Distributed computing services: cluster grids, HPC systems, clouds.

COMPUTE RESEARCH SCHOOL COURSE NTF004F

Evolution of science paradigms

Data exploration (**e-Science**)

- Unifies the rest to explore **Big Data**

Computational science

- Simulations

Theoretical science

- Models

Empirical science

- Descriptive

after Jim Gray

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Data tsunami

All scientific research needs **data** (testing models, finding patterns)

All data and information is **digitised**

Modern instruments produce digital data in **huge amounts**

Instruments and data are **accessible by all scientists** on the planet

Modern science is impossible without **global distributed infrastructures** to handle data

Why are Big Data distributed?

There is no Big Storage

- Even Cloud storage is distributed

Preservation

- More copies – better preservation

Instruments are distributed

- Sensors, CT scanners, telescopes, even accelerators

Scientists are many and everywhere

- Local copy is nice to have

e-Science needs e-Infrastructures

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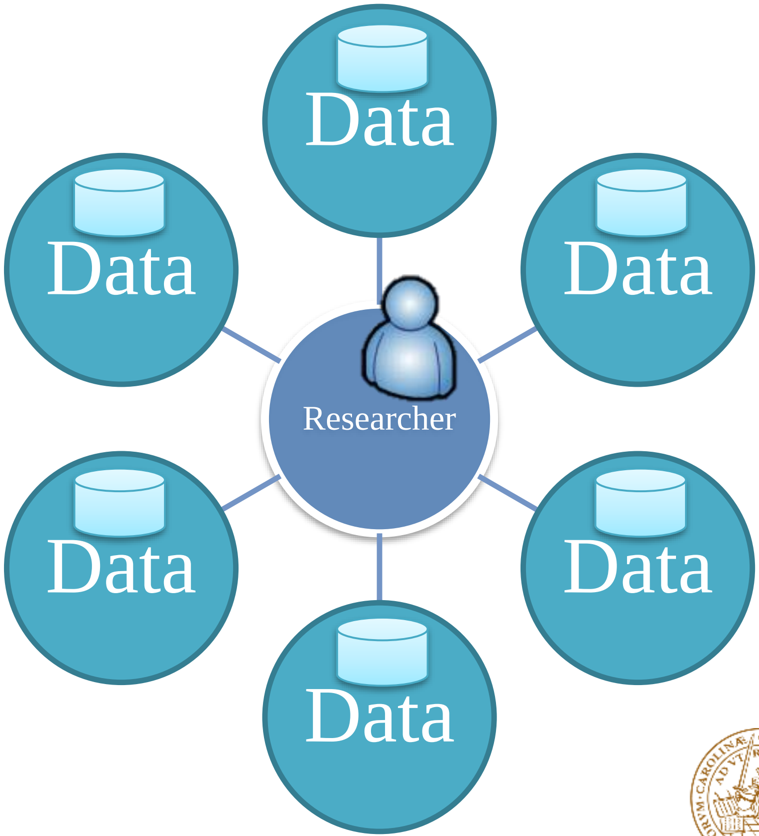
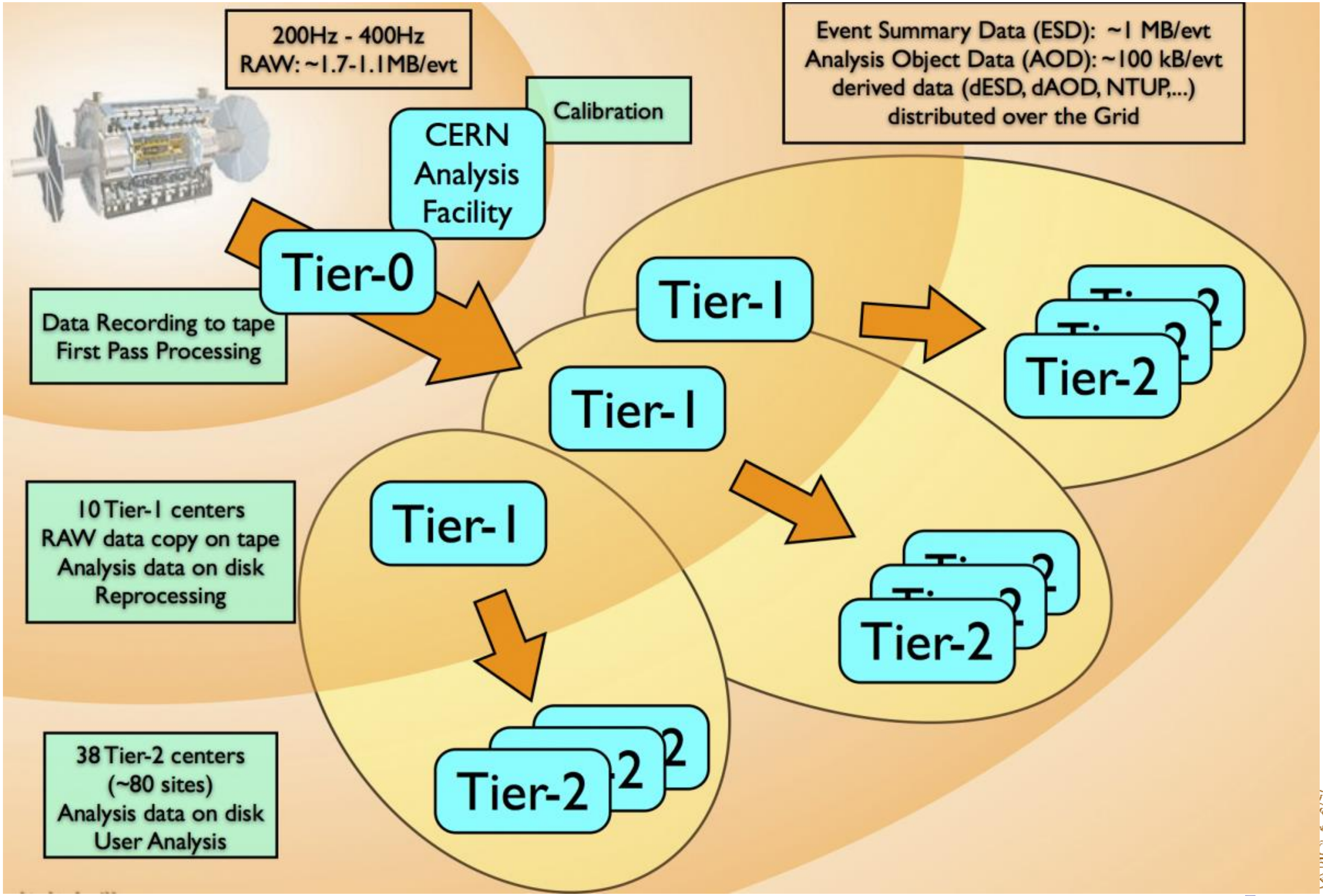
Different data access concepts

Traditional

Distributed data



Distributing collected data – CERN way



Graphics by iSGTW

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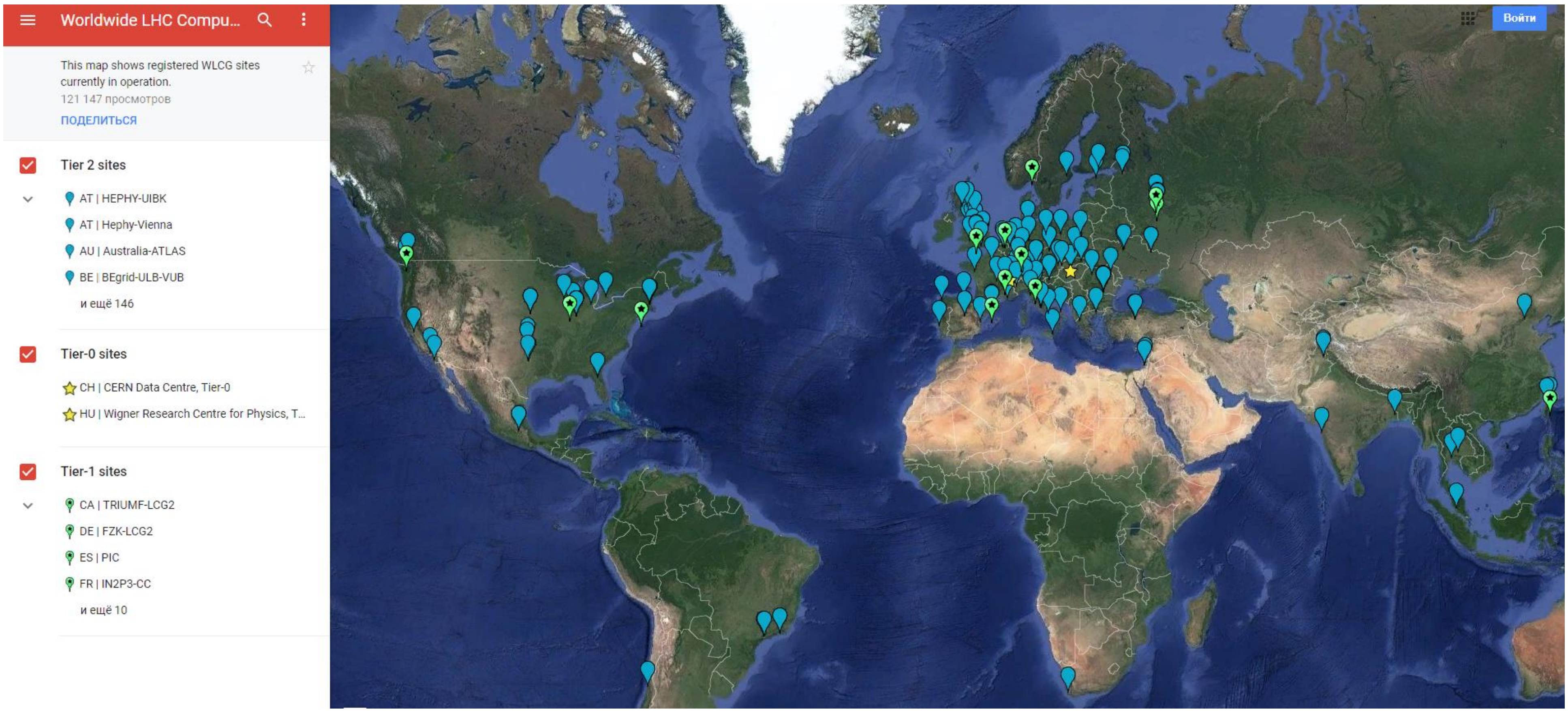
CERN Data and Computing Sites



Check yourself at http://wlcg.web.cern.ch

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Recall: scientific computing scenarios

A Infrequent tasks with moderate resource consumption

- E.g. Excel macros, simple image processing etc

B Large batches of similar (simple) independent tasks: serial jobs

- Processing of many images, analysis of accelerator collision events etc

C Lengthy resource-consuming tasks: often parallel jobs

- Pattern recognition, complex system simulation, parameter scanning, lattice QCD
  - Parallel jobs share memory, or exchange information by other means

Typical of massive data processing

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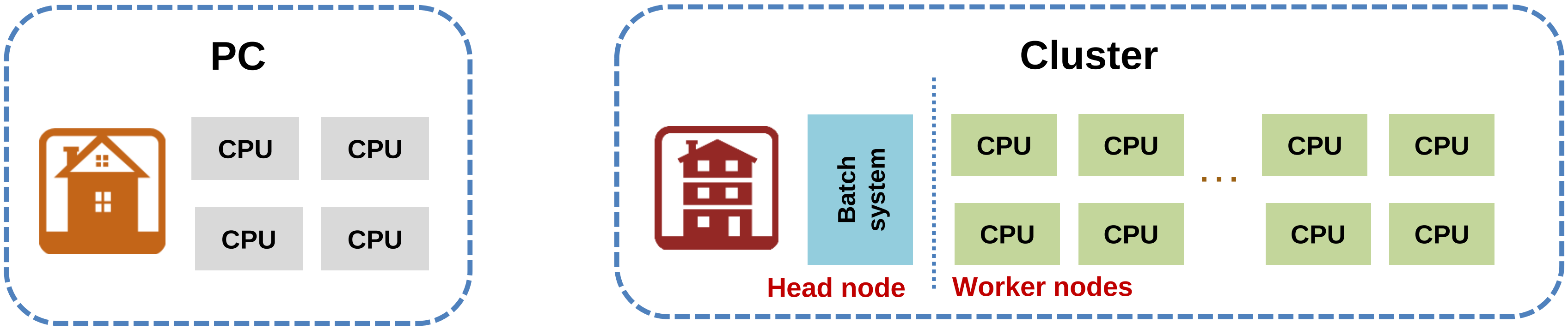
Recall: customized shared service – clusters, supercomputers

- One system serves many users
- One user can use many systems
- Systems are typically provided as public service (by universities and labs)

- Systems are customized, but each can serve many different users
- When many different systems jointly offer common services (login, storage etc), they create a computing *Grid*

