HPC AND CURRENT EU DEVELOPMENTS

Raymond Oonk (SURF , NL)

SURF

Program

Agenda GEO-OPEN-HACK 2024

OPEN EARTH MONITOR

Time	Sunday 23-Jun-24	Monday 24-Jun-24	Tuesday 25-Jun-24	Wednesday 26-Jun-24	Thursday 27-Jun-24	Friday 28-Jun-24
08.00-08.30					Canadian Pancake Breakfast IIASA Schlossrestaurant	
08.30-09.00		Get together IIASA WODAK meeting room	Get together IIASA WODAK meeting room	Get together IIASA WODAK meeting room		Get together IIASA WODAK meeting room
09.00-09.30		Keynote Raymond Oonk, SURF	Keynote Tom Hengl, OGH	Keynote Jan Verbesselt & Dainius Masiliunas	Keynote Edzer Pebesma, Uni Münster	Keynote Wolfgang Wagner, TU Wien & EODC
09.30-10.00		Giuseppe Amatulli Geo-Processing with HPC	Pieter Kempeneers Geo-python with HPC	Keynote Patrick Griffiths, ESA	Claus Michele & Valentina Premier openEO	Anne Fouilloux & Tina Odaka Pangeo
10.00-12.30				Antonio Fonseca ML with HPC		
12.30-13.30		Lunch break IIASA Gvishianhi meeting room	Lunch break IIASA Gvishianhi meeting room	Lunch break IIASA Gvishianhi meeting room	Lunch break IIASA Gvishianhi meeting room	Lunch break IIASA Gvishianhi meeting room
13.30-14.00		Big Data Story Giuseppe Amatulli	Big Data Story Milutin Milenković & Florian Hofhansl	Big Data Story Yu-Feng Ho & Johannes Heisig	Big Data Story Valentina Premier	Big Data Story Leandro Parente
14.00-17.30		Working with your data	Park Visit Laxenburg Park -- START: 16.00h Working with your data	Working with your data	Working with your data	Open floor sessions OEMC and other open initiatives. OEMC data platform & feedback. Where to implement my big data problem?
18.00-21.00	Ice Breaker Event Rest. Stöckl im Park Prinz-Eugen-Strasse 25 1030 Vienna			Social Event IIASA Schlossrestaurant Herzog Albrecht-Strasse 1 2361 Laxenburg		

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No.101059548

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Outline

1) Introduction
2) Compute architecture
3) Large-Scale Computing Services (LSCS)
    - Supercomputer (traditional HPC) , HTC , Cloud
4) Europe’s digital transition
    - common European Data Spaces , SIMPL , EuroHPC, DestinE
5) Possible misconceptions (if time allows)
6) EESSI (if time allows)

Introduction

Your guide today: (J. B.) Raymond Oonk

- Sr. Advisor SURF Cooperative (NL)
- Distributed Data Processing & Big Data innovation lead
  - High throughput computing (e.g., Copernicus, CERN, SKA)
  - European projects (e.g., EOSC, Green Deal Data Space, C-SCALE)

- PhD Astronomy (Leiden University 2011)
- Postdoc (Leiden University , ASTRON)
- Research: Astrophysics (Intergalactic medium)

“ Role of an advisor is to try to understand the research problem & workflow, and see if/how it can fit on a large-scale computing (and data) infrastructure “

SURF

Service Provider	Innovator	Association	Goals
ICT infrastructure & services (ISO 27001)	Push digital innovation & transformation	Knowledge sharing: Expertise, training, meeting & support	Acceleration of 100+ member goals via collaboration

SURF is the collaborative organisation for IT
in Dutch education and research

SURF
R. Oonk

SURF Services

SURF develops IT services for education and research. Members and non-members can make use of these (50+) services: https://www.surf.nl/en/services

- Compute services
- Data services
- Network connectivity
- IaaS (Cloud / VRE)
- Security, Trust & Identity
- Digital Platforms
- Agreements with market parties
- Expertise, advice & training

(Tape library 2022)

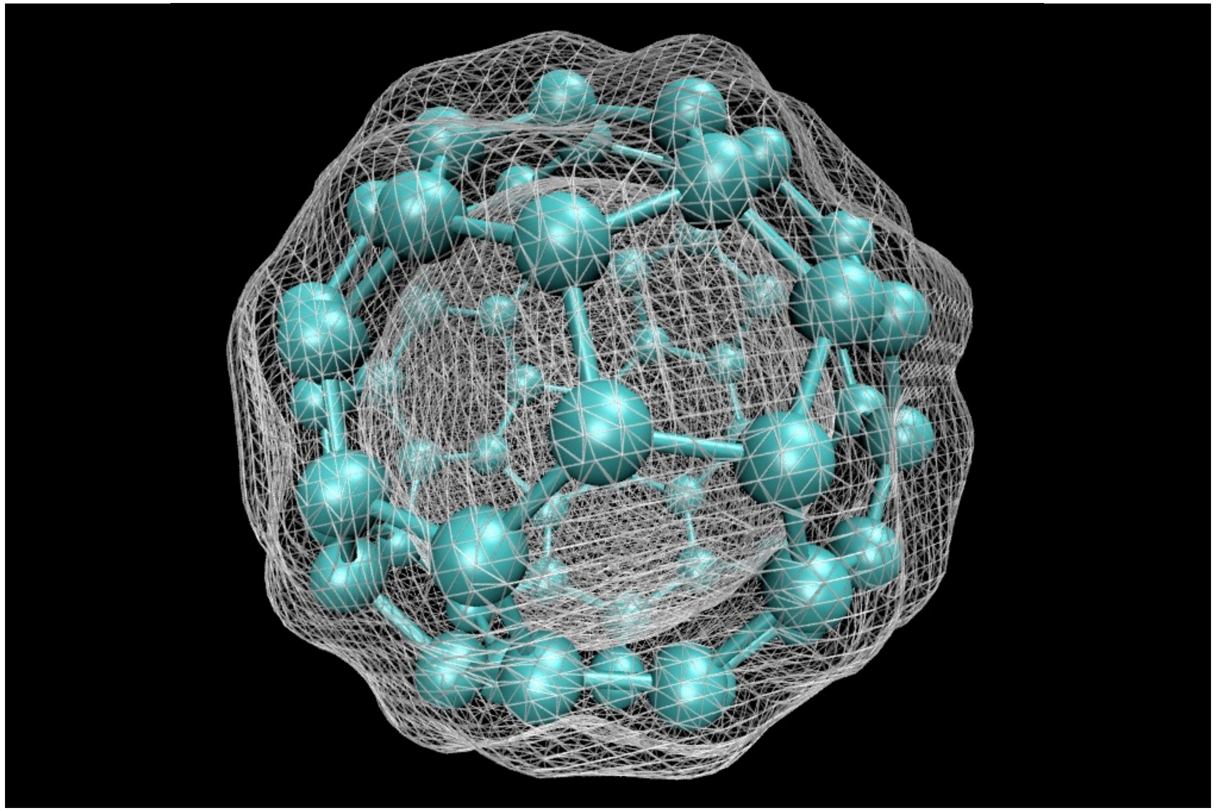
SURF Cooperative has 100+ member institutions in Dutch academia

Compute architecture

Outline

- Introduction to High Performance Computing (or equivalently large-scale computing)
  - Definitions
  - Parallel programming
- Running jobs
  - Definitions for jobs
  - (Hands-on exercises)

