a remote registry
   - DockerHub is the public registry maintained from the Docker company
3. Pull (i.e. download) the image on a target machine and run the container



2. Push to Docker Hub

```
FROM debian
RUN apt-get ...
RUN make ...
```

1. Create Docker image

3. Pull image and run container

Key terms

- **Image**: standalone, executable package that includes everything needed to run a piece of software
  - code, runtime libraries, environment variables, configuration files

- **Container**: runtime *instance* of an image
  - What the image becomes in memory when actually executed
  - Runs completely isolated from the host environment by default
    - only accessing host resources if configured to do so

So… how are containers useful?

Containers give the possibility to create (scientific) applications that are:

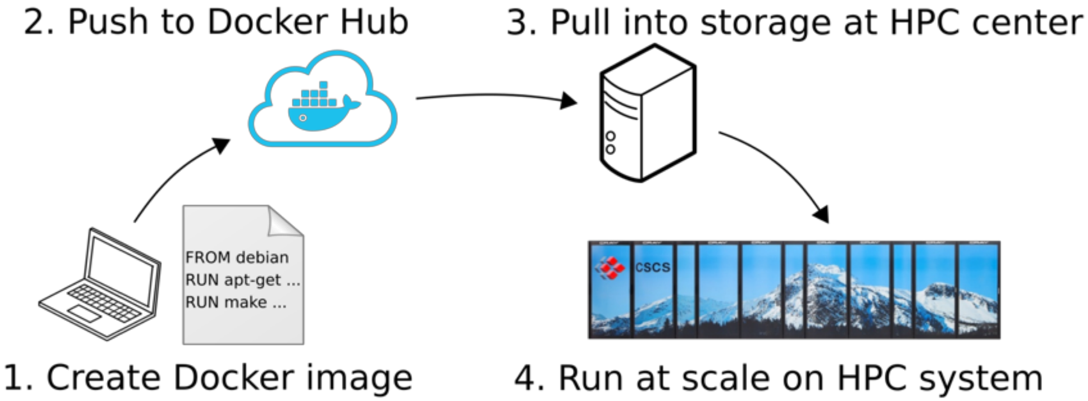
1. Portable
2. Reproducible
3. Easy to deploy
4. Easy to test

Unfortunately Docker containers are not a panacea for HPC environments because of:

- ➢ Security concerns
  - root in the container means root on shared parallel file systems
- ➢ Performance Portability
  - Performance is important in HPC (it’s in the name…)

Shifter

- Shifter is a *Docker-compatible* container platform specifically developed for HPC and addressing:
  - Security
  - Accounting
  - Native performance from custom HPC hardware
  - Integration with site infrastructure
- Enables flexible and convenient user workflows:



2. Push to Docker Hub

3. Pull into storage at HPC center

```
FROM debian
RUN apt-get ...
RUN make ...
```

1. Create Docker image

4. Run at scale on HPC system

Shifter development @ CSCS

- The Infrastructure & Development Services group works on extending Shifter with a focus on:
  - Usability
  - Features
  - Performance
- Previous work:
  - Native GPU support: automatic import of host's CUDA driver and devices
  - Native MPI support
    - Transparently swap container's MPI libraries with the host's at runtime
    - Enables full performance from vendor-specific implementations (e.g. Infiniband, Cray Aries)
    - Relies on MPICH ABI compatibility (http://www.mpich.org/abi/)