From PCs to Clusters and HPC systems



- Clusters started as loosely coupled PC boxes
  - Now industry solutions exist
    - » Even virtual
- HPC: High Performance Computing systems
  - Supercomputers or very advanced clusters
    - » Shared memory, fast interconnect etc

The workhorse of scientific computing: clusters

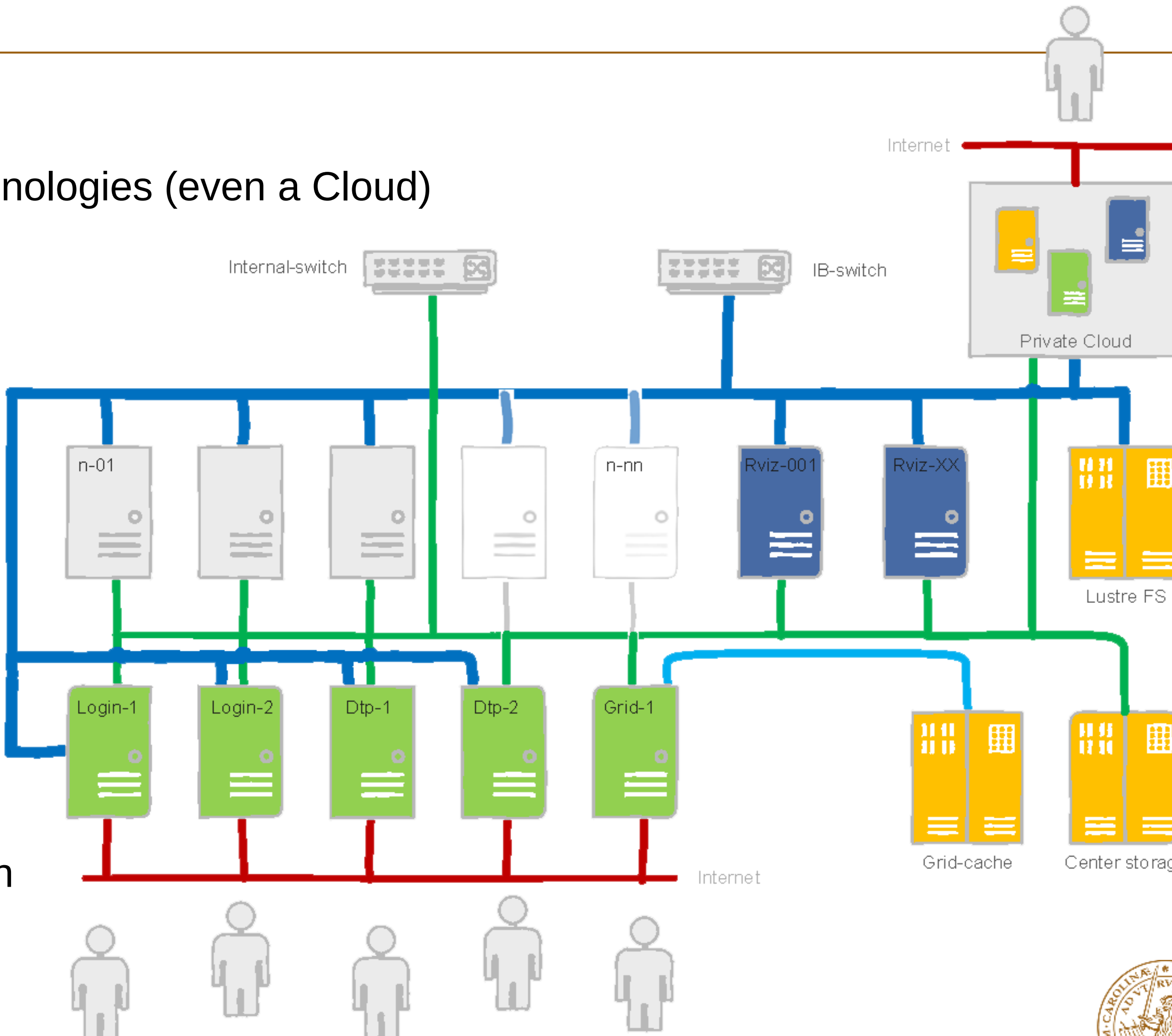
- Computing facilities in universities and research centers are usually Linux <u>clusters</u>
  - Some supercomputer-grade facilities are often clusters, too
- A cluster is a (comparatively) loosely coupled set of computing systems presented to users as a single resource
  - 0-level **distributed computing**, because of loose coupling
  - A typical cluster has a <u>head node</u> (or a few) and many <u>worker nodes</u>
    - » A node is a unit housing processors and memory – a server
  - Distribution of load to worker nodes is orchestrated by means of Local Resource Management Systems (a.k.a. <u>batch systems</u>)
    - » Many batch systems exist on the market: SLURM, PBS, SGE, HTCondor etc
- Every cluster is a heavily customised resource built for a range of specific applications

Clusters in the LUNARC center

Photo: Gunnar Menander, LUM

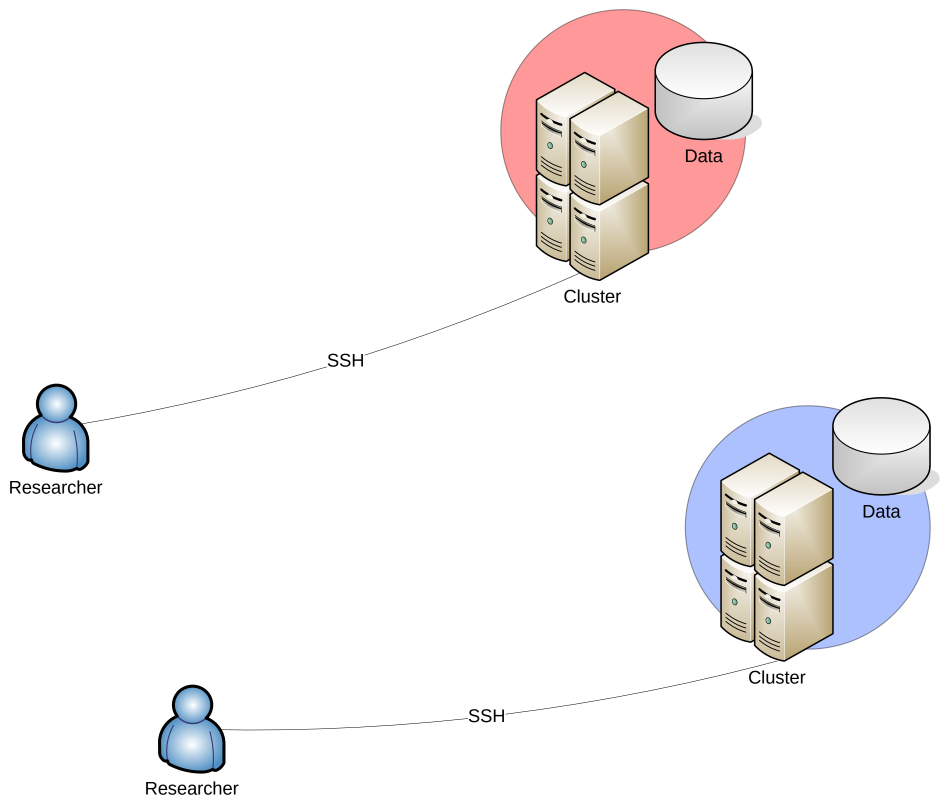
Aurora cluster at LUNARC

- Combines many different technologies (even a Cloud)
- Offers many different services
  - Computing (of course)
  - Storage
  - Remote desktop
  - Etc
- 180 base nodes + over 50 nodes owned by research groups
  - Each node has 2 Haswell processors, 20 cores each



Graphics by J. Lindemann

Typical workflow on clusters



- Users connect to the **<u>head node</u>**
  - Typically, using Secure Shell - SSH
- Necessary software is installed
  - For example, your own code
    - » Usually centrally by admins
- Specialised scripts are used to launch tasks via **batch systems**
  - A task can be anything, from adding 2 and 2, to bitcoin mining
  - A single task is called a **job**
- Data are placed in internal storage – not really distributed
  - Cluster worker nodes often have no network

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Jobs and queues

- A batch system is software that schedules computational tasks to worker nodes according to given criteria and requirements
- A single unit of scheduling is called a **job**; some job requirements are:
  - A job can use a single core (serial job), or several cores at once (parallel job)
  - Consumes CPU time and astronomic (wall-clock) time
    - A well-parallelized job will consume less wall time, but a comparable CPU time to a serial one
  - A job also consumes memory and disk space
  - A job may do intensive input/output operations (data processing)
  - A job may require public network connectivity (for example, for database queries)
- When there are more jobs than resources, **queue** management is needed
  - A cluster may have several queues for different kinds of jobs (long, short, multicore etc)
  - A queue is actually a persistent partition of a cluster, exists even if there are no jobs

Different tasks use different jobs

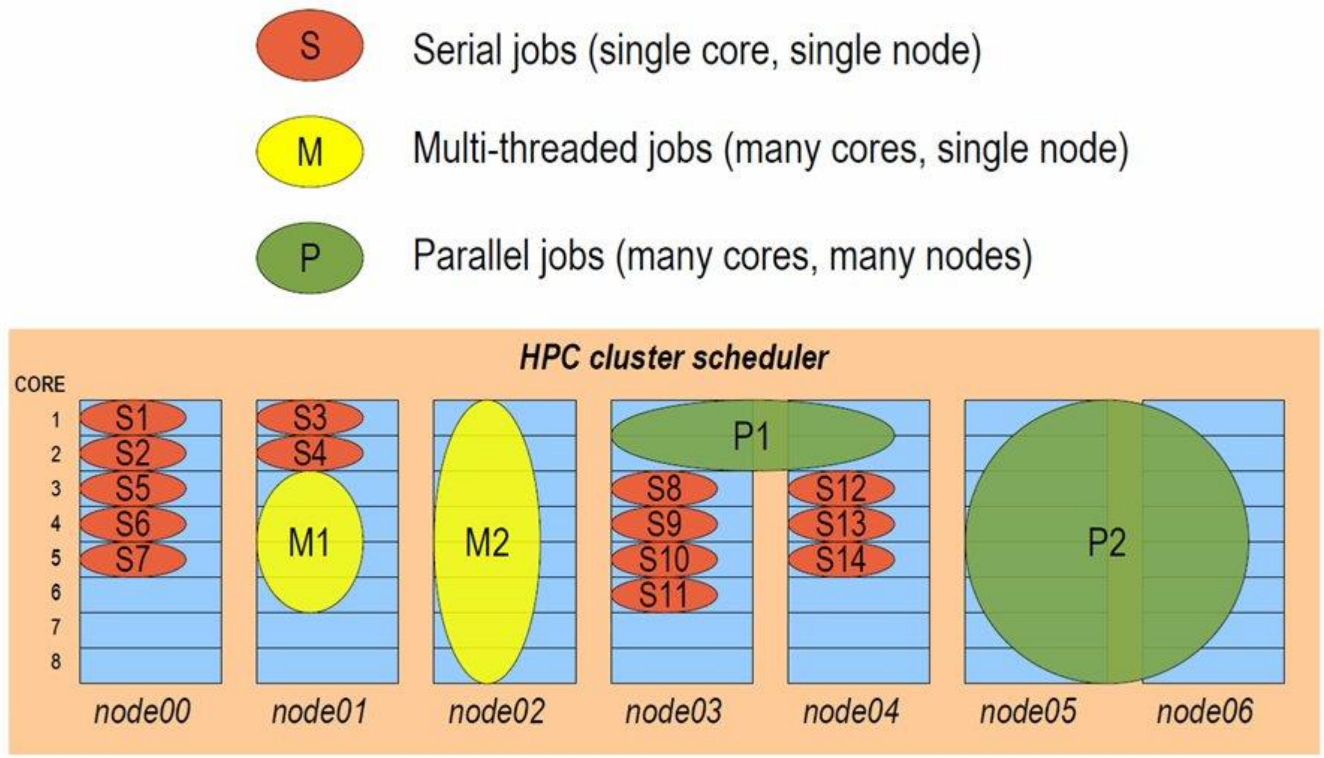
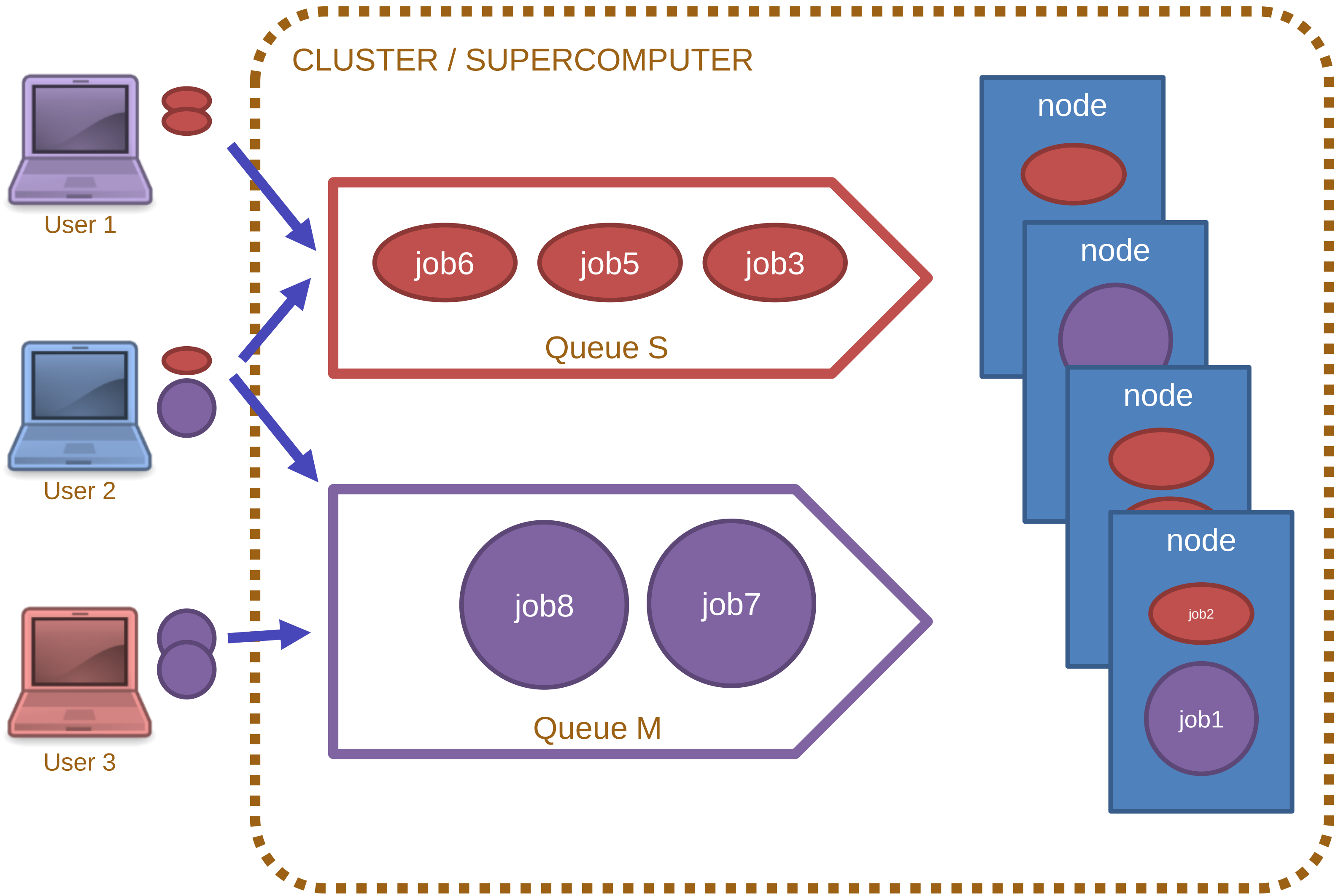