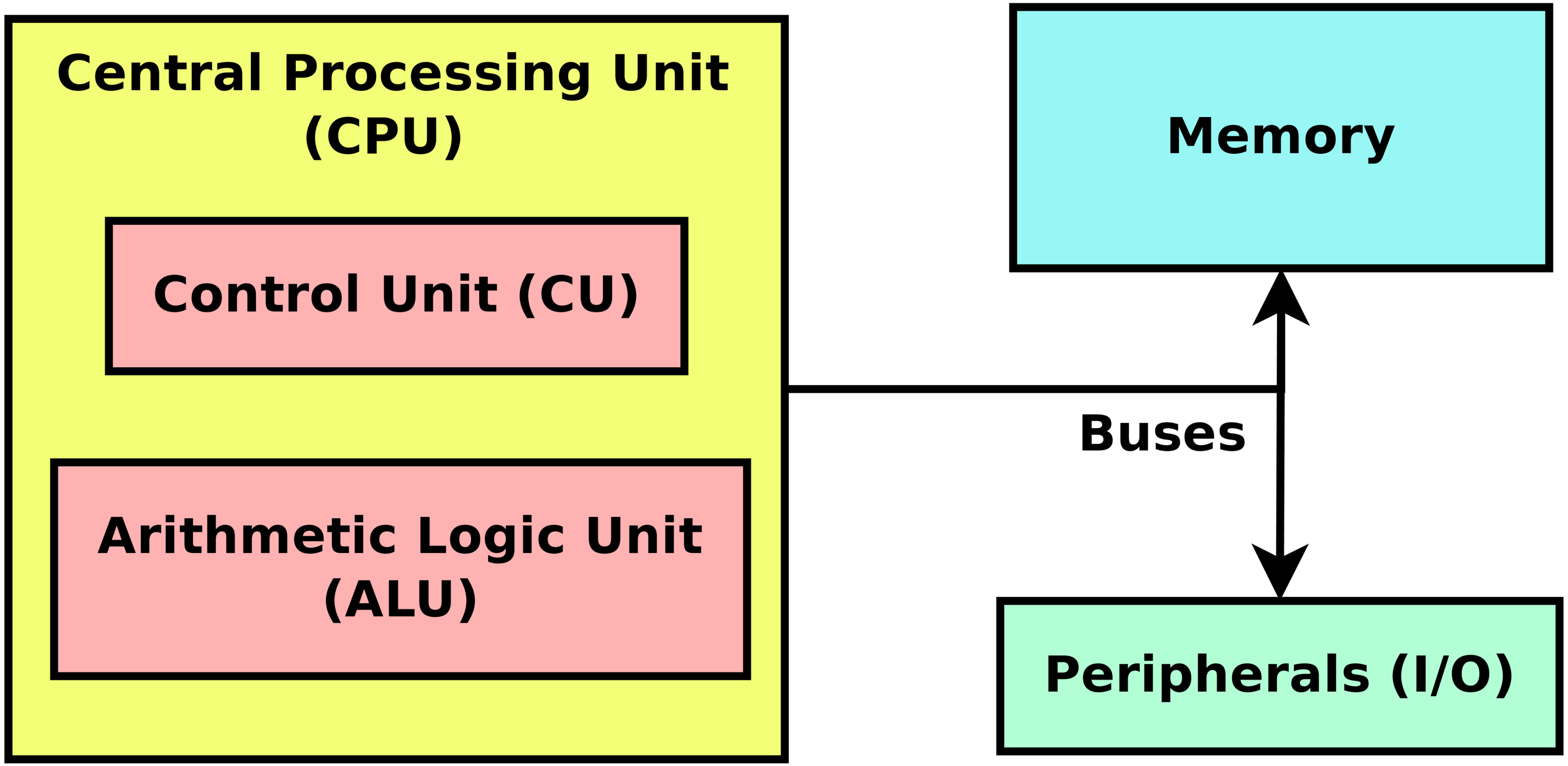
High-performance computing (HPC) is …



Large-scale or high-performance computing (HPC) is …

- *… an area of computer-based computation. It includes all computing work that requires a high computing capacity or storage capacity.*
- *… the use of parallel processing for running advanced application programs efficiently, reliably and fast.*
- *… the practice of orchestrating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business.*

A computer is …



… and Boolean logic (0’s and 1’s)

A central processing unit (CPU) is …

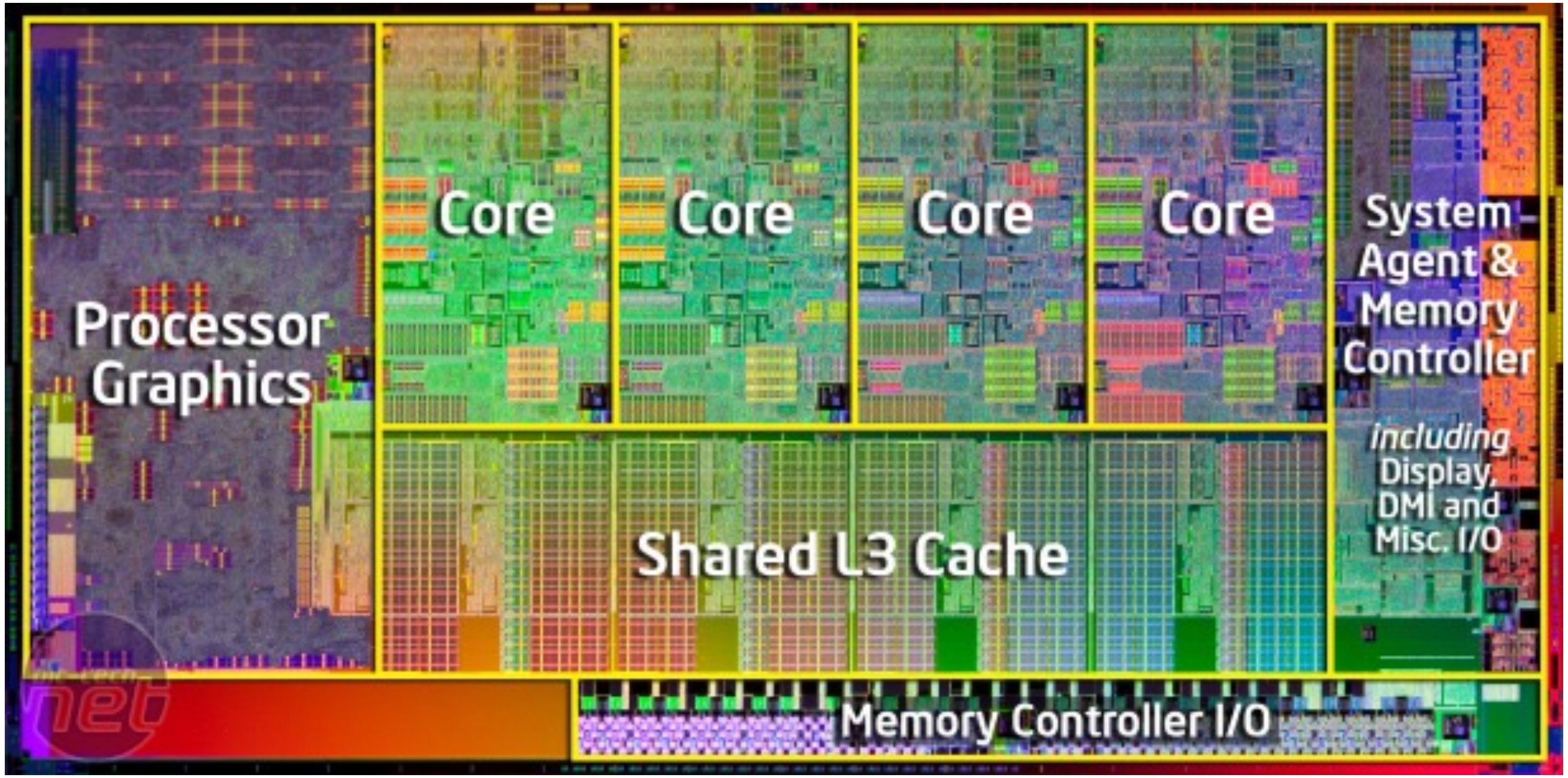


Image source: https://bit-tech.net/reviews/tech/cpus/intel-sandy-bridge-review/1/