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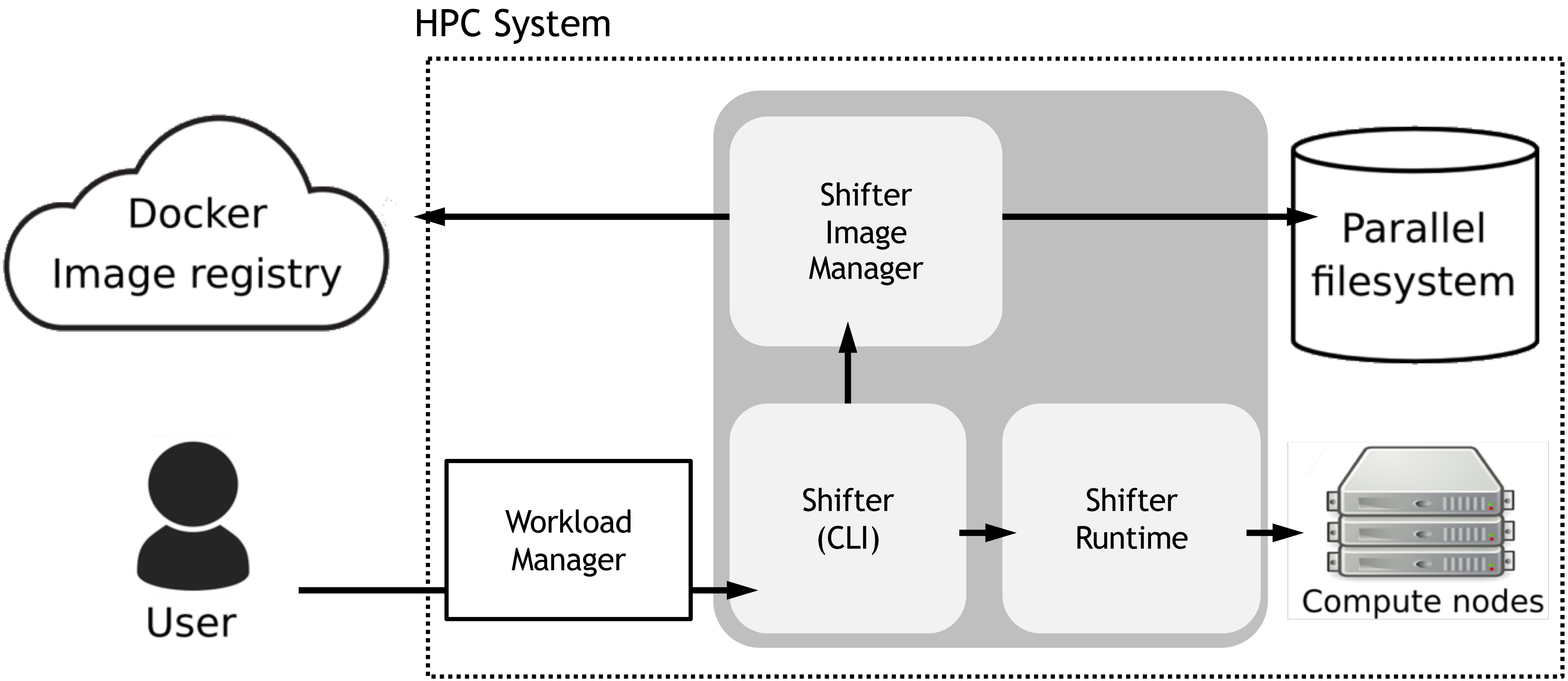
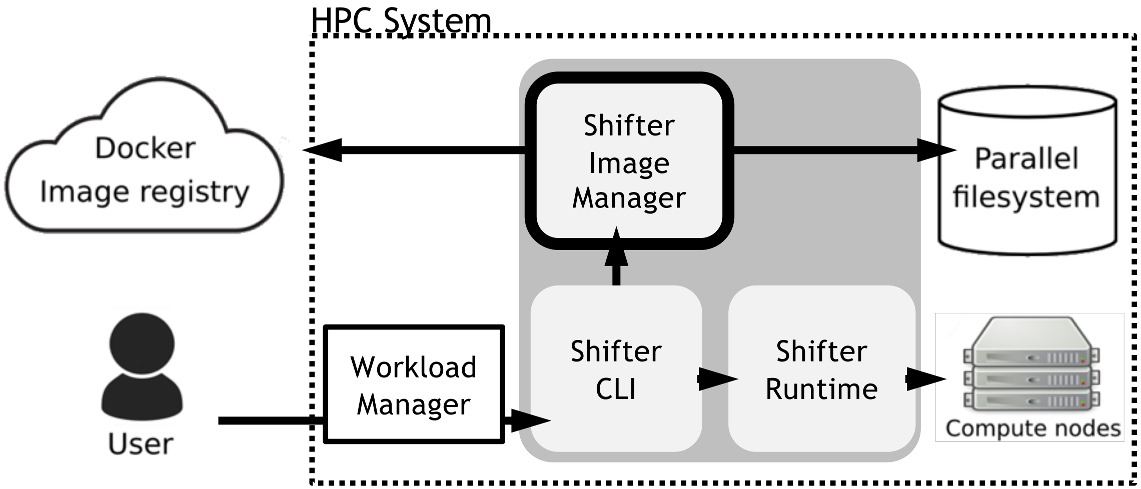
Shifter development @ CSCS – (cont.)