Image from https://alces-flight.com

- Batch scheduling is like playing Tetris – only you can't rotate pieces (says Gonzalo Rodrigo)

Scheduling usually relies on queues



What clusters and HPC systems are good for:

- Executing many tasks at once
  - Use scheduling algorithms
- Serving many users at once
  - Use fair-share algorithms
- Executing tasks that need massive resources
  - Processing capacity, but also memory
  - Word of the day: Exascale
    - » Countries compete to build ExaFLOP-capacity machines

What if we need many clusters/HPCs?

- Not everybody has an ExaFLOP machine
- Scientists often have access to several clusters and HPC systems
  - Different accounts
  - Different passwords
  - Even different operating systems
  - And different sysadmins!
- Solution: equip every system with a dedicated service that will:
  - Work with digital identities
  - Adapt your workload to local system peculiarities
    - » And make sure the system has the software you need
  - Facilitate access to data wherever they are
- This solution is called **Grid**

Some Grid precursors

Distributed file systems: AFS, NFS4

- First implementation in ~1984
- Allow different systems to have common storage and software environment

Condor/HTCondor pools

- High Throughput Computing across different computers
- Started in ~1988 by pooling Windows PCs
- A variant often used as a cluster batch system

Networked batch systems: LSF, SGE

- Could use single batch system on many clusters since ~1994
- Variants of regular cluster batch systems

Volunteer computing: SETI@HOME, BOINC

- Target PC owners since ~1999
- Supports only a pre-defined set of applications

Grid concept – formulated in ~1999

Abstracted interfaces from systems
- No need for common batch systems or common file systems

Introduced security infrastructure
- Single sign-on
- Certificate-based authentication and authorisation

Introduced resource information system
- Necessary for batch-like job management

Ideal for distributed serial jobs
- Initially was thought to be suitable even for parallel jobs

Grid is a technology enabling federations of heterogeneous conventional systems, facilitated by fast networks and a software layer that provides single sign-on and delegation of access rights through common interfaces for basic services

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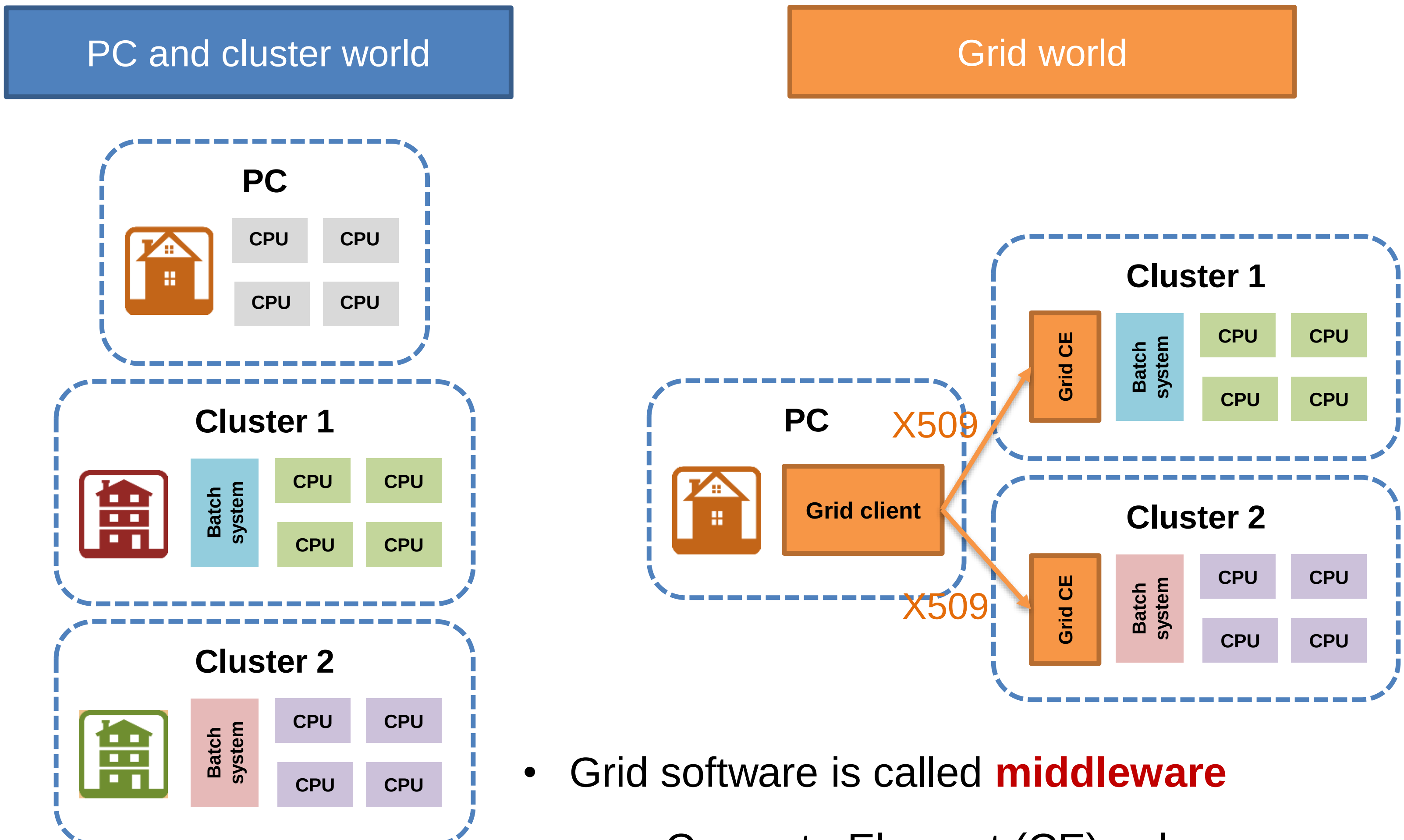
Grid as abstraction layer for computing



- Grid software is called **middleware**
  - Compute Element (CE): a layer between the system and applications

Workflow: Grid vs PC/cluster

PC/cluster

- **Log in via SSH**
  - Different logins on different machines
- **Familiarize with the environment**
  - OS, installed software, storage space, batch system, sysadmin etc
- **Customize the environment**
  - Pathes, environment variables, own software, scripts, data files etc
- **Prepare for batch submission**
  - Interactive execution of short jobs, optimization of batch scripts
- **Submit jobs to the batch system, check their status**
  - Different batch systems (or none) on different machines
- **Log out**
- **Log in later to fetch the output**

Grid

- **Create proxy**
  - One for all machines
- **Create a Grid job description document**
  - Generalization of batch scripts, plus input/output data location etc
- **Test a couple of jobs, fix job description**
- **Submit jobs to the Grid, check their status**
  - Same commands for all machines
- **Watch output appearing in the desired location**
  - Or fetch it manually

Key differences

Operation	PC/Cluster	Grid
Log in	Interactive SSH session	No actual log in: delegation
	Different passwords	Single sign-on
Job description	Shell script with batch-system-specific variables	Specialized language
	Different scripts for different batch systems	Same document for all systems
Environment	Can be personalized	Pre-defined, generic
	Can be explored in detail	All details can not be known
Job monitoring and management	Requires log in	Remote
Data management	Manual	Can be automatic

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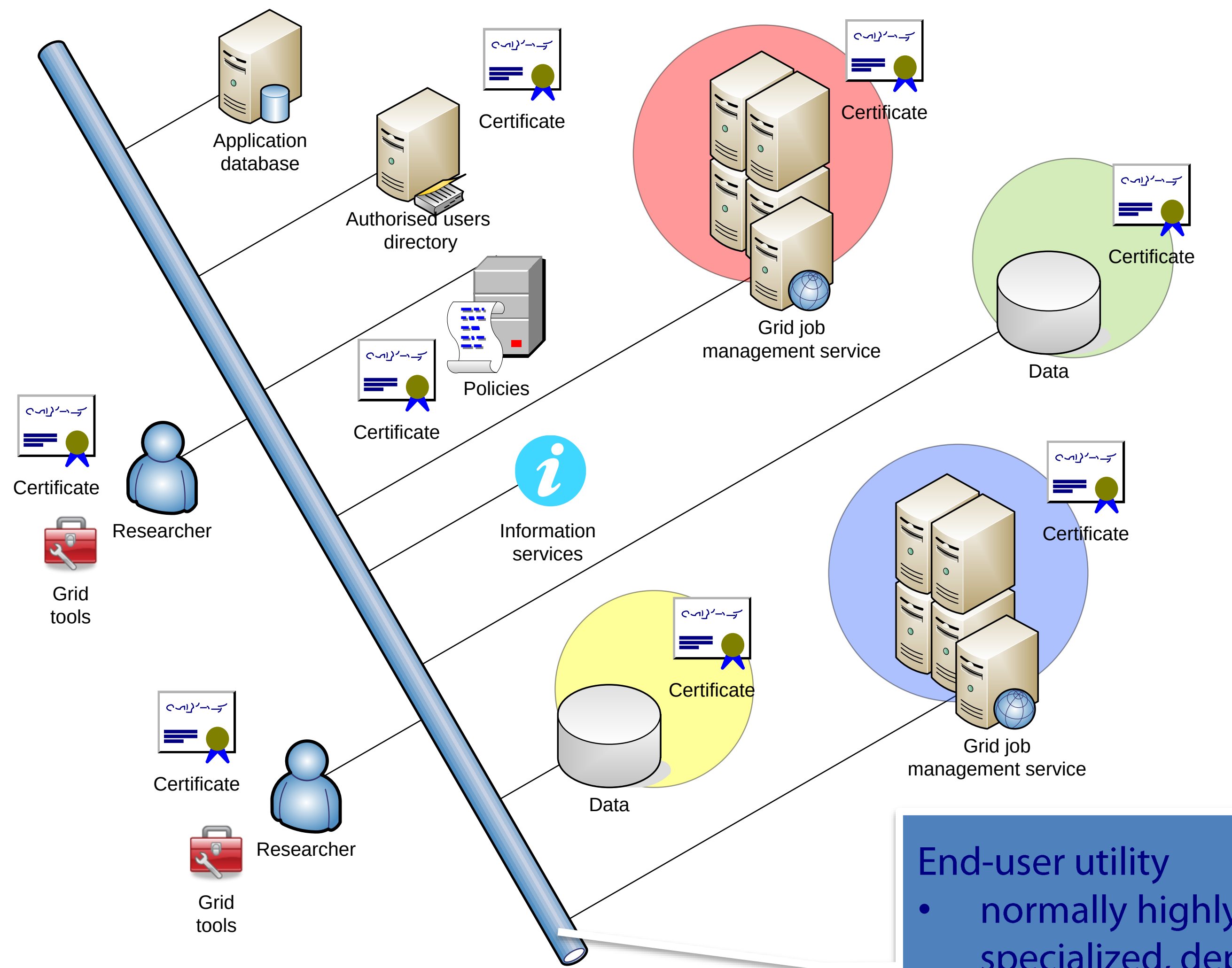
Overview of generic Grid components