Image source: https://www.computerhope.com/jargon/s/sandybri.htm

A central processing unit (CPU) is …

LONG TIME: X86_

NOW: INCREASING COMPLEXITY

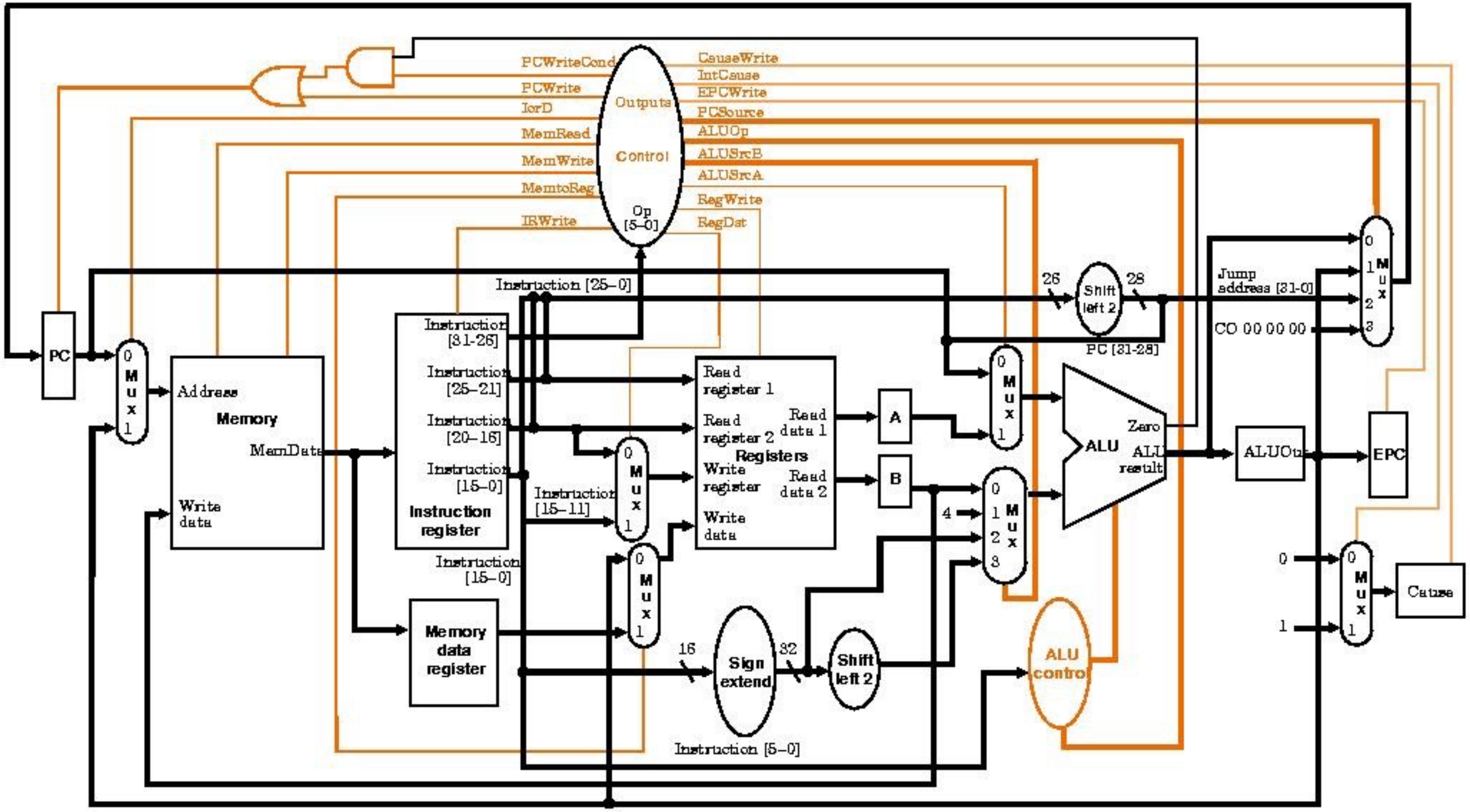
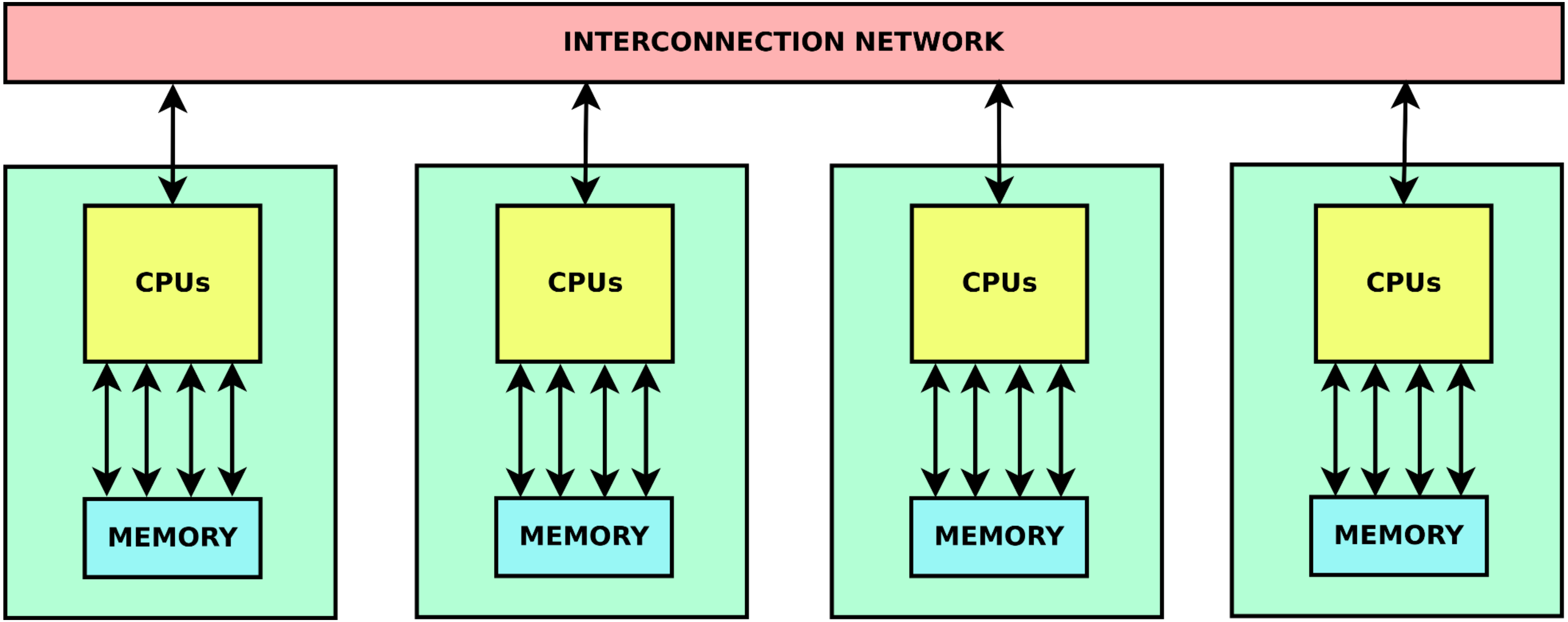
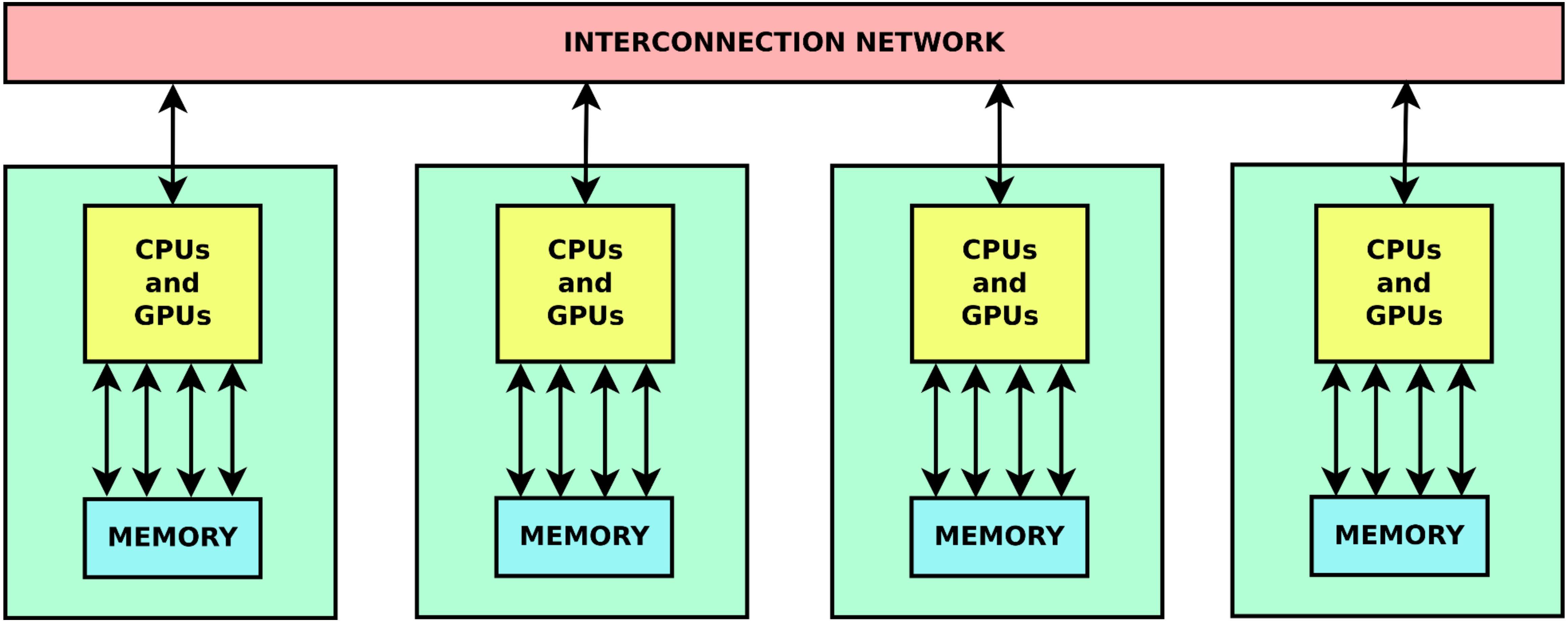