- Software Architecture
  - Single executable, no background service
  - Image Manager component: robust, fast, designed from scratch
- Docker-like command line interface
- Improved container customization
  - User-specified mounts
  - “Writable volatile” directories

Shifter Architecture – CSCS branch



Shifter Image Manager



- Container image management component written in C++
- Pull/query/remove images in **user owned** repositories
- **Import** images from tar files
- Parallel and robust layer download
  - automatic retry in case of errors
- Improved image expansion and local filesystem use

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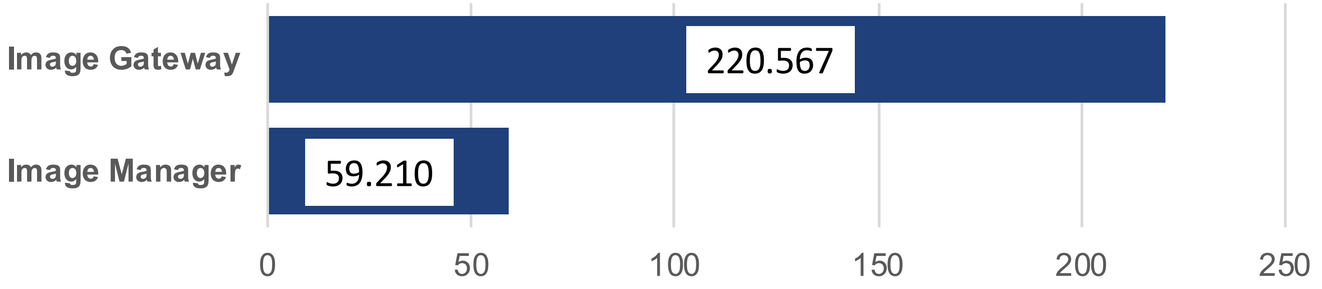
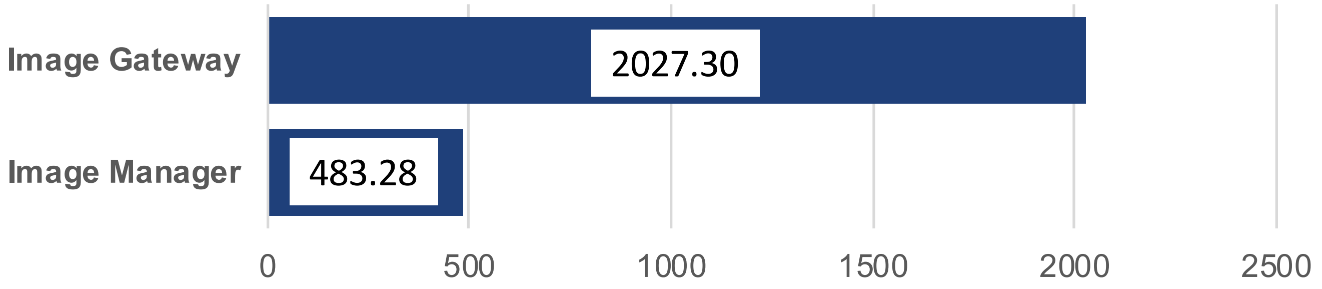
Image Manager performance



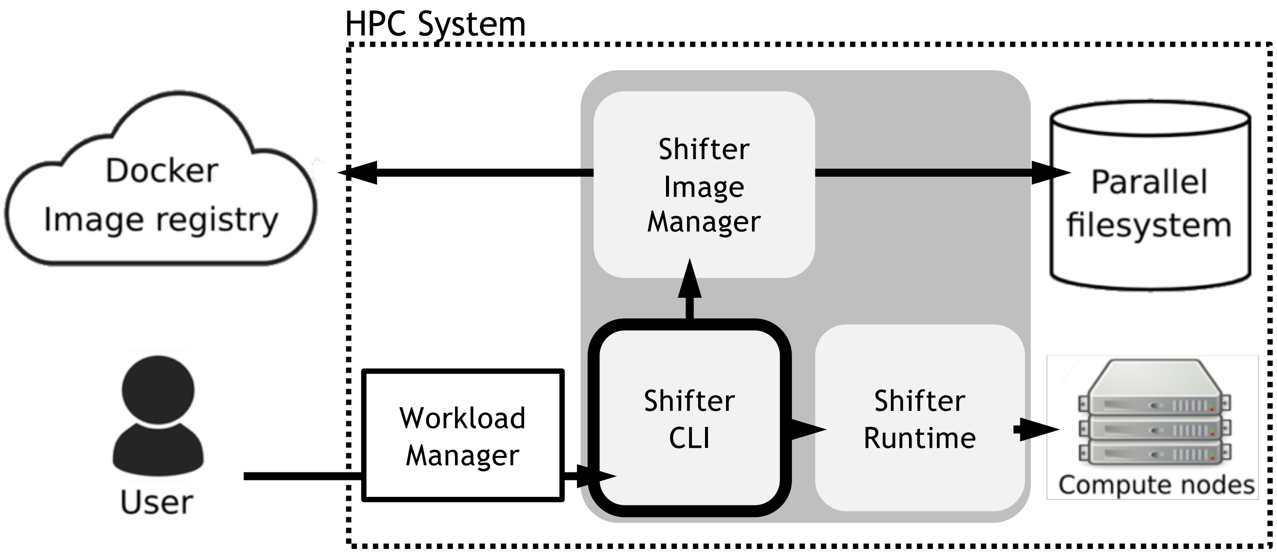
- Image: NVIDIA CUDA 8.0 Toolkit on CentOS 7 (official image)
- Size on Docker Hub: 1 GB (6 layers)
- Total speedup: **3.73x**

Image Manager performance



- Image: Microsoft Cognitive Toolkit (CNTK) custom build
- Size on Docker Hub: 6 GB (32 layers)
- Speedup: **4.20x**

Shifter CLI



- Command line processing component
- Goal was providing an in interface as close as possible to Docker
  - Consistent experience
  - Smoother transition between platforms

CLI comparison

- Shifter

```
# run container
$ shifter run [options] <image>[<:tag>]
<args>

# pull image
$ shifter pull [options] <image>[<:tag>]

# show list of images
$ shifter images

# remove image
$ shifter rmi <image>[<:tag>]

# import image
$ shifter import [options] <file> <image>
```

- Docker

```
# run container
$ docker run [options] <image>[<:tag>]
<args>

# pull image
$ docker pull [options] <image>[<:tag>]

# show list of images
$ docker images [options] [repo[<:tag>]]

# remove image
$ docker rmi [options] <image> [image…]

# import image
$ docker import [options] <file>|<URL>|-
```

Support for private & 3rd party registries

- Authentication option for private registries (`--login`)

```
$ shifter pull user/privateRepo:tag --login
username  : user
password  :
…
```

- Support for 3rd party registry services
  - `$ shifter pull <server>/<namespace>/<image><:tag>`
  - e.g. NVIDIA GPU Cloud

```
$ shifter pull nvcr.io/nvidia/caffe:17.12 --login
username  : $oauthtoken
password  :
…
```

Shifter Import

- Import image from a tar file created by `docker save`
- Deploy an image to the HPC system without using the cloud

```
$ shifter import ./debian.tar my_debian

 > expand image layers ...
 > extracting     :
/tmp/debian.tar/7e5c6402903b327fc62d1144f247c91c8e85c6f7b64903b8be289828285d502e/layer.tar
 > make squashfs ...
 > create metadata ...
 # created: <user dir>/.shifter/images/import/library/my_debian/latest.squashfs
 # created: <user dir>/.shifter/images/import/library/my_debian/latest.meta
```

Container customizations

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User-specified Mounts

- Map some paths from the Host to another location within the container
- Requested at launch time with the `--mount` option
- Reproduces the same option syntax from Docker

```
$ ls -l /data
 -rw-r--r--.  1 root root 1048576 Feb  7 10:49 data1.csv
 -rw-r--r--.  1 root root 1048576 Feb  7 10:49 data2.csv

$ shifter run --mount=type=bind,source=/data,destination=/input debian bash

[user@container]$ ls –l /input
 -rw-r--r--. 1 root 0 1048576 Feb  7 10:49 data1.csv
 -rw-r--r--. 1 root 0 1048576 Feb  7 10:49 data2.csv
```

Writable volatile directories

- Directories originating from the container image are mounted as read-only
- Some use cases have specific requirements (e.g. create file in `/var/lock`)
- The `--writable-volatile` option of `shifter run` can be used to make such directories writable
- Original contents of the directory keep owners and permissions, but it is possible to create new files and work with them (thus, *"writable"*)
- Any modification made to the directory is lost when the container exits (thus, *"volatile")*

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Writable volatile directories

```
$ shifter run --writable-volatile=/usr/local debian bash

[user@container]$ ls –l /usr
 drwxr-xr-x  2 root                   0 3560 Oct  9 00:00 bin/
 drwxr-xr-x  2 root                   0    3 Jul 13 13:01 games/
 drwxr-xr-x  2 root                   0    3 Jul 13 13:01 include/
 drwxr-xr-x 20 root                   0  324 Oct  9 00:00 lib/
 drwx------ 10 <user name>  <group name>  105 Oct  9 00:00 local/
 drwxr-xr-x  2 root                   0  961 Oct  9 00:00 sbin/
 drwxr-xr-x 41 root                   0  670 Oct  9 00:00 share/
 drwxr-xr-x  2 root                   0    3 Jul 13 13:01 src/

[user@container]$ echo "Hello world" > /usr/local/hello.txt
[user@container]$ ls –l /usr/local/
 ...
 -rw-r--r-- 1 <user name>  <group name> 12 Dec 19 15:18 hello.txt
 ...

[user@container]$ cat /usr/local/hello.txt
 Hello world
```