End-user utility

- normally highly specialized, depending on the research task

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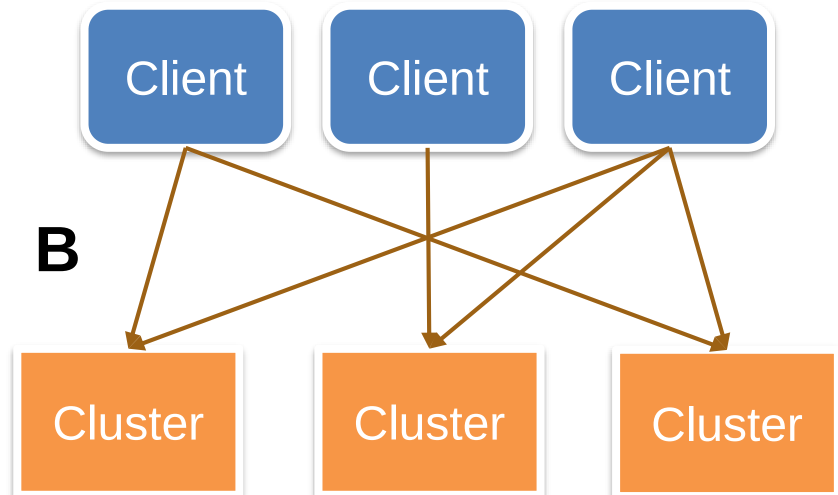
The core of the Grid: Computing Service

- Once you got the certificate (and joined a Virtual Organisation), you can use Grid services
- Grid is primarily a distributed **computing** technology
  - It is particularly useful when **data** is distributed
- The main goal of Grid is to provide a layer for:
  - Common authorization, **single sign-on** – by means of proxies
  - Common task specification (**job description**)
  - Common protocols and interfaces for job and data management
  - Common accounting and monitoring
- All this is provided by Grid **Computing Services**
  - A single instance of such service is called a **Computing Element** (CE)
    - » You also need a Grid **client** software to communicate to Grid services (CE, storage etc)
    - » More during the last class

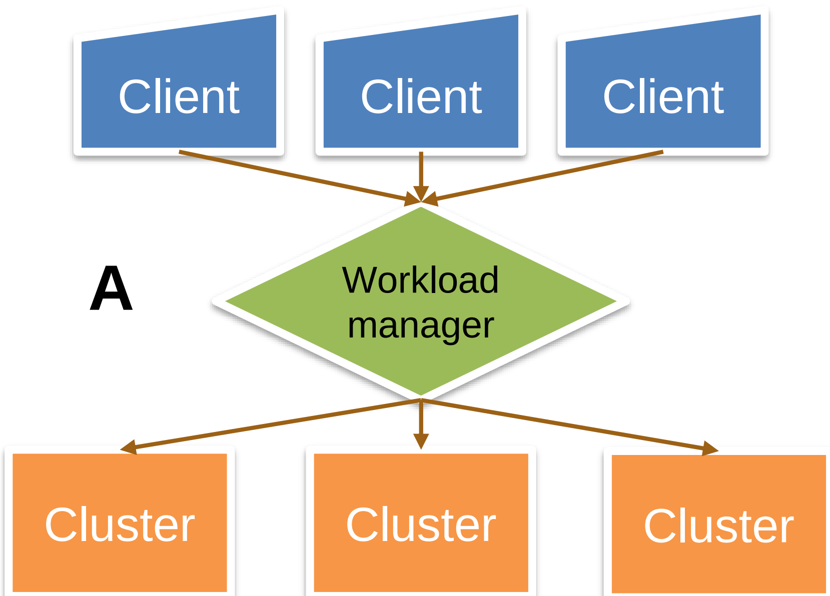
Grid workload management concepts

- Traditional approach **A**:
  - One central service to orchestrate the workload
  - Meta-queue on top of other queues
- Problems:
  - Limited scalability
  - Single point of failure

B



A



- Alternative approach **B**:
  - Every client can submit jobs to any cluster
  - No single point of failure
- Problems:
  - Non-optimal workload
  - Rather complex clients
  - Slow interaction with users

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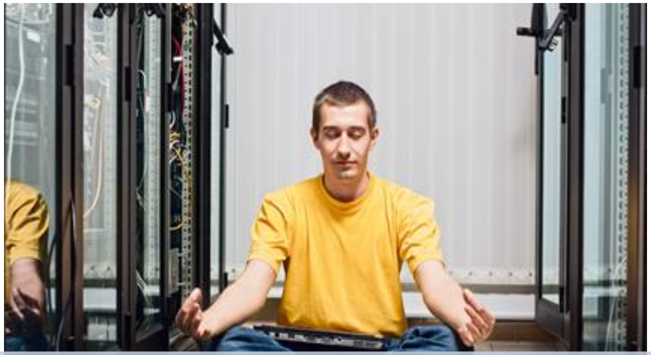
What's wrong with clusters / HPCs / Grids?

Authentication required (typically, SSH)

Batch queues – interactive work discouraged



Only sysadmins can really install software

Applications need to be tailored for each site

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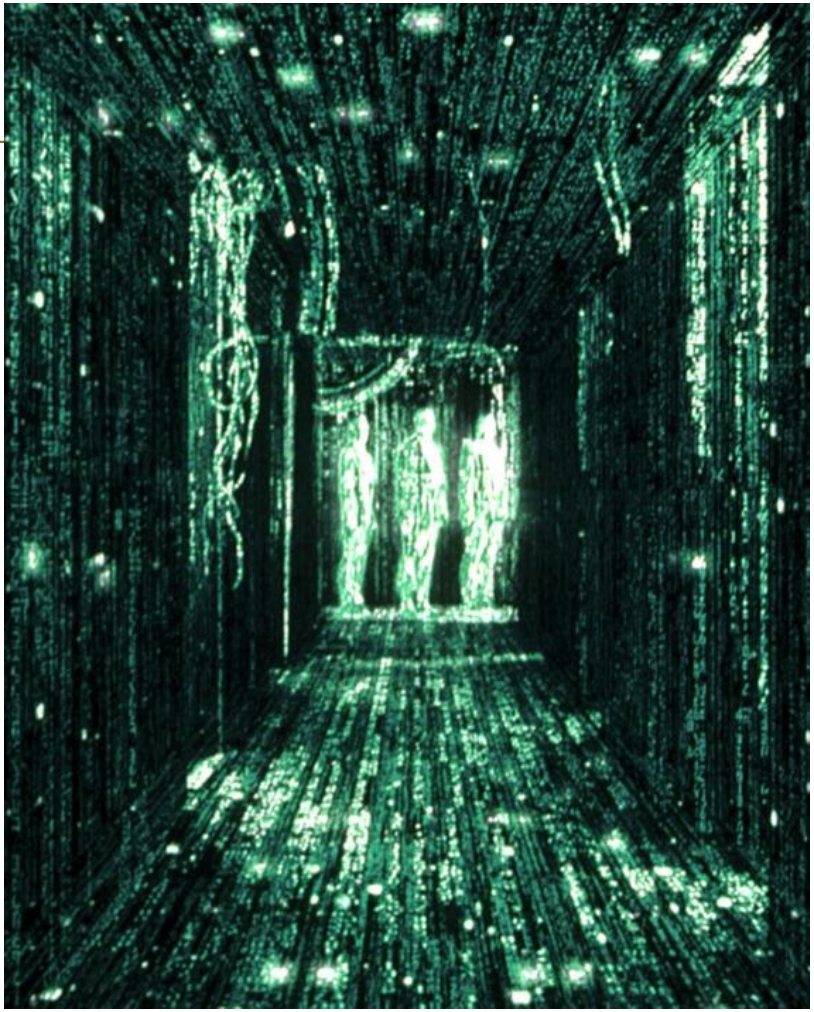
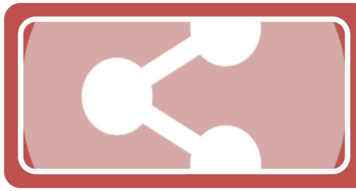
Enter Clouds

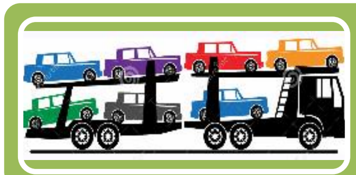
- Cloud is like Matrix for computers
  - You can build your own virtual PC with virtual CPU, virtual memory, virtual network, virtual everything, with your real application inside
  - You can save all this in one file – "image"
  - Load this image into the ~~Matrix~~ Cloud and enjoy instant computing power!
  - And you can even build your own virtual cluster where you are the sysadmin
    - » If you have enough money



Practical motivations for Clouds



Easy to create a platform for shared access – like e.g. Google Docs



Each real machine can host several virtual ones – “**elasticity**”

Convenient way of offering different operating systems on the same hardware, like e.g. in universities

Preservation of software and data: save a snapshot of an old system, no need to re-build for new ones

Recovery and migration of services: when a virtual server crashes, it is trivial to restart it on a healthy host

Isn't Cloud another word for Grid?

- Yes, by inference: Grid is inspired by BOINC, BOINC requires virtualisation, virtualisation is used by Cloud
  - Jokes aside, both Grid and Cloud are technologies to abstract underlying infrastructures
- No: Grid is Communism, Cloud is Capitalism
  - Clouds typically have clear ownership, Grids are federated infrastructures
- Maybe: virtual clusters become common in Grids
  - Infrastructure as a Service
  - More in the next part!

Virtualization and Containers

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General-purpose computing: Theory

1)Write code

2)Compile on ANY target platform

3)Run on ANY target platform

General-purpose computing: practice

1. Write code
   1. Add specific code to adapt to each platform
2. Compile on target platform
   1. Install **all required development libraries** on target platform
      a. decide: binaries (dynamic) or sources (static)?
   2. Setup the **toolchain**: instruct your build system about which tools to use and where to get them
   3. Setup the **build environment**: instruct your build system about which tools to use and where to get them
   4. Write a script to do 2.1, 2.2, 2.3 automatically
3. Run on target platform
   1. Install **runtime dependencies**
   2. Instruct the code where to find runtime dependencies
   3. Write a script to do 3.1, 3.2 automatically
4. TEST ON EVERY POSSIBLE PLATFORM