Image source: http://people.cs.pitt.edu/˜don/coe1502/current/Unit4a/Unit4a.html

A larger computer actually is …



A larger computer actually is … (incl. accelerators)



Large-scale or high-performance computing (HPC) …

- *… is an area of computer-based computation. It includes all computing work that requires a high computing capacity or storage capacity.*
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- *… is the part of computing focused on making computers collaborate effectivey and efficiently (hardware and software) up to very large scales*

Note: diversity in architectures and optimizations is increasing starkly and this requires more technical knowledge for efficient use of infrastructure by researchers – relative code performance is decreasing!

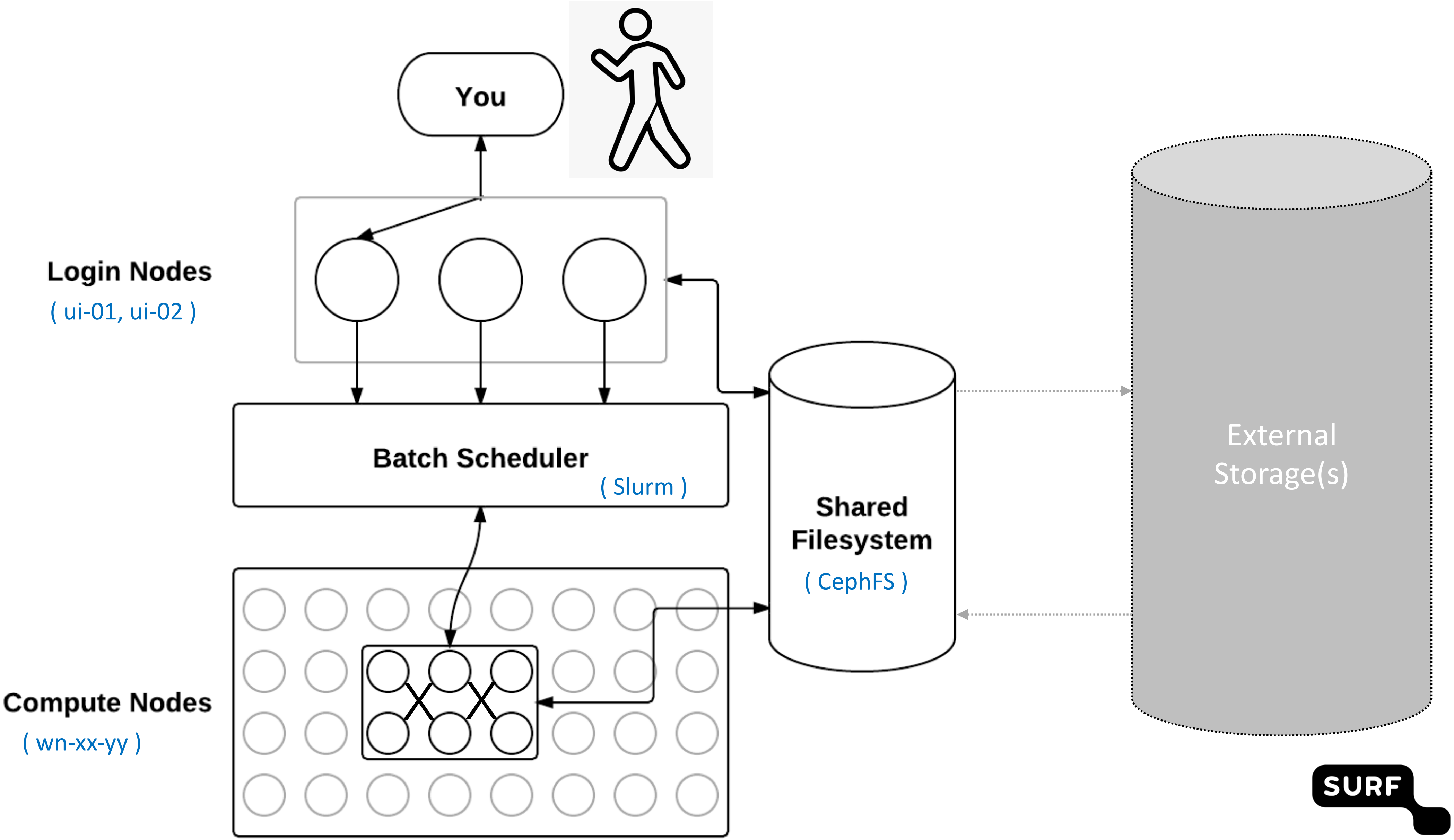
Dutch national supercomputers: performance increase