Wrap-up

- Improved deployment and operation
  - Simpler architecture
  - Streamlined build/installation process
  - No background service
- Improved user experience
  - Docker-like CLI for a more consistent workflow
  - Robust, faster image pulling
  - Import images bypassing the cloud
  - Support private and 3rd party repositories
  - User owned image repositories improve privacy
  - Mount custom directories in the container
  - Writable volatile directories
- More information available at
  - https://user.cscs.ch/tools/containers/

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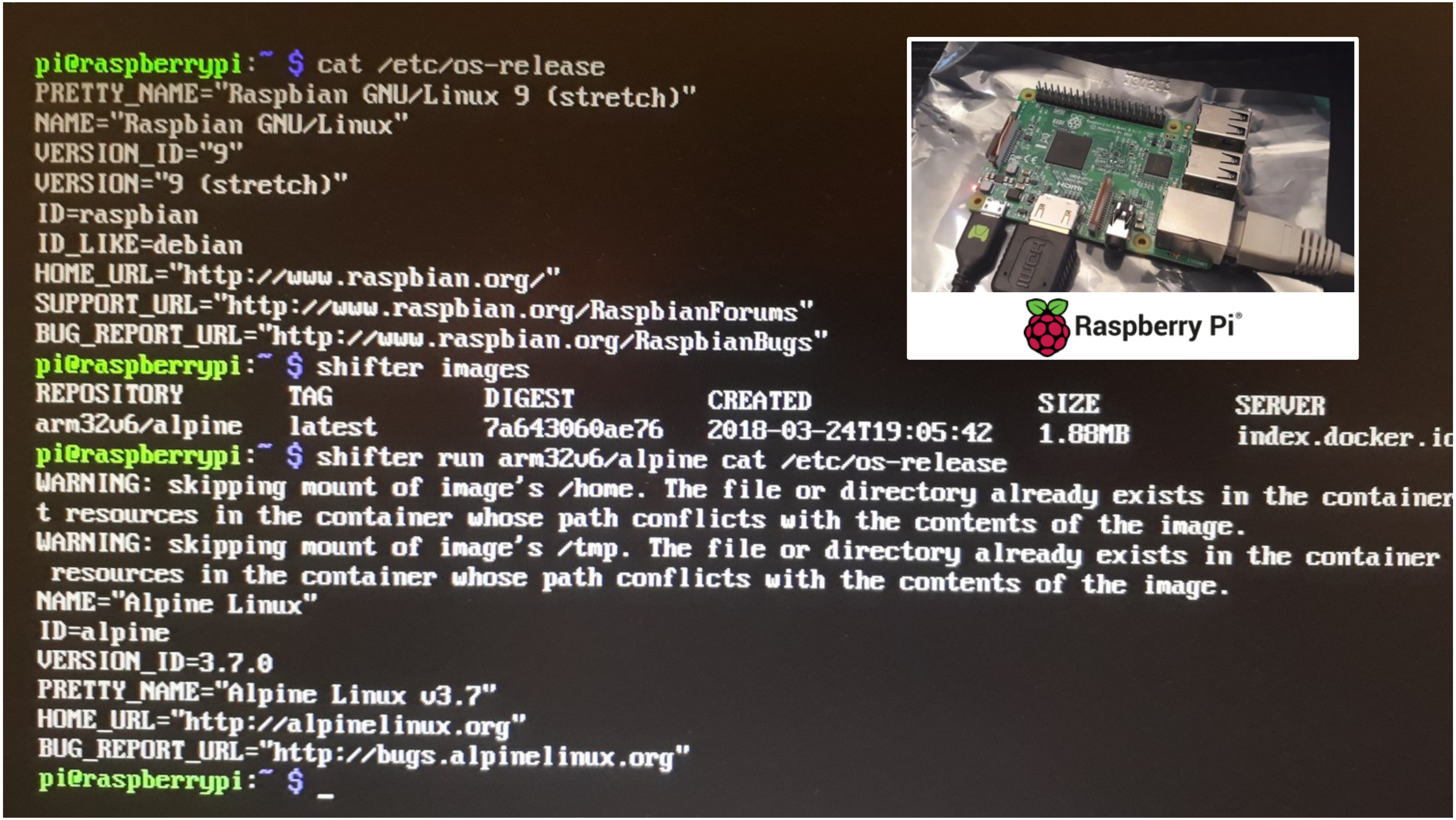
Cheatsheet

Step-by-step guides: https://github.com/eth-cscs/containers-hands-on

```
docker pull <repo/image:tag>
docker run <image:tag> <command>
docker run –it <image:tag> bash
docker run <image:tag> mpiexec –n 2
docker images
docker build –t <repo/image:tag> .
docker login
docker push <repo/image:tag>
```

Shifter is not just for HPC!



```
pi@raspberrypi:~ $ cat /etc/os-release
PRETTY_NAME="Raspbian GNU/Linux 9 (stretch)"
NAME="Raspbian GNU/Linux"
VERSION_ID="9"
VERSION="9 (stretch)"
ID=raspbian
ID_LIKE=debian
HOME_URL="http://www.raspbian.org/"
SUPPORT_URL="http://www.raspbian.org/RaspbianForums"
BUG_REPORT_URL="http://www.raspbian.org/RaspbianBugs"
pi@raspberrypi:~ $ shifter images
REPOSITORY      TAG         DIGEST          CREATED                SIZE        SERVER
arm32v6/alpine  latest      7a643060ae76    2018-03-24T19:05:42    1.88MB      index.docker.ic
pi@raspberrypi:~ $ shifter run arm32v6/alpine cat /etc/os-release
WARNING: skipping mount of image's /home. The file or directory already exists in the container
t resources in the container whose path conflicts with the contents of the image.
WARNING: skipping mount of image's /tmp. The file or directory already exists in the container
 resources in the container whose path conflicts with the contents of the image.
NAME="Alpine Linux"
ID=alpine
VERSION_ID=3.7.0
PRETTY_NAME="Alpine Linux v3.7"
HOME_URL="http://alpinelinux.org"
BUG_REPORT_URL="http://bugs.alpinelinux.org"
pi@raspberrypi:~ $ _
```

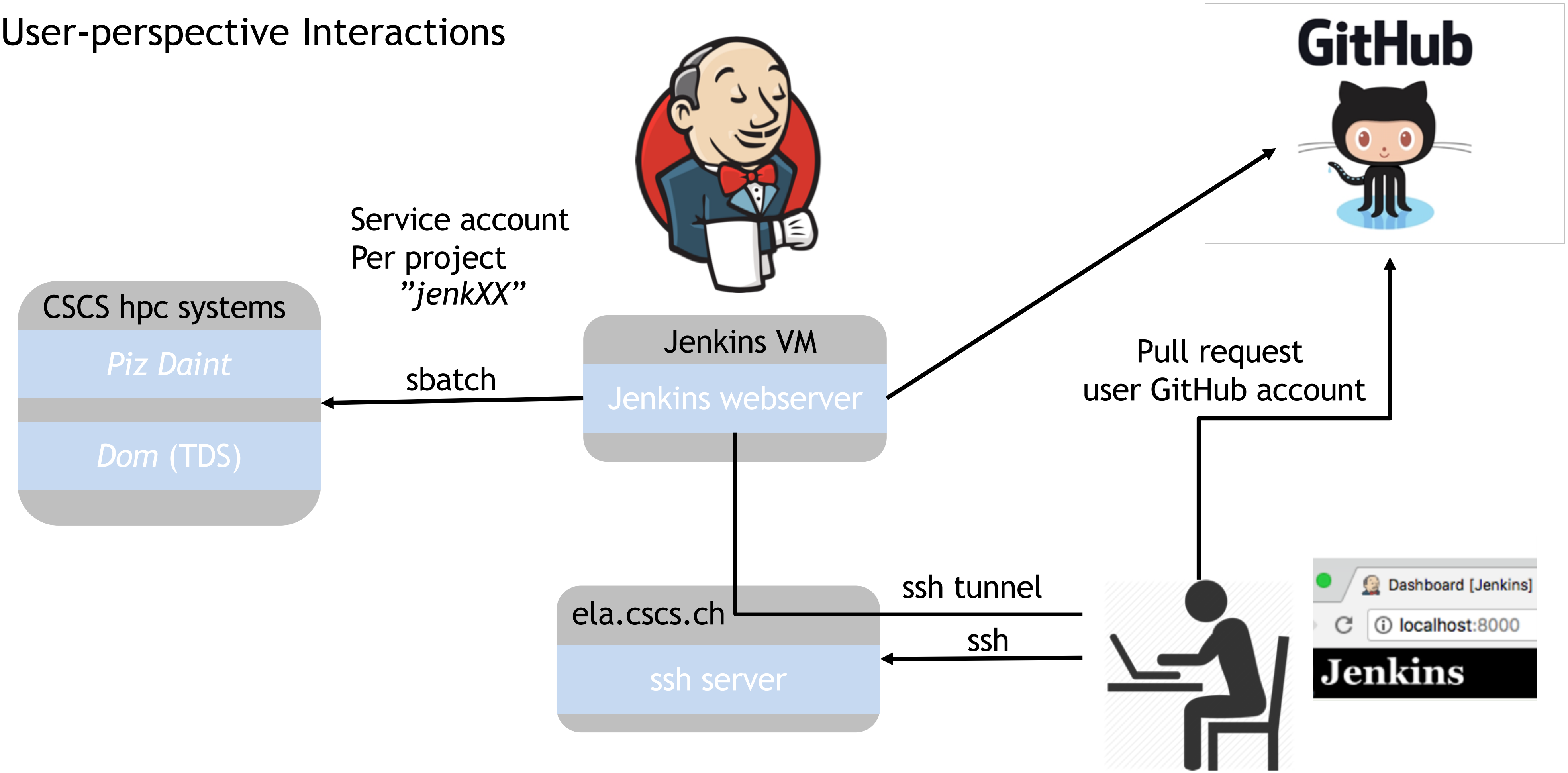
Service Detail:
Continuous Integration

Jenkins CI Overview

- **CSCS provides the Java-based open source Jenkins interface as an automation server**
  - Can be used as a simple continuous integration (CI) server or turned into a CI tool for projects
  - Each project is assigned a Jenkins folder with the corresponding project name on the Jenkins instance
  - The Jenkins jobs related to the project have to be created in the above folder
  - Credentials can be added to be used with version control systems, etc.
  - Each project is assigned a Jenkins node which will manage the corresponding Jenkins jobs
  - Each project is additionally assigned a Jenkins user which is going to be used by the Jenkins node to access *Piz Daint*
- **Since the CSCS Jenkins is not visible in public web, it is not possible to communicate with Github and trigger builds via webhooks. Two alternatives are recommended:**
  - Use polling with a reasonable timestep to poll your remote repository for changes.
  - Use the GitHub Pull Request Builder (ghprb) plugin

Overview of Jenkins Service Interactions

User-perspective Interactions



CSCS hpc systems

Piz Daint

Dom (TDS)

Service account
Per project
"jenkXX"

sbatch

Jenkins VM

Jenkins webserver

Pull request
user GitHub account

ela.cscs.ch

ssh server

ssh tunnel

ssh

Service Detail:
JupyterHub Service at CSCS

Using JupyterHub at CSCS

- This service enables the interactive execution of Jupyter Notebook on *Piz Daint* over both single and multiple nodes.
  - The supported python version is python3.
- The service is accessed through the address
  - https://jupyter.cscs.ch
  - users should provide their HPAC credentials in order to login
- Once logged in, the user is redirected to a job setup page
  - Allows typical job configuration options to be selected in order to allocate the resources that are going to be used to run Jupyter
    - account
    - type of *Piz Daint* node type (gpu or mc)
    - number of nodes
    - wall-clock time limit
- More information at: https://user.cscs.ch/tools/interactive/

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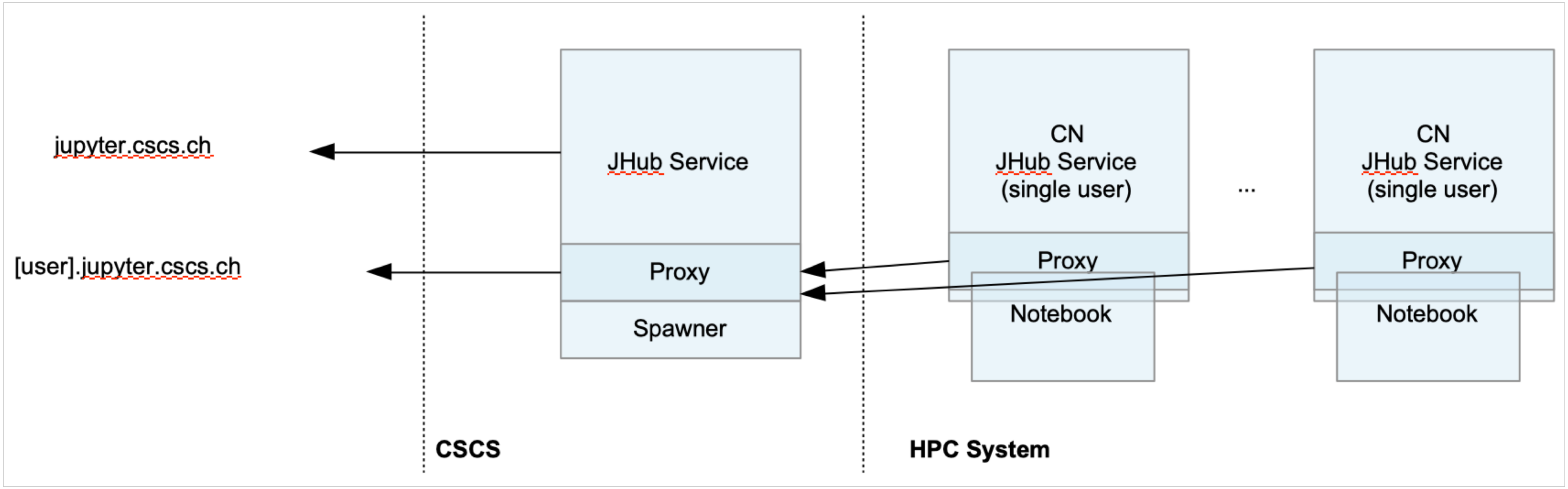
JupyterHub Service Architecture (1)

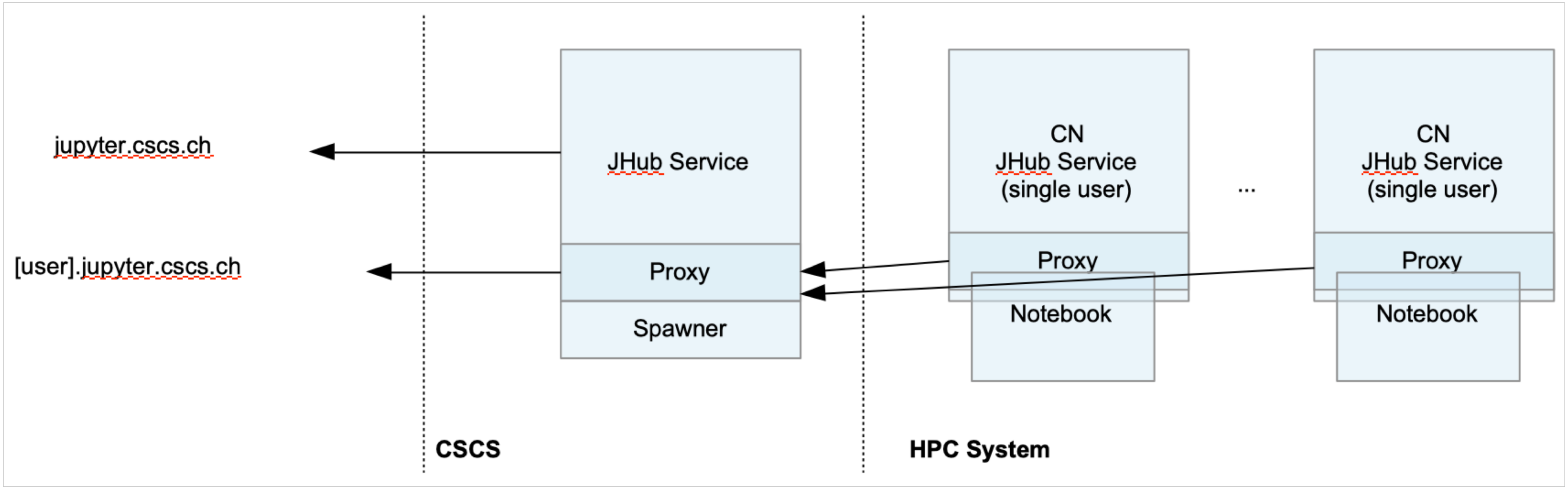
- The **current** architecture protects the notebook in each compute node (CN) by launching a JupyterHub Service along with it



JupyterHub Service Architecture (2)

Notebooks v4.3 and newer are protected with a per-session tokens

- Avoids the creation of several custom spawners
  - Ideally we want one CSCS spawner only
- Will be integrated with an Infrastructure Services API (UNICORE or similar)
- The frontend will be kept outside of the HPC system



How to get Help or More Information

General Contact for HPAC Platform:

- HPAC Platform: https://collab.humanbrainproject.eu/#/collab/264/nav/2378

How to apply for resources:

- Send your proposals to: icei-coord@fz-juelich.de

Getting help:

- Send emails to: hpac-support@humanbrainproject.eu

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Thank You

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