General-purpose computing: practice

1. Write code
   1. Add specific c
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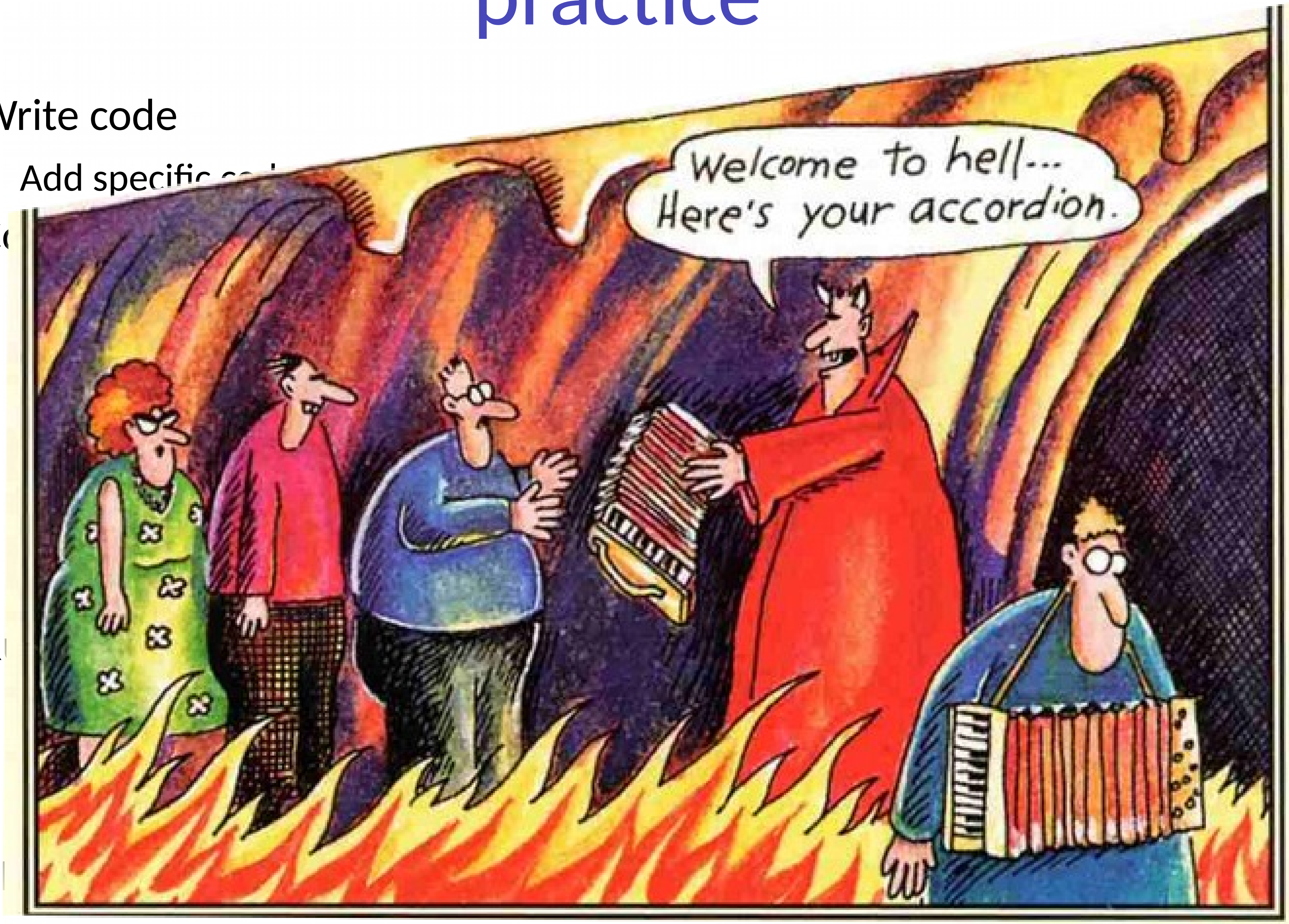


Setting up the build & runtime env

- No real unified way.
- Experiments have their own scripts/packages/suite/tools/ whatever
  - tools to create/discover toolchains and envs (autotools, cmake)
- CERN: `cvmfs` or shared filesystems with custom scripts
- In HPC/HTC, DIY or ask sysadmin
  - Software to build development and runtime libraries (`EasyBuild`)
  - modules (module or lmod) to load an unload environments on demand

Packaging. A wish

- What if I could package my software all together with the libraries to create and run it?

Packaging. You wish...

CERN software for ATLAS:

- Custom system packages required for each operating system
- The most skilled sysadmins in Umeå tried 3 years ago to compile all software and gave up after 2 years. Continuous updates and new libraries where the main issue

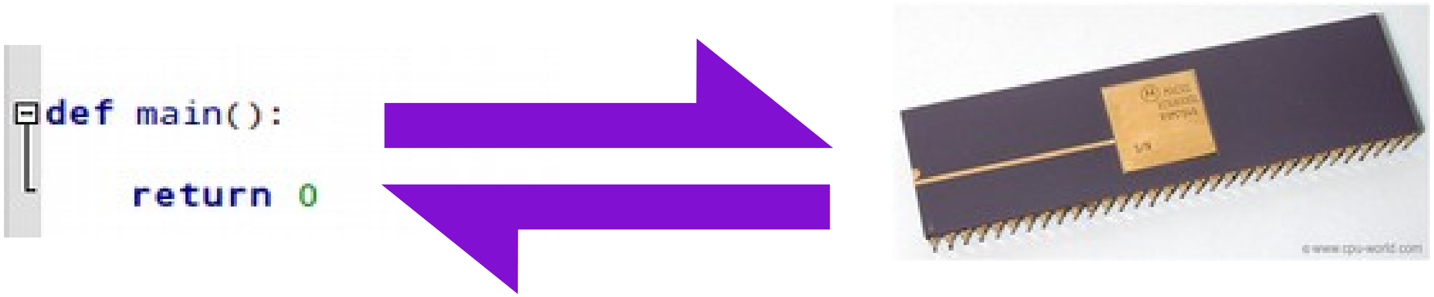
Packaging. Another wish

- ~~What if I could package my software all together with the libraries to create and run it?~~
- Ok what if I send around my preconfigured computer

Send around a machine

- It’s clear that shipping hardware around the world is not the solution:
  - It might get lost
  - someone might compromise it on the way
  - There exist only one copy of it, unless you buy bunches. Bit expensive.
- Solution: have a “software” representation of a machine. Is that possible?

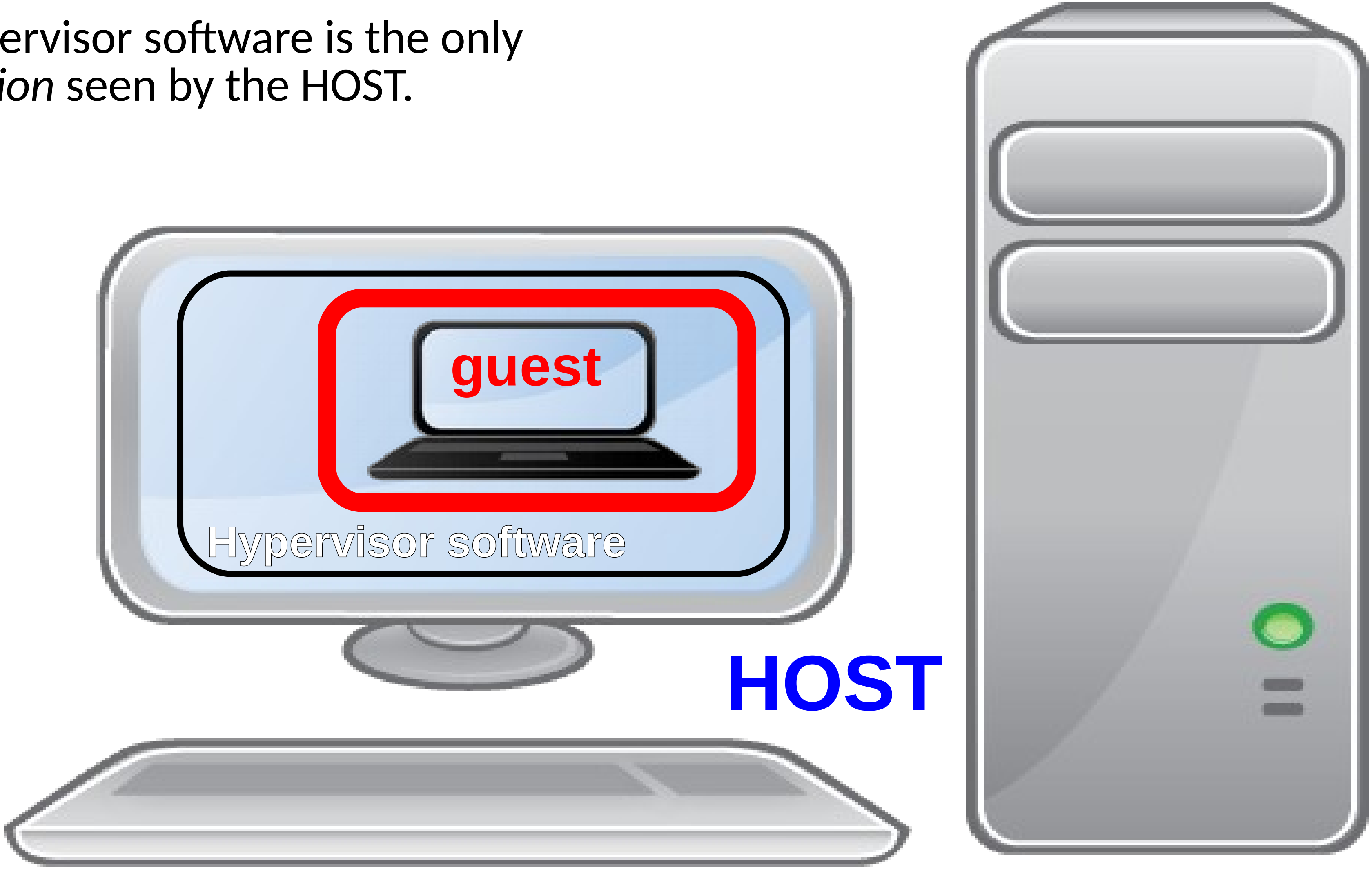
Hardware-Software equivalence



- Everything that can be modeled via software can be created in hardware and vice-versa
- This poses the foundation for machine (hardware) **simulation** and **emulation**
  - **Simulation**: software that behaves exactly like some piece of hardware, internally and externally. For prototypes and testing
  - **Emulation**: software whose *external* behavior *acts as a* piece of hardware. The internals can differ. It ”pretends” to be some hardware.

Virtualization

- Running a virtual computer (guest) inside a physical computer (host)
- The Hypervisor Software *emulates* real hardware
- The Hypervisor software is the only *application* seen by the HOST.

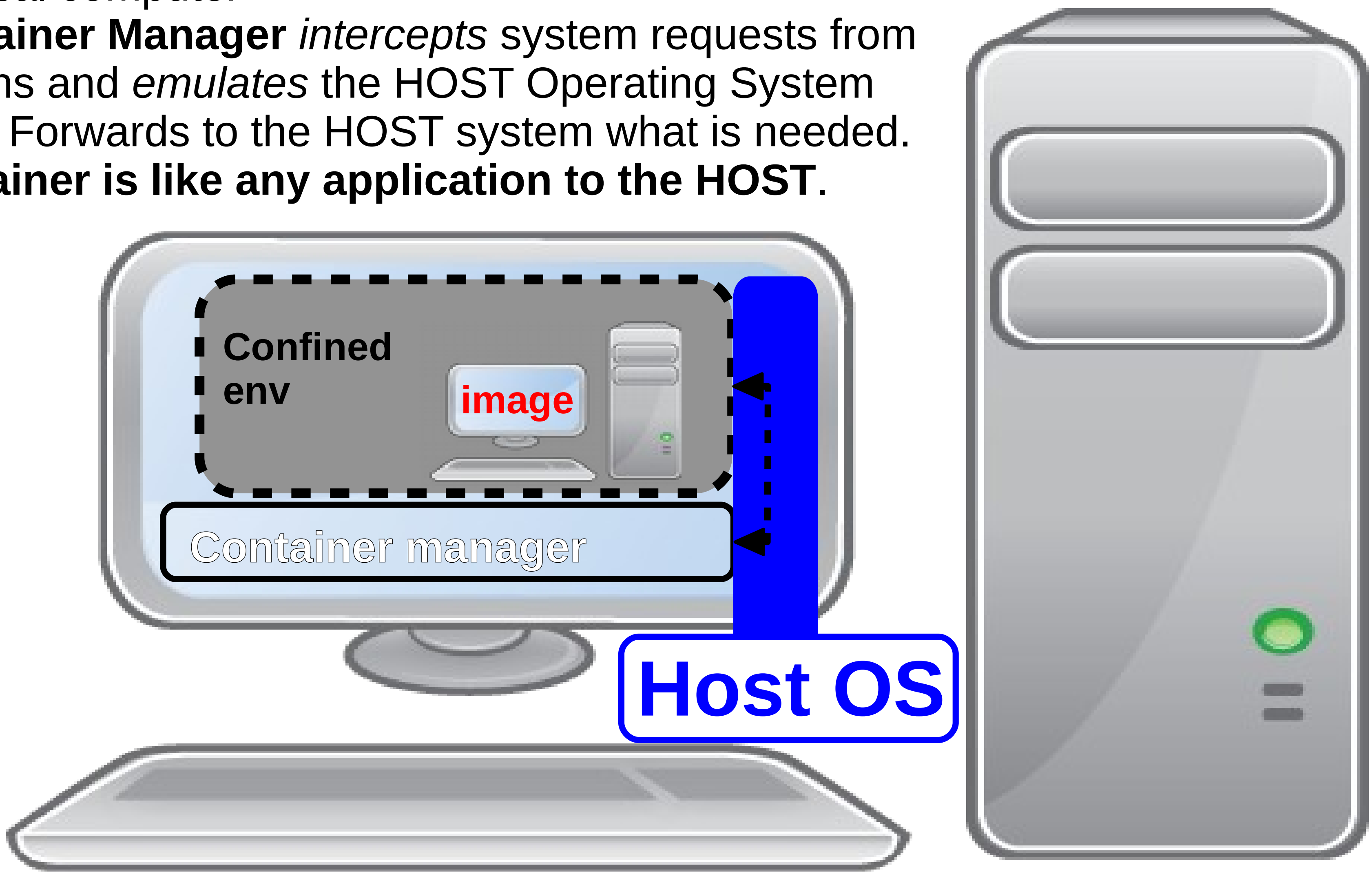


Virtualization

- Running a computer (guest) inside a computer (host)
- The guest machine is usually called Virtual Machine. It carries a full representation of an hardware configuration.
- The Host machine manages the guest machine using something called Hypervisor. The user can manage the machine using the tools provided by the hypervisor.
- The host offers software simulated or emulated hardware, plus it can offer **real** hardware to the guest machine
- The guest machine sees all the software simulated/emulated/virtualized hardware as it was real hardware, but it can also be aware that it is virtualized to boost performance
- A virtual machine can contain ANY operating system regardless of the Host OS. (Windows, Linux, Mac, BSD, Android?)
- Was invented mostly for
  - Ease of management of multiple machines in big data centers, without the need to buy dedicated hardware for each machine
  - Emulate hardware and run multiple operating systems on the same machine