Year	Machine	R_{peak} (GFlop/s)	kW	GFlop/s/ kW
1984	CDC Cyber 205 1-pipe	0.1	250	0.0004
1988	CDC Cyber 205 2-pipe	0.2	250	0.0008
1991	Cray Y-MP/4128	1.33	200	0.0067
1994	Cray C98/4256	4	300	0.0133
1997	Cray C916/121024	12	500	0.024
2000	SGI Origin 3800	1,024	300	3.4
2004	SGI Origin 3800 +SGI Altix 3700	3,200	500	6.4
2007	IBM p575 Power5+	14,592	375	40
2008	IBM p575 Power6	62,566	540	116
2009	IBM p575 Power6	64,973	560	116
2013	Bull bullx DLC	250,000	260	962
2014	Bull bullx DLC	~ 1,000,000	520	1923
2017	Bull bullx DLC + KNL	~ 1,840,000	850	2168
2021	Lenovo AMD (1st phase)	~ 6,100,000	610	10000
2023	Lenovo AMD (2nd phase)	~ 17,900,000	1150	15565
2016	*Raspberry PI 3 (35 euro)*	*0.44*	*0.004*	*110*

Outline

- Introduction to High Performance Computing (or equivalently large-scale computing)
  - Definitions
  - Parallel programming
- Running jobs
  - Definitions for jobs
  - (Hands-on exercises)

Schematic overview of a supercomputer (batch system)



Running jobs: how-to guide

- Schedulers distribute work to *batch nodes*
- Workflow:
  - 1. **You** upload your data from your computer to the cluster system
  - 2. **You** create a job script with the work steps
  - 3. **You** submit the job script to the scheduler
  - 4. **The scheduler** looks for available computers to run your work
  - 5. When a batch node with the requirements you specified becomes available, your work runs
  - 6. When the job is finished, **you** download the results to your computer
- Batch scheduler on Spider: SLURM (http://slurm.schedmd.com)

Running jobs: useful commands of the SLURM scheduler

- sbatch *<jobscript>* - submit a job to the scheduler
- squeue -j *<job_id>* - inspect the status of job *<job_id>*
- squeue –u *<user_id>* - inspect all jobs of user *<user_id>*
- scancel *<job_id>* - cancel job *<job_id>*
- scontrol show job *<job_id>* - show estimated job start

Types of Large-Scale Computing Services (LSCS)

Large-scale computing systems are per definition complex

Why should anyone consider using these?

- Some problems do not fit on a single machine
- Time to result is reduced
- Shared systems typically have better utilization
- Expertise can be bundled effectively
- Knowledge can be shared effectively
- Economy-of-scale effects for investment

Fitting your problem to a LSCS may (initially) be challenging

Supercomputer (traditional HPC)

A **supercomputer** is a type of computer with a high level of performance as compared to a general-purpose computer. The performance of a supercomputer is commonly measured in floating-point operations per second (FLOPS). Nowadays we measure in PFLOPS (10^{15} FLOPS) or EFLOPS (10^{18} FLOPS) for the largest systems.

All of the world's fastest 500 supercomputers run on Linux-based operating systems.

One of defining aspects of supercomputers is fast interconnects (e.g., infiniband) between computer servers and the use of Message Passing Interface (MPI) to enable parallel processing on **complex tightly coupled calculations** (e.g., simulations) in an efficient manner.

Source: Wikipedia

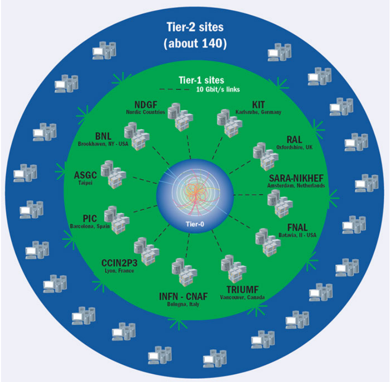
TOP 500: https://top500.org/

High Throughput Computing (HTC)

High-throughput computing (**HTC**) is the use of many computing resources over long periods of time to accomplish a **data intensive** computational task (often semi-continuous data streams).

The HTC community is also concerned with robustness and reliability of jobs over a long-time scale. That is, being able to create a reliable system from unreliable components. This research is similar to transaction processing, but at a much larger and often distributed scale.

A typical example for HTC is Grid computing and in this context HTC is defined as *"a computing paradigm that focuses on the efficient execution of a large number of* ***loosely-coupled*** *tasks"*, while Supercomputer (HPC) systems tend to focus on tightly coupled parallel jobs, and as such they must execute within a particular site with low-latency interconnects.



Source: Wikipedia

Cloud Computing (public, private)

Cloud computing can be defined as the practice of using a network of remote servers hosted on the internet to store, manage, and process data, rather than a local server or a personal computer.

To facilitate rapid (on-demand) availability of computer (and data) resources, cloud computing often makes use of **virtualization techniques** to offer a subset of a physical server in virtual form (e.g., virtual machines, containers). HPC and HTC can in certain cases also be provided via cloud computing techniques.

Cloud is a technique to offer resources. One can try to discriminate between Public (commercial) and Academic (private research) Cloud as follows:

- Public Cloud: “infinite resources” (i.e., there is always significant spare capacity to allow for instantaneous provisioning and the pricing incorporates this – demand driven)
- Private Cloud: “infinite work/jobs” (i.e., there is always more work than capacity and hence work is typically regulated by a queuing and scheduling system – capacity driven)

Source: Wikipedia, Oxford Languages

Spider (HTC / batch): accessible to you this week

Interactive data processing
Interactive data visualization
Interactive monitoring

Interactivity

Event-driven processing
Customizable frameworks
Software portability & containers

Scientific workflows

Role-based project spaces
Data publication & redistribution
Access federation

Collaboration

User-facing utilities

Fast local disks for high I/O

Scalable Petabyte staging storage

Data Archive storage

External Scalable Distributed storage

Storage integration

Scalable batch processing cluster

Private project-tailored clusters

Private project-tailored nodes

ANSIBLE

Platform Deployment

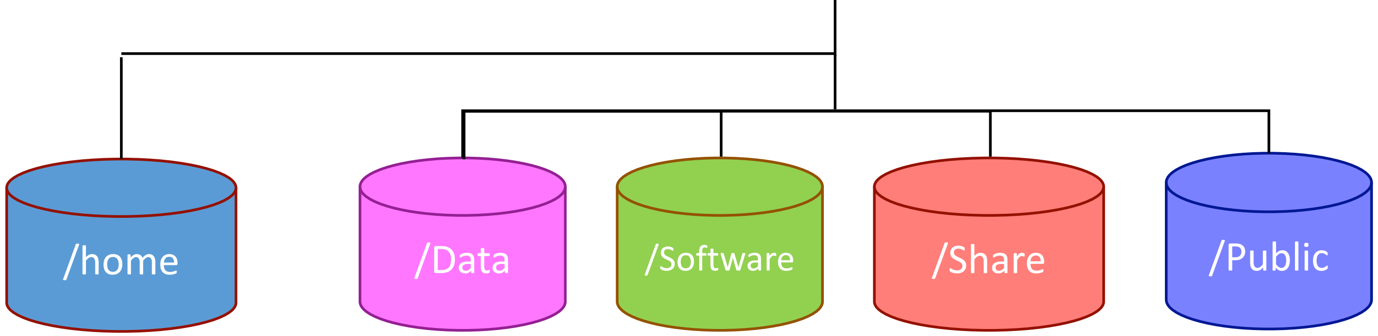
Elastic Cloud

SURF

Terraform

Resource Provisioning

File systems on Spider



- **/home**
  - Part of (slow) shared filesystem (CephFS) that is globally mounted of all nodes
- **/project**
  - Part of (slow) shared filesystem (CephFS) that is globally mounted of all nodes
  - Role-based access control (https://doc.spider.surfsara.nl/en/latest/Pages/about.html)
  - 4 sub-folders (Data, Software, Share, Public)
- **scratch via $TMPDIR**
  - Fast NVME storage that is locally mounted on a worker node
  - Data is directly removed after job finishes (i.e., copy output to /home, /project)
  - Info see *scontrol show node*
  - https://doc.spider.surfsara.nl/en/latest/Pages/compute_on_spider.html

!! DATA IS NOT BACKED UP !!

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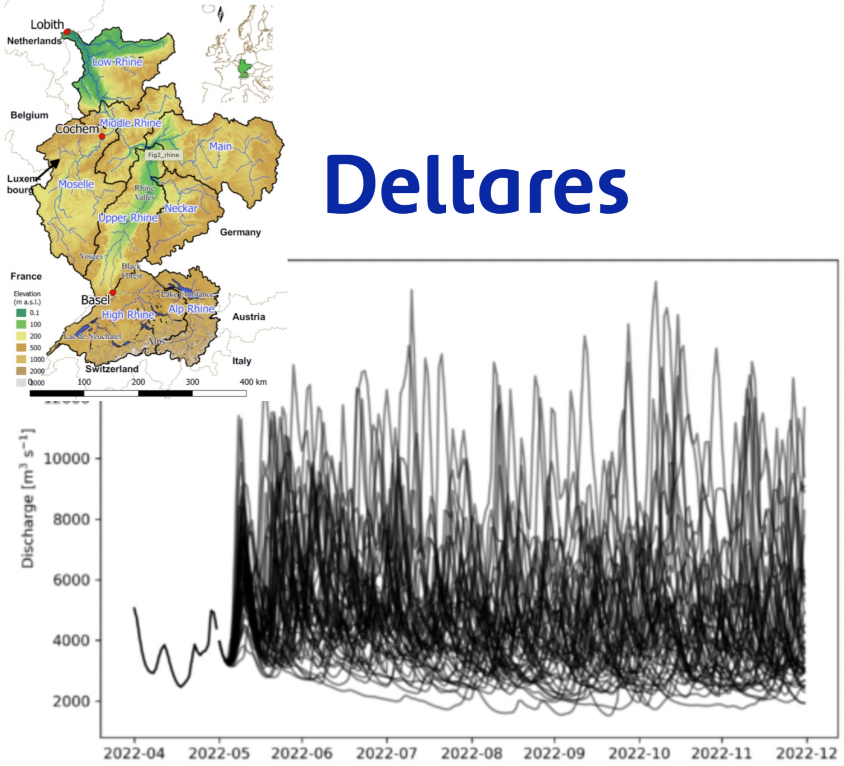
Use case: “High resolution, seasonal, ensemble river discharge (flow) forecast for a river basin of interest”

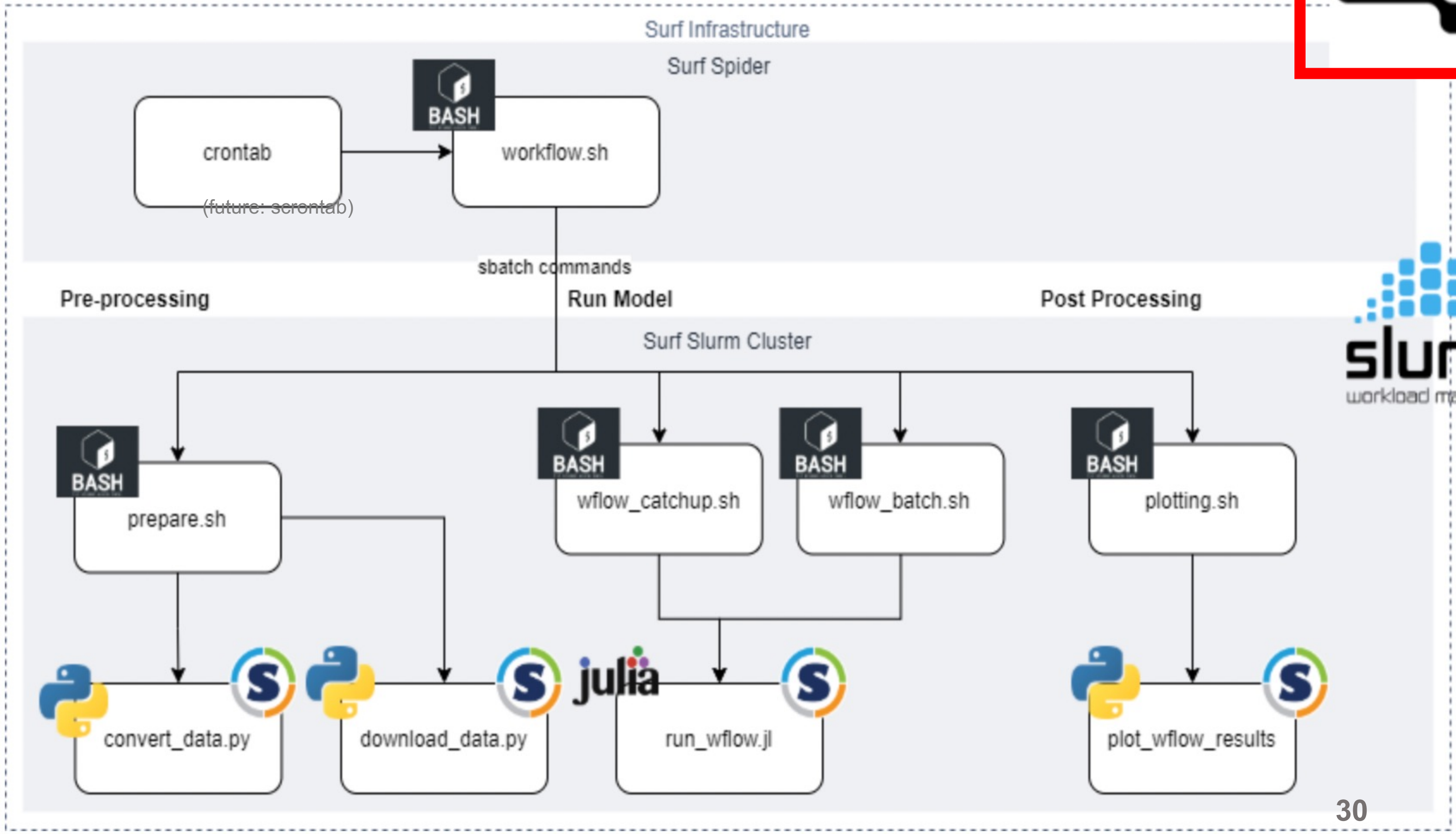
Easily deploy a workflow that produces a monthly high resolution, seasonal, ensemble river discharge forecast for a river basin of interest.



Deltares

Courtesy: B. Backeberg (Deltares)

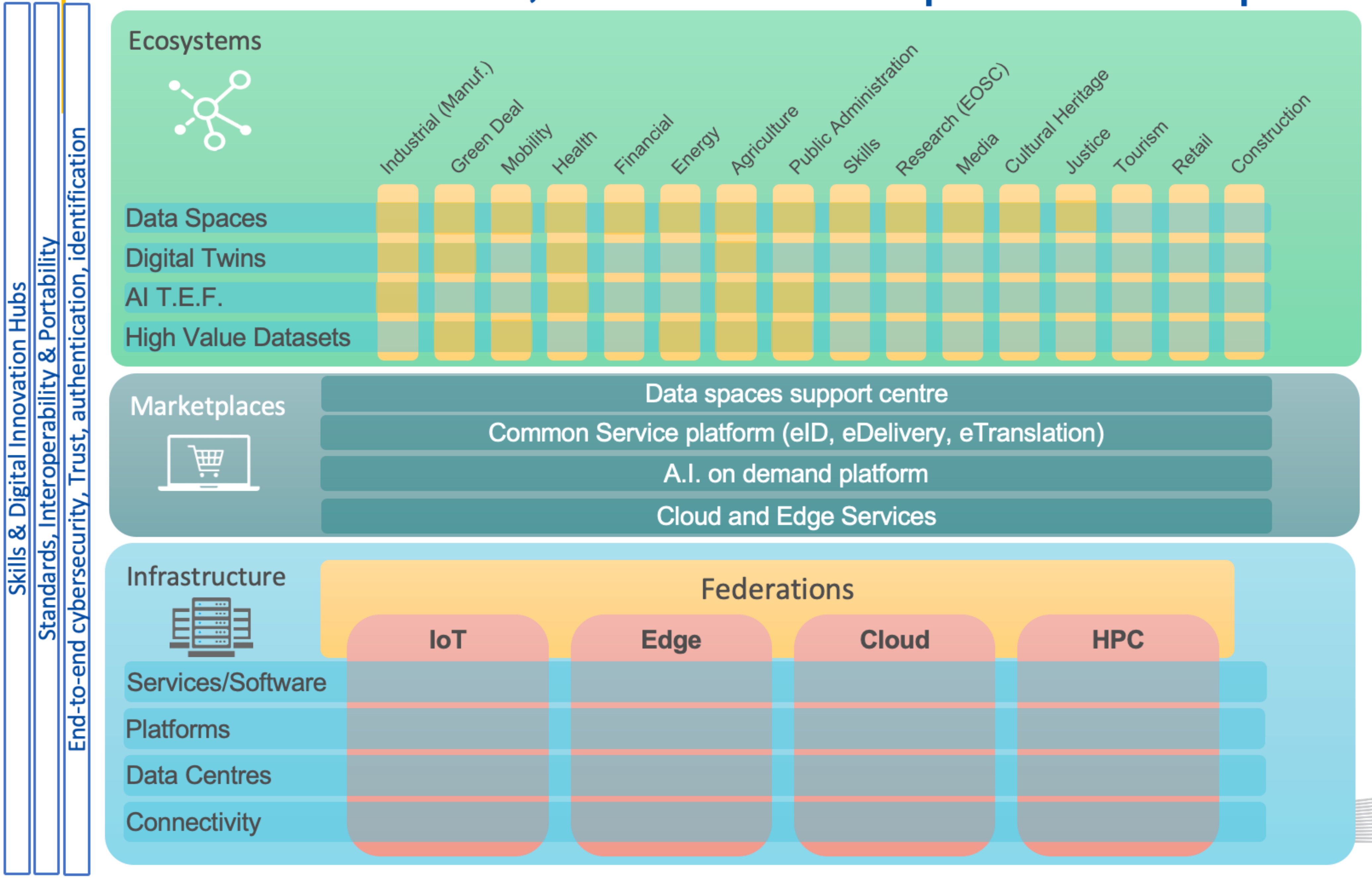
SURF



slurm
workload manager

European Infrastructure and Projects

EC vision: Cloud, Common European Data Spaces and AI

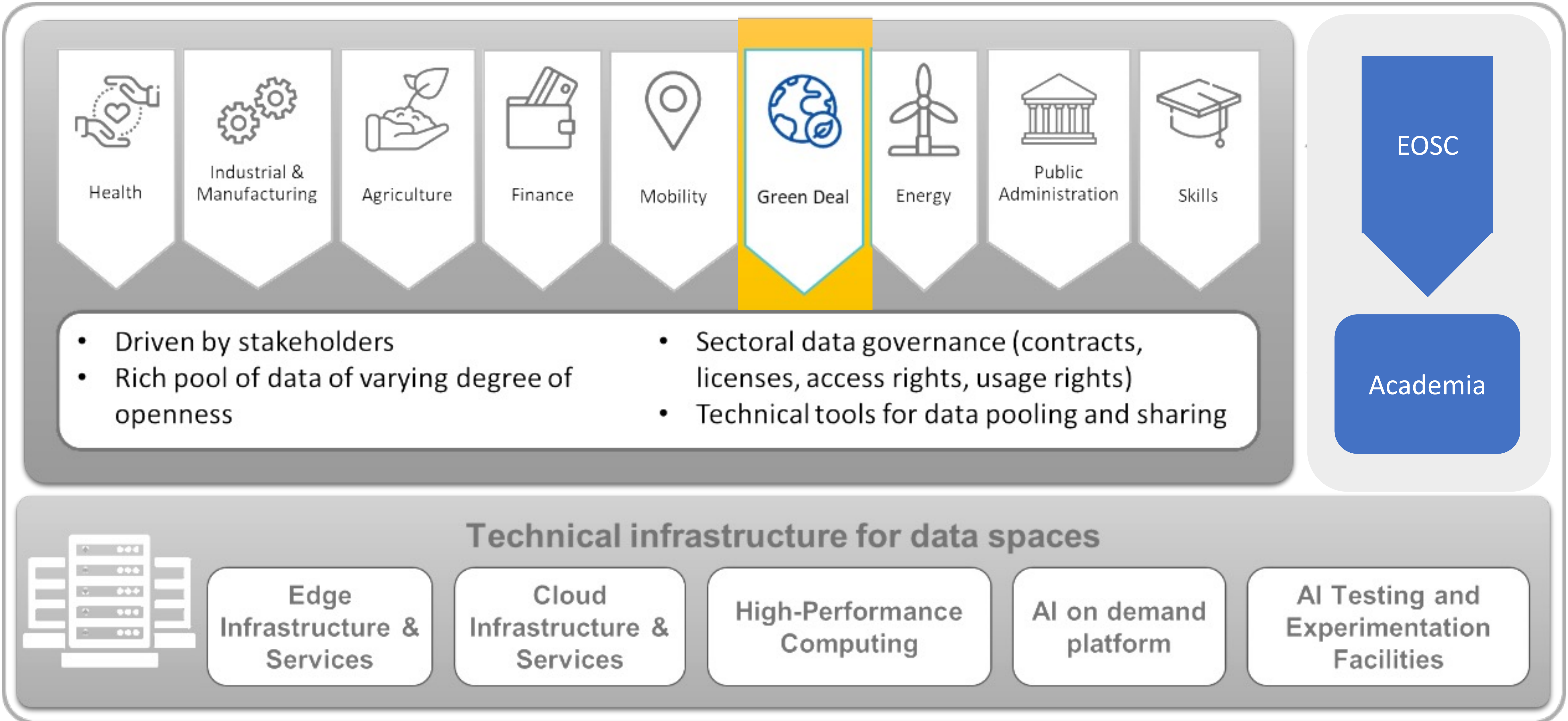


Data Spaces will be built over federated data infrastructure with common technical requirements (where possible)

Services and middleware developed to enable a federation of cloud-to-edge capacities will be at the disposal of all data spaces

Common European Data Spaces

Funded by the European Union



Common European Data Spaces – a single market for data

European Open Science Cloud (EOSC): *" to provide European researchers, innovators, companies and citizens with a federated and open multi-disciplinary environment where they can publish, find and reuse data, tools and services for research, innovation and educational purposes* [a] *"*

Green Deal Data Space (GDDS): *" will interconnect currently fragmented and dispersed data from various ecosystems, both for/from the private and public sectors. It will offer an interoperable, trusted IT environment, for data processing, and a set of rules of legislative, administrative and contractual nature that determine the rights of access to and processing of the data* [b] *"*

SIMPL: " open source, smart and secure middleware platform that supports data access and interoperability among European data spaces [c] "

a https://research-and-innovation.ec.europa.eu/strategy/strategy-2020-2024/our-digital-future/open-science/european-open-science-cloud-eosc_en

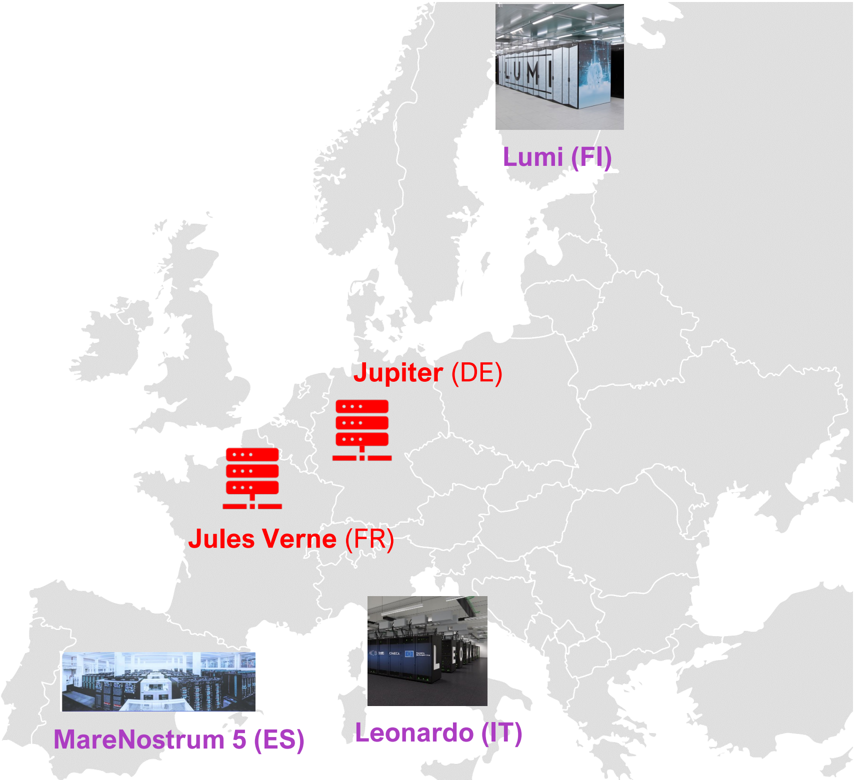
b https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/opportunities/topic-details/digital-2024-cloud-ai-06-greendeal

c https://digital-strategy.ec.europa.eu/en/policies/simpl

EuroHPC Mission

Develop, deploy, extend and maintain in the Union a world leading federated, secure and hyper-connected ***supercomputing****,* ***quantum*** *computing, service and data infrastructure ecosystem; support the production of innovative and competitive supercomputing systems based on a supply chain that will ensure components, technologies and knowledge limiting the risk of disruptions and the development of a wide range of applications optimised for these systems; and, widen the use of this supercomputing infrastructure to a large number of public and private users, and support the development of key skills for European science and industry.*

(Courtesy G. Kalbe)



- 15 HPC Centres of Excellence
- National HPC Centres of Competence
- EPICURE –HPC application support service, Application Support Teams (ASTs)
- European-wide HPC application support service
- Education/Skills: EUMaster4HPC

Destination Earth (DestinE)

esa ECMWF EUMETSAT

Key initiative, announced in:

A European Green Deal (2019)

A European strategy for data (2020)

Shaping Europe's digital future (2020)

EuroHPC Joint Undertaking

GREEN DEAL DATA SPACE

Aim and goals

Develop a **very high precision digital model of the Earth (Digital Twin)** of the Earth to monitor and simulate natural and human activity and to develop and test scenarios for

- more sustainable development and achievement of the EU green deal objectives
- saving lives
- avoiding large economic downturns
- **support EU policy-making and implementation**
- reinforce Europe's industrial and technological capabilities in advanced computing, simulation, modelling, predictive data analytics and Artificial intelligence (AI)

European Commission

https://destination-earth.eu/
https://digital-strategy.ec.europa.eu/en/policies/destination-earth
https://destine-data-lake-docs.data.destination-earth.eu/en/latest/index.html

Some potential misconceptions

Some misconceptions related to LSCS for research

1) The average CPU in my laptop is faster than the average CPU in a supercomputer ?!
2) The average filesystem response (disk+network) is faster on my laptop than on a supercomputer ?!
3) The software I built on my laptop does not work on a supercomputer ?!

An LSCS is a bit like a factory where work is orchestrated according to well-defined processes. As a user you only benefit from the factory if you use many nodes/cores simultaneously (i.e., many jobs or very complex jobs.

Efficient work orchestration often requires a technical understanding of a LSCS (e.g., node setup and job scheduler). In some cