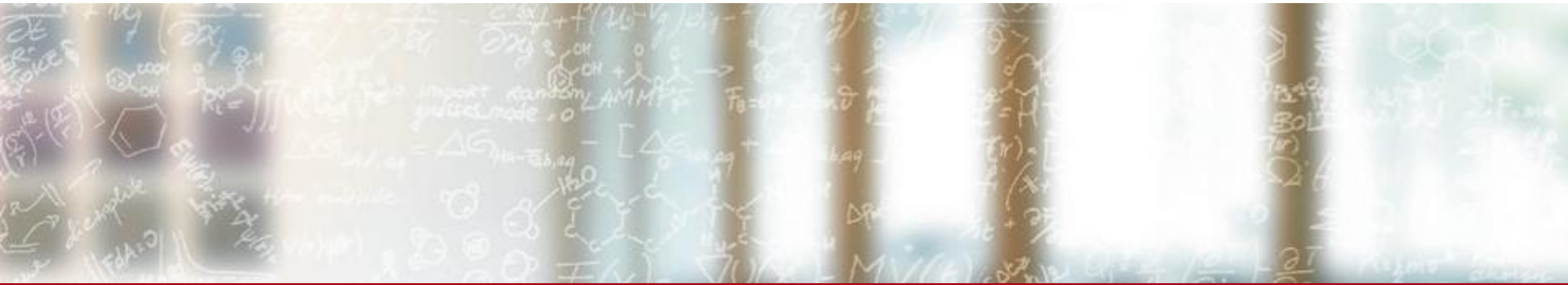




**CSCS**

Centro Svizzero di Calcolo Scientifico  
Swiss National Supercomputing Centre

**ETH** zürich



# CSCS Services to support your scientific work

Pablo Fernandez

CSCS User Lab Day, September 11<sup>th</sup>, 2018

# Service Overview

- User Lab
  - Peer-reviewed
  - Different allocation schemas
- Computational Services for Science
  - Swiss research institutions and consortia with their own funding can take advantage of the services provided by CSCS.
  - Shared with User Lab when possible, but also dedicated
  - Individual PIs with can easily use “cscs2go”

All share the same service catalog

# Our partners

## Call for Proposals

- User Lab
- PRACE Tier 0

## Housing

- BlueBrain for EPFL
- Euler for ETH Zurich

## Hosting (dedicated systems)

- MeteoSwiss
- Mönch Cluster for ETH Zurich (dismantling)
- Phoenix for CHIPP (new also as non dedicated system)

## Services on non dedicated systems

- Empa
- ETH Zurich
  - C2SM (storage)
  - Prof. Petros Koumoutsakos
  - Prof. Nicola Spalding
  - Prof. Matthias Troyer
- Hilti
- MARVEL
- PartnerRe
- Paul Scherrer Institute
- Swiss Data Science Center
- Università della Svizzera Italiana
- University of Geneva / CADMOS
- University of Zurich

# Pay-as-you-go – Service Highlights

- Highly standardized offering
  - Clearly defined packages with different price tags
  - Access to our service catalog
- Low entry barriers
  - Online creation of accounts and payments (goal: immediate access)
  - Inexpensive entry level package for testing
  - Reduced bureaucratic load



[Overview](#)

[Contractual Partners](#)

[Service Catalog](#)

[User Regulations](#)

cscs2go

[Services](#) | [Service Catalog](#)

## SERVICE CATALOG

### CATEGORIES



#### COMPUTE RESOURCES

##### GPU Hybrid (@Piz Daint)

Computing node-hours on a CPU/GPU hybrid partition (Cray XC50) of the Piz Daint supercomputer. This service includes access to



#### STORAGE RESOURCES

##### Home Directory

Every user is assigned their own home directory with sufficient storage space to store codes and documents (/home)



#### INTERACTION AND WORKFLOW TOOLS

##### Job Queue

Access to compute nodes is provided with the use of an integrated workload manager (Slurm). This provides traditional batch processing services

# Service Catalog Categories

- Compute resources
- Storage resources
- Interaction and Workflow tools
  
- Scientific applications
- Data Science and Machine Learning applications
- Visualization applications
- Programming environment
  
- Helpdesk & training

# Compute and Storage resources

Consumable resources, billable

- MultiCore @ Piz Daint
- GPU Hybrid @ Piz Daint
- Manycore @ Grand Tavé
- OpenStack @ Pollux
- Cluster-on-demand @ Mythen
- Homes
- Online (+Object)
- Data Protection

# From Mönch to Mythen up to Fulen: Virtualization of Cluster Services

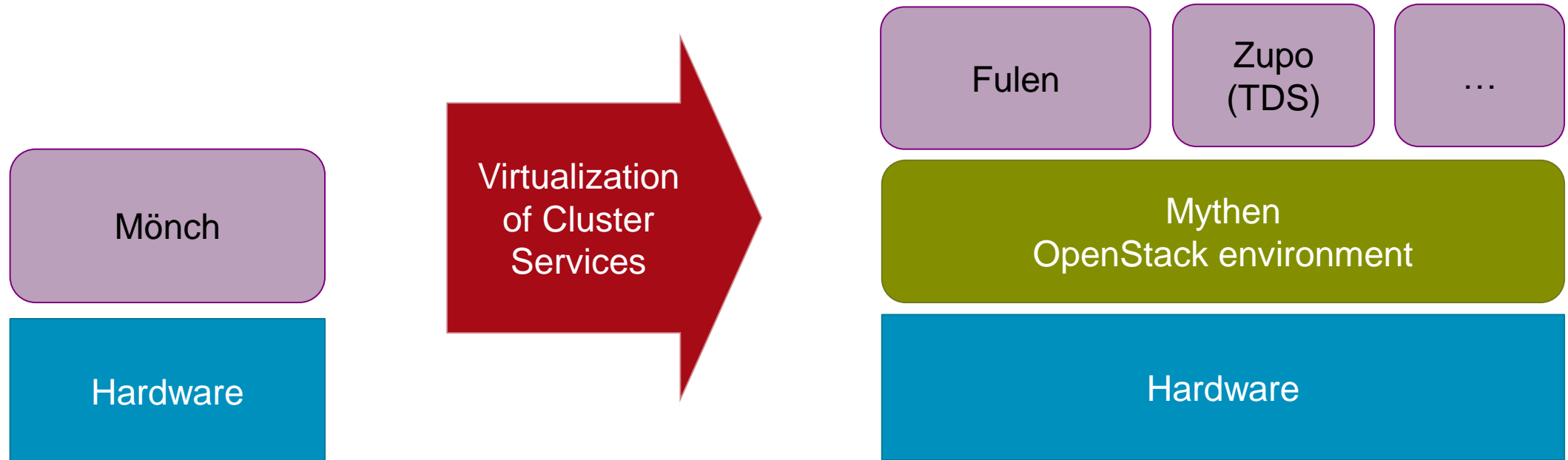
## Mönch

- A cluster dedicated to research groups at ETH Zurich
- 10 rack NEC Intel-based system: 376 standard compute nodes, 40 large-memory compute nodes, 24 huge-memory compute nodes
- One physical / logical cluster





# From Mönch to Mythen up to Fülen: Virtualization of Cluster Services



# From Mönch to Mythen up to Fulen: Virtualization of Cluster Services

## Mythen

- A physical OpenStack environment optimized for HPC applications
  - 20 compute nodes (16 CPU, 2 Big Mem, 2 GPU)
- Can be extended with different kind of compute nodes
- Mythen is not made directly available to customers but is used to create virtual clusters

## Fulen

- The first "logical" cluster implemented on Mythen
  - Virtual 84 compute nodes (from 10 to 104 cores) plus additional service nodes
- Can "dynamically" grow in size depending on customers need

# Interaction and Workflow tools



- Job Queue
- Containers, Docker/Shifter
- High Throughput Scheduler, Greasy
- OpenStack, infrastructure-as-a-service
- Data Transfer
- JupyterHub
- Continuous Integration

# Interaction and Workflow tools - Data transfer

- Move datasets (>TB) around (and in/out) CSCS
  - High throughput (> GB/s)
  - Main file systems @ CSCS (/scratch/snx..., /project, /store)
- Internal transfers
  - Xfer queue
  - Can chain with jobs using SLURM dependencies
- External transfers
  - Globus Online / GridFTP

# Interaction and Workflow tools - JupyterHub

- Allows users to run their Jupyter Notebooks in a dedicated node
  - A small partition of Piz Daint is free for single-node notebooks
  - Bigger notebooks can run on the normal job queue
  - Multicore or Hybrid
- Charged against your project

 **CSCS** [Home](#) [Token](#)  [Logout](#)

## Spawner Options

Piz Daint node type


Reservation

Number of Nodes













Job duration

Account (leave empty for default)

Spawn

 **Test** [Logout](#) [Control Panel](#)

File Edit View Insert Cell Kernel Help  | Kernel

        Run     

```
In [1]: print ("hello world!")  
  
hello world!
```

```
In [ ]:
```

# Interaction and Workflow tools – Continuous Integration



# Jenkins

- Helps automate the non-human part of the software development process, with continuous integration and delivery
- Builds take place on the compute nodes of Piz Daint and therefore software is tested on the actual hardware/software
- For CSCS projects that need it, the PI should ask us at [help@cscs.ch](mailto:help@cscs.ch)

- Up
- Status
- Configure
- New Item
- Delete Folder
- People
- Build History
- Project Relationship
- Check File Fingerprint
- Move
- Open Blue Ocean
- Credentials
- New View

SCS

[add description](#)

All +						
S	W	Name ↓	Last Success	Last Failure	Last Duration	Fav
		<a href="#">Test_Arbor_Demo</a>	6 hr 22 min - <a href="#">#17</a>	1 day 21 hr - <a href="#">#15</a>	16 min	
		<a href="#">Test_Reframe_CI</a>	4 days 2 hr - <a href="#">#10</a>	4 days 2 hr - <a href="#">#4</a>	2 min 4 sec	
		<a href="#">TestDomVMFeatures</a>	1 mo 15 days - <a href="#">#3</a>	1 mo 15 days - <a href="#">#2</a>	0.61 sec	
		<a href="#">TestPipeline</a>	1 day 0 hr - <a href="#">#19</a>	1 day 0 hr - <a href="#">#14</a>	22 sec	
		<a href="#">UserLabDay</a>	20 hr - <a href="#">#17</a>	20 hr - <a href="#">#16</a>	2 min 9 sec	

Icon: [S](#) [M](#) L[Legend](#) [RSS for all](#) [RSS for failures](#) [RSS for just latest builds](#)

Build Queue

No builds in the queue.

Build Executor Status

master

- 1 Idle
- 2 Idle

s299\_daintvm1 (offline)

s577\_daintvm1 (offline)



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# Okay, but what can I actually do inside the machine?

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# Scientific applications

- Amber
- CP2K
- CPMD
- GROMACS
- LAMMPS
- NAMD
- Python
- Quantum Espresso
- VASP
- (+libs: Trilinos, FFTW, HDF5, Blas, NetCDF)

# Data Science and Machine Learning applications

- Spark
- TensorFlow
- Theano
- ABCpy
- Jupyter Notebook
- Cray Graph Engine
- Dask
- Intel BigDL
- Anaconda Python & R

# Visualization applications

- ParaView
- VisIt
- VMD

# Programming environment

- Cray/Intel/GNU/PGI compilers
- DDT debugger
- CrayPat performance tool
- VI-HPS performance tool
- CUDA Toolkit
- NVIDIA SDK performance tool
- Easybuild framework

# Helpdesk & training

- We are here to help: [help@cscs.ch](mailto:help@cscs.ch)
- Watch out for upcoming training events:  
<https://www.cscs.ch/publications/tutorials/>
- Coming soon: User Management Portal
  - To allow PIs and users to manage their projects

# Discussion

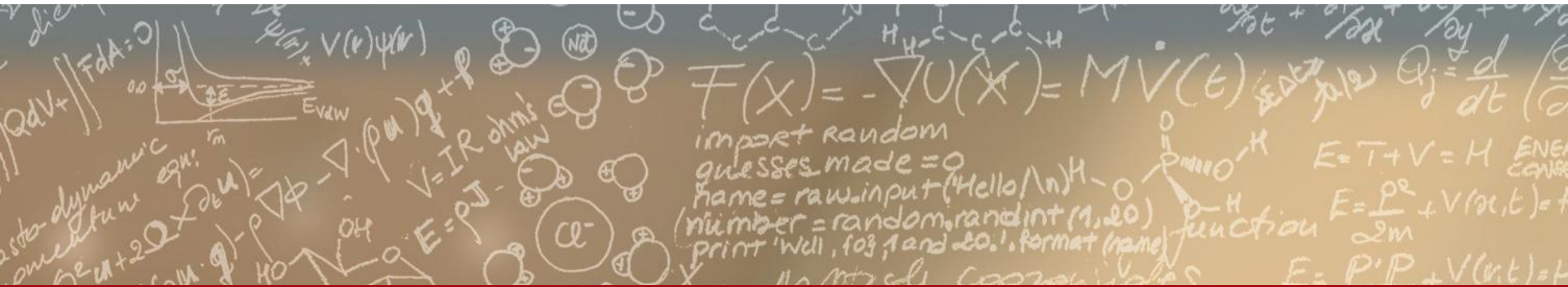
- Are you missing something from our service catalog?
- Is your scientific area well represented within our set of installed applications?
- Do you have any workflow other than just submitting a job in the queue and wait for the result? Have you tried to use the Data Transfer queue?
- Are you planning to build a mobile or web application, or a portal, that need to use HPC resources?
- Do you (plan to) use Amazon / Google / Azure cloud services? What for?



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**Thank you for your attention.**

# Service Catalog

Compute Resources

MultiCore, GPU Hybrid, Manycore, OpenStack, (Cluster-on-demand)

Storage Resources

Homes, Online (+Object), Data Protection

Interaction and Workflow tools

Job Queue, Containers, High Throughput Scheduler, OpenStack, Data Transfer, JupyterHub, Continuous Integration

Scientific Applications

Amber, CP2K, CPMD, GROMACS, LAMMPS, NAMD, Python, Q. Espresso, VASP (+libs: Trilinos, FFTW, HDF5, Blas, NetCDF)

Data Science & Machine Learning

Spark, TensorFlow, Theano, ABCpy, Jupyter NB, CGE, Dask, BigDL, Anaconda Python & R

Visualization

ParaView, VisIt, VMD

Programming environment

Cray/Intel/GNU/PGI, DDT, CrayPat, VI-HPS, NVIDIA SDK, Easybuild

Customer/Support Services

Help Desk, Training