Containerization

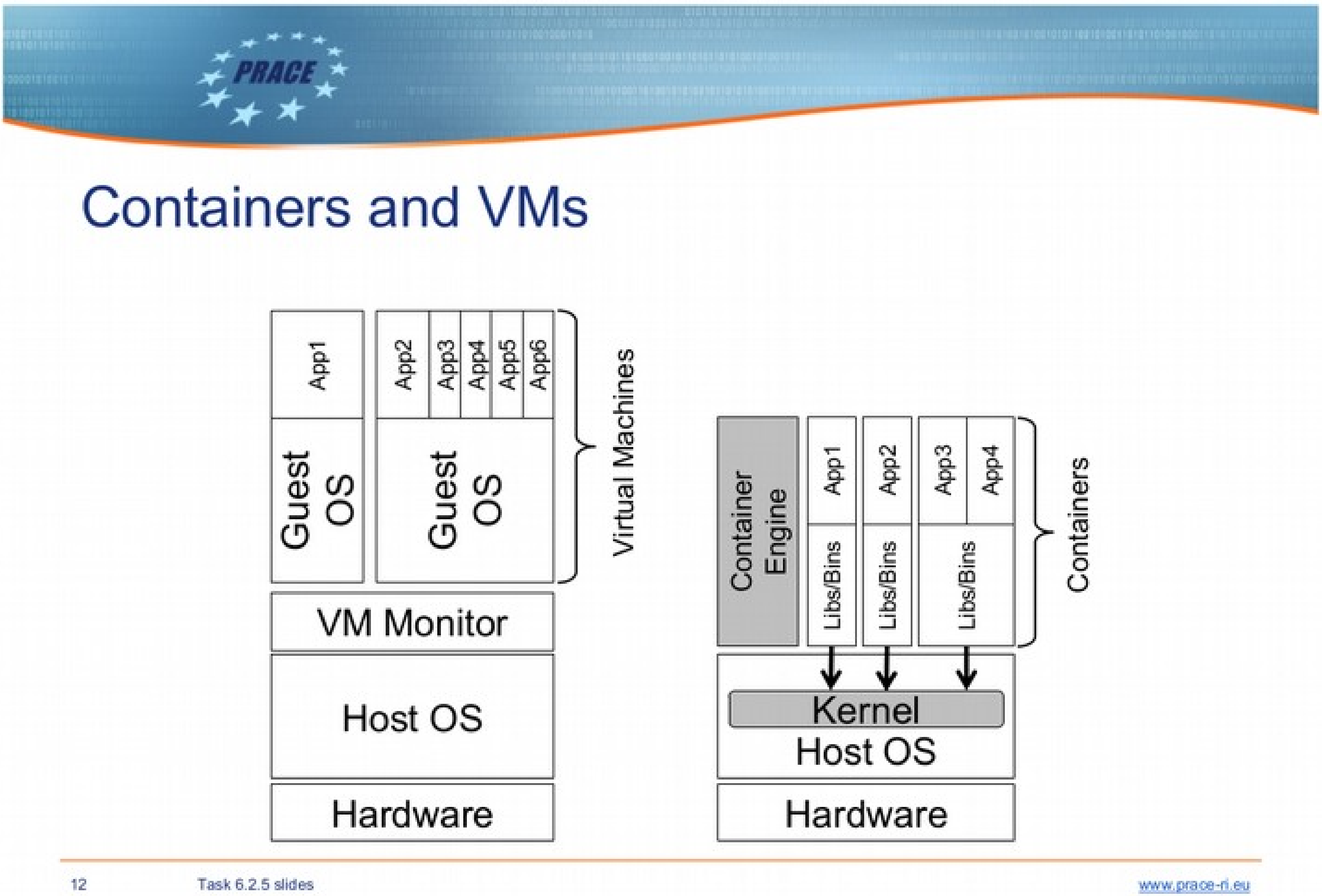
- Running a different* Operating System **image** inside a *confined environment* inside the HOST Operating System of a physical computer
- The **Container Manager** *intercepts* system requests from applications and *emulates* the HOST Operating System response. Forwards to the HOST system what is needed.
- **The container is like any application to the HOST**.



Containerization

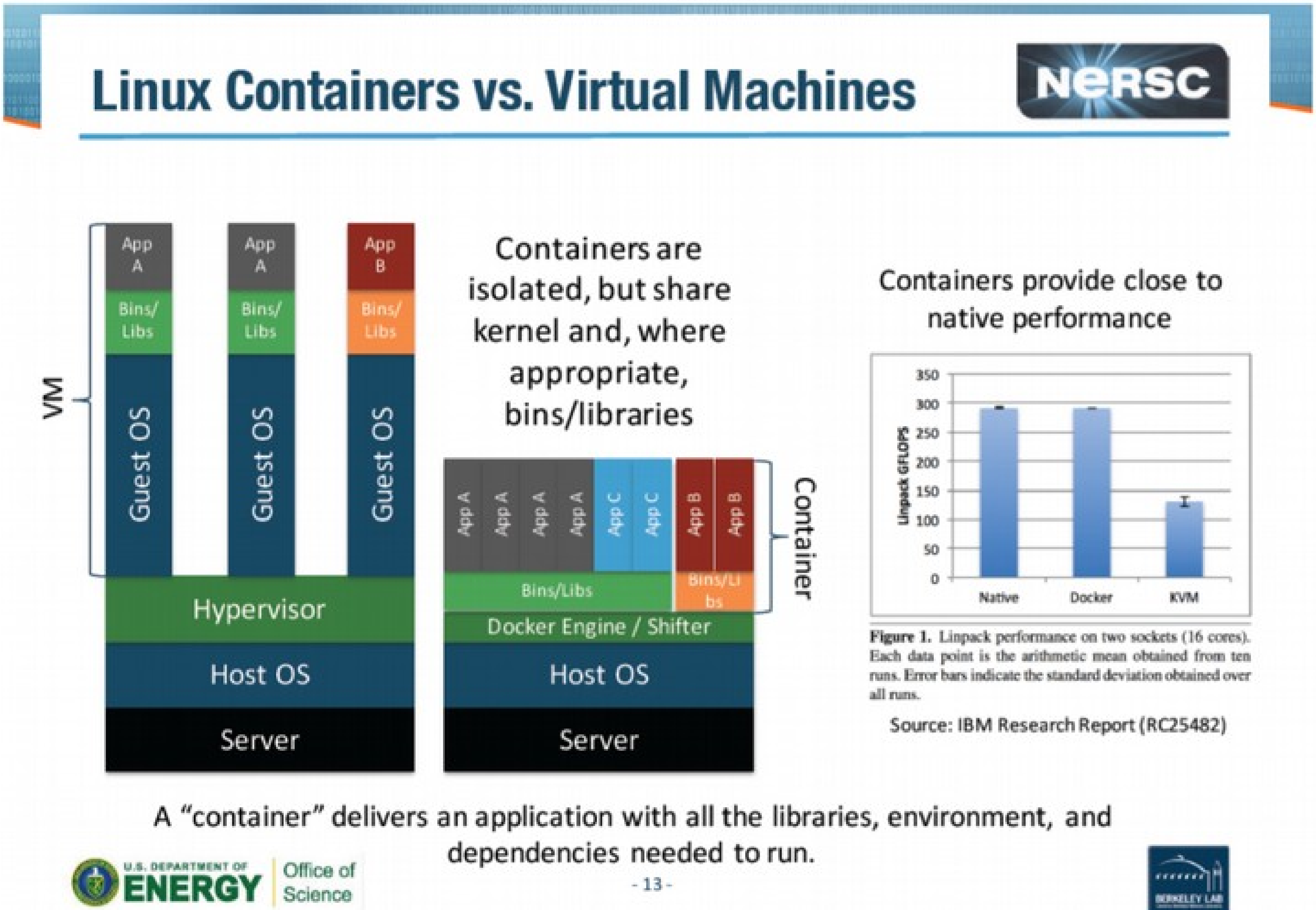
- Running an Operating System **Image** inside a **confined environment** in an existing host operating system)
  - *Different OS: Not all operating systems can work in a container. Only those that share a similar *kernel architecture*, that is,
    only Linux machines on a Linux Host OS.
    In case of a different kernel, the kernel requests are *translated* to the Host Kernel.
  - **Image**: a “snapshot” of the files in a system
- The user can manage the **Image** using something called Container manager, a set of tools and commands to deploy/start/stop/install/configure the contents of the image.
- The Host OS treats the container and its applications like a single application running in the OS. The OS activity inside the container is *emulated* by the container system.
- The application in the Image sees only the containerized OS and NOT the Host OS. It sees the exact same hardware that the Host OS has.

Architecture summary



Credit: Abdulrahman AZAB, PRACE technical talk, NorduGrid 2018, Garching Bei München, Germany
http://indico.lucas.lu.se/event/908/session/3/contribution/12

Architecture facts



Credit: Abdulrahman AZAB, PRACE technical talk, NorduGrid 2018, Garching Bei München, Germany
http://indico.lucas.lu.se/event/908/session/3/contribution/12

When to use what?

Virtualization:

- Environments in which you have total control
- Environments that must run a different operating system technology within a HOST OS (Example: running a Windows VM inside a Linux HOST)
- Complex setups that involve different platforms (OS technology, hardware architecture)

Containers:

- Systems with similar OS technology (i.e. multiple linux versions/distros)
- Application confinement
- Complex test setups that involve multiple distributed systems

“a ghost is haunting computing”

- Virtualization and containerization was so cool that hardware vendors included the so-called virtualization instructions
- A VM/Container is allowed to *see and use* the actual hardware
- 2018: Meltdown and Spectre security vulnerabilities
  - Every processor since 1995 (few exceptions)
  - A process can *leak* its memory info to *some other process*
  - The fixes out there slow down performance of at most 20%
  - Source: https://meltdownattack.com/
- *=> Virtualization and containers are considered intrisically insecure until a new generation of processors is born*
- => It’s hard to convince a sysadmin virtualization is good!

The Cloud

- With a huge computing power, say an entire data center, one can create a large number of virtual machines or containers on demand
  - *Cloud interfaces* to request resources (computing or storage)
    - **IaaS,** Infrastructure as a service : request a computer architecture or a whole network of computers. It only provides the hardware (virtualized or not)
    - **PaaS**, platform as a service: request some hardware and an operative system inside, along with some management software (could be docker for example)
    - **SaaS,** Software as a service: the user just requests a service to use. A common historical example is web hosting, nowadays one can think of services like Jupiter Notebooks servers or Online latex editors like overleaf.
  - Products: OpenStack, Google Kubernetes, Amazon EC2 / S3...
    - **Not compatible with each other, for marketing reasons.**
- Users can create their own predefined setup and make it available on the internet.

Next steps

- In this course: Containerization
  - **Docker**: do-it-yourself container technology with online repositories
  - **Singularity**: HPC-level container technology.
- NOT in this course: Virtualization
  - VirtualBox: desktop Hypervisor
  - See slides from our MNXB01 course if curious http://www.hep.lu.se/courses/MNXB01/

Containerization in Scientific Computing

- Goal: provide a container ready with the environment for your kind of research

1) Create a container on your laptop and test it

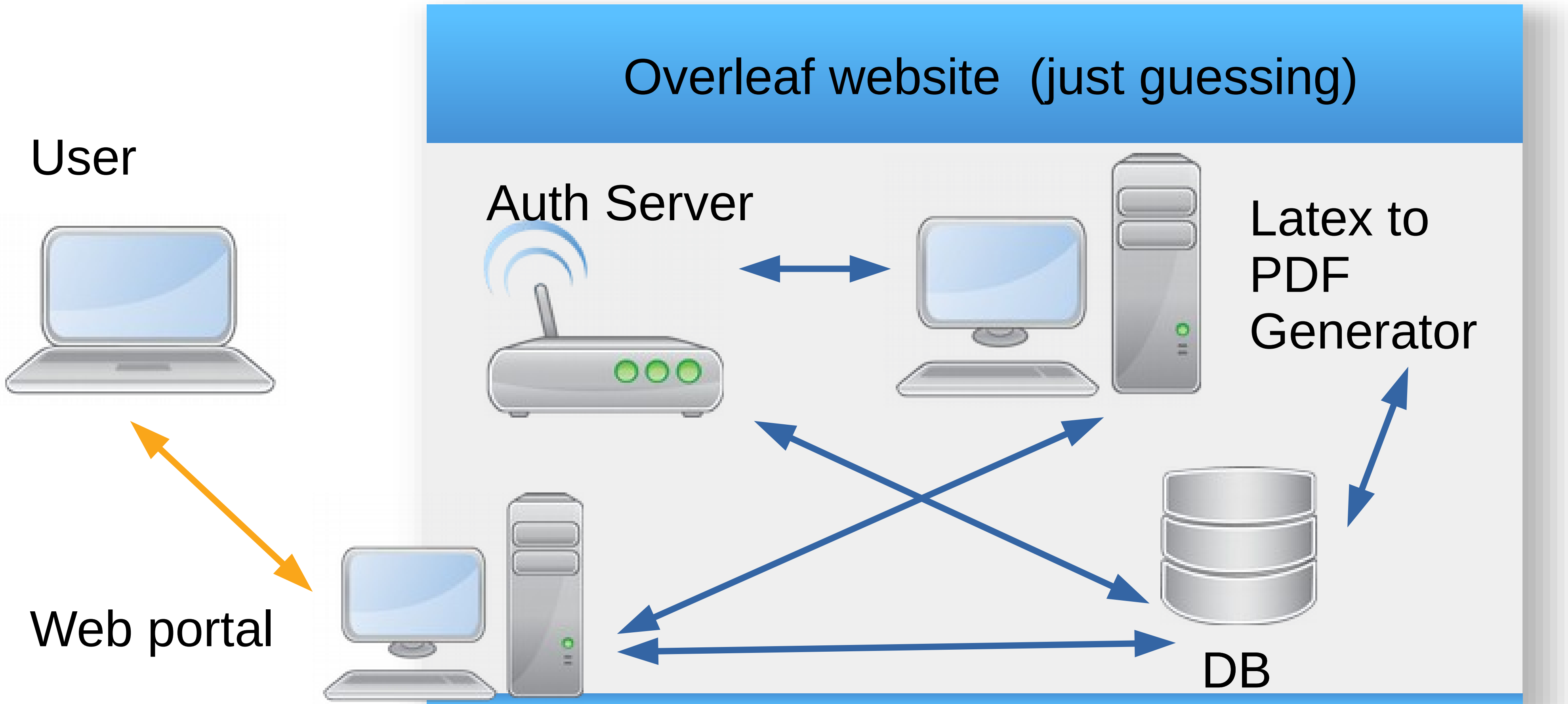
2) Use the container on a research facility (or on the cloud) where that container technology is supported

Technologies: Docker

- https://www.docker.com/: commercial solution
- https://www.docker.com/products/docker-engine community solution that we will use
- Installation and configuration (Will do on the 23rd): https://hub.docker.com/search/?type=edition&offering=community
- Tutorials (TODO: evaluate one):
  - https://training.play-with-docker.com/beginner-linux/ Homework! More info via email.
  - https://docs.docker.com/get-started/ Will do on the 23rd

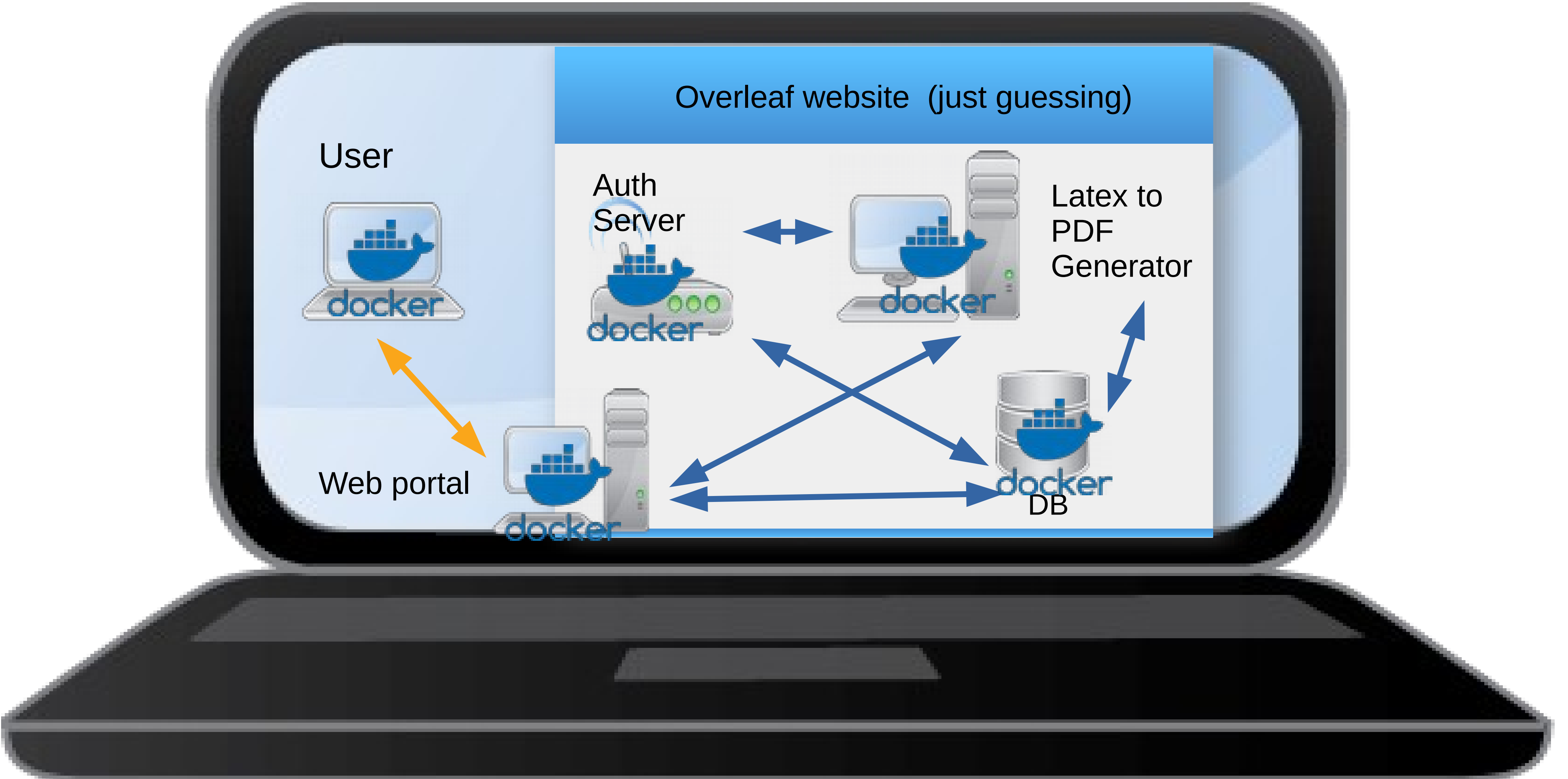
Docker

- Was invented mostly for complex applications that involve different servers (typically, web applications)



Docker

- So that the developer can have everything in their machine to test
- Arrows: docker's own virtual (emulated) network



How will we use docker

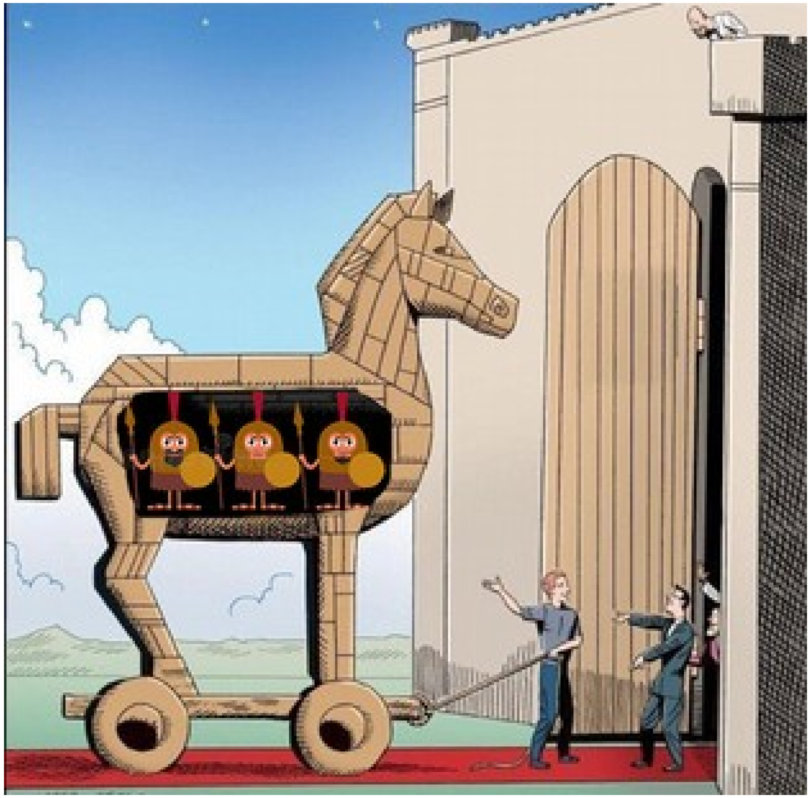
- Create an environment that runs your application
- Give it to other researchers to reproduce your results or to do their research in a similar environment

Problems: security

- Trojan-horse potential
- Datacenters and sysadmins do not like root users
  - An unskilled user might harm the whole system by mistake!

=> **in Datacenters** :

- Images have to be **certified** to be not harmful
- User **cannot be root**
- Images are **readonly**



Implications

- It's not possible to modify the content of the image
- It's not possible to get data out of the image
- It's not easy to install new software in the image

An alternative for HPC: Singularity

- Runs a container in user space
- Mounts local folder inside the container transparently
- Security can be fine-tuned by the sysadmin
- Question: Docker-Singularity compatibility?

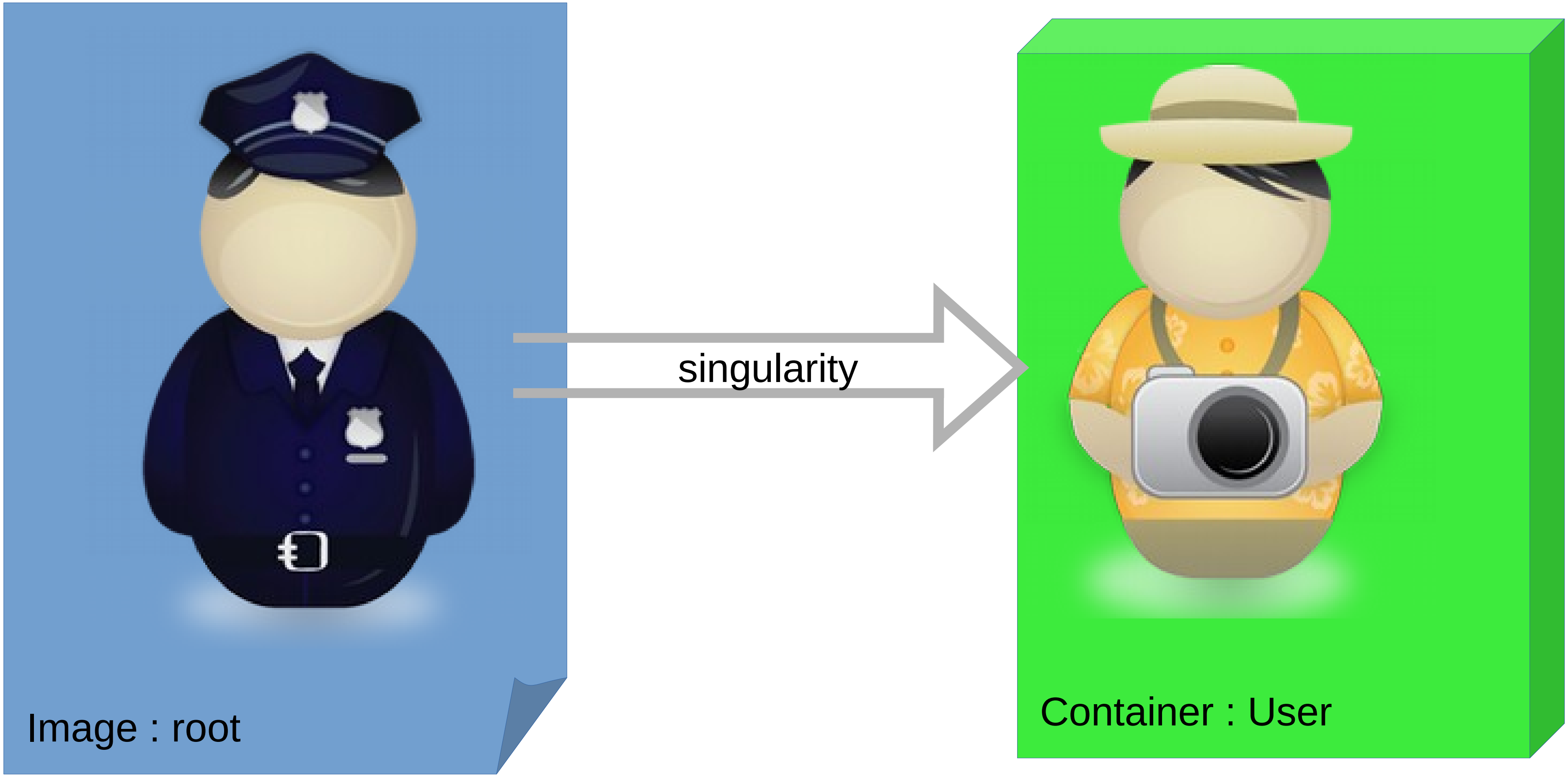
Technologies: Singularity

- https://www.sylabs.io/docs/
- Can be installed by user, but
  we will not discuss this in this course
- A container it’s a file, that is also
  an executable
- A user can invoke the environment for a job by just
  running the container

```
./singularityimage myscript.py
```

Singularity approach

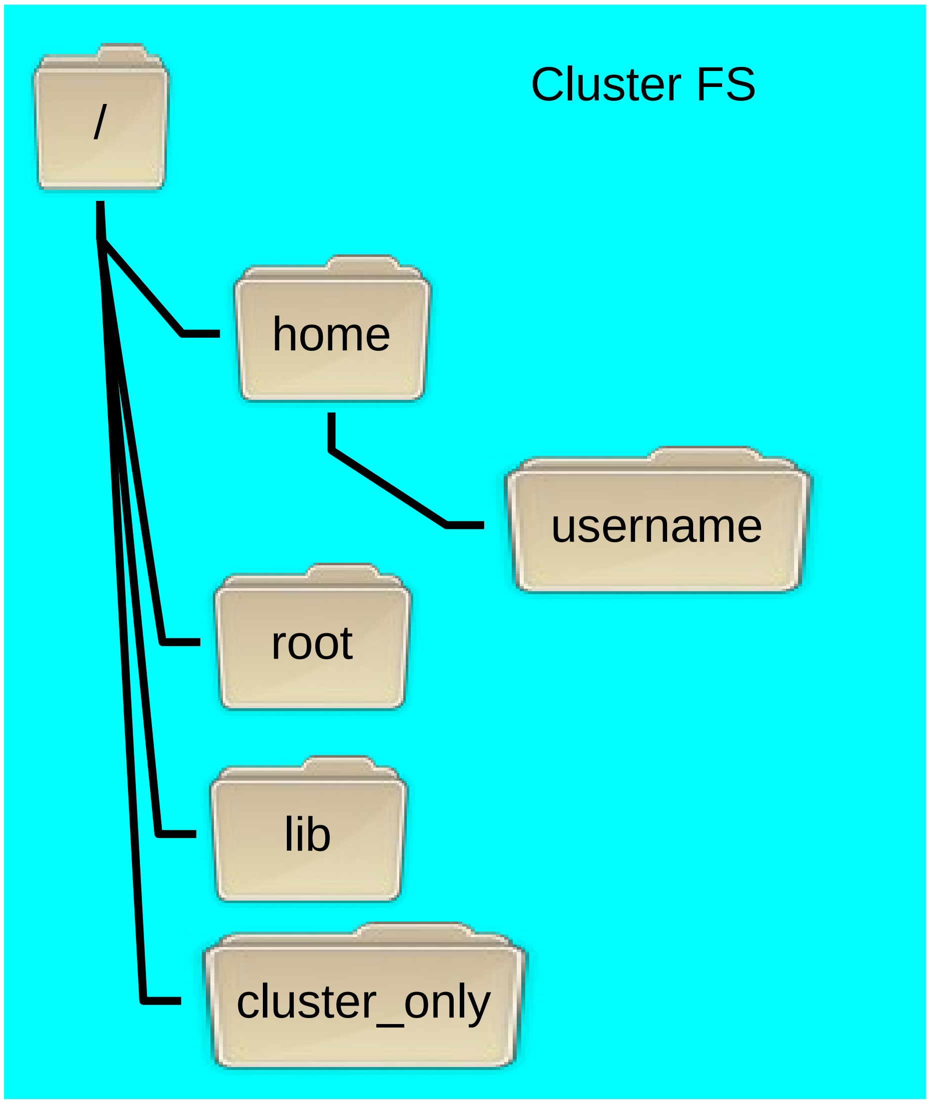
- Root in the image becomes a normal user in the container, hence can't modify the image/container.

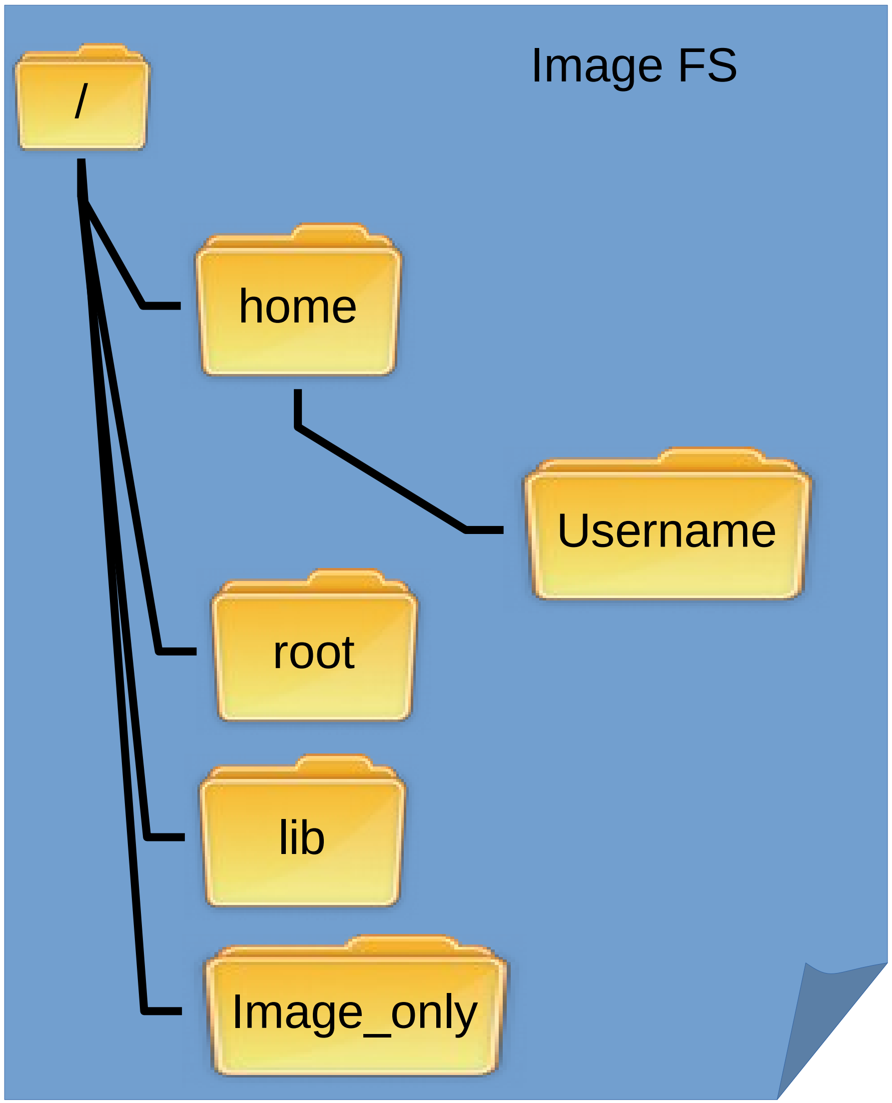


Singularity approach

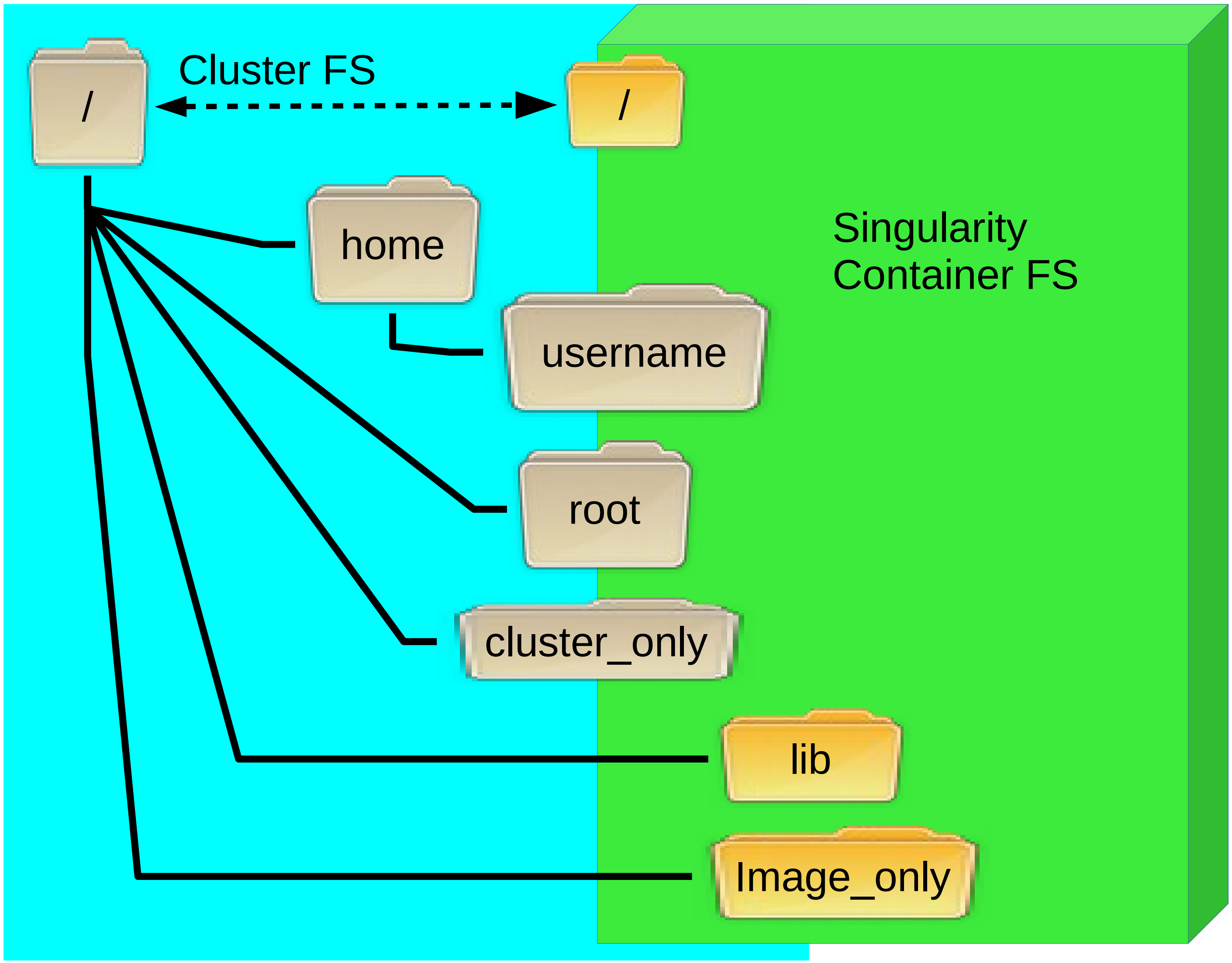
- The user home folders on the cluster are mounted inside the container environment. The user **can write** in their home while inside the container.
- Other paths of the cluster filesystem **that are not present in the image** are automatically mounted in the container.
- Paths in the container that exist on the cluster are **overridden** by the containers one, that is, the user can only see the containers one (overlay effect)

Overlay – before:





Overlay – After:



Prepare for tutorial 18/4

- Completely new to bash command line? Please do this tutorial: https://linuxsurvival.com/linux-tutorial-introduction/
- Need some refresh of linux command line stuff? http://rik.smith-unna.com/command_line_bootcamp/
- Feeling brave? Here’s a tutorial to learn bash scripting. We will use some of this knowledge during 18/4 https://www.learnshell.org/en/Welcome
- Requirement: need to be able to use a text editor on the cluster. We will show you options.

Images references

- Libreoffice Gallery
- Gary Larson, The Far Side, taken from http://www.dedics.co.uk/temp/welcome%20to%20hell.jpg
- https://knowyourmeme.com/photos/1393740-trojan-horse-object-labels
- https://meltdownattack.com/
https://meltdownattack.com/

Software references

- `EasyBuild`, tool to build devlopment libraries
  https://github.com/easybuilders
- `Lmod`, tool to manage build/runtime environments
  https://github.com/TACC/Lmod
- `autotools`, suite to configure build environments for compilation
  https://www.gnu.org/software/automake/
- `cmake`, suite to configure build environments for compilation
  https://cmake.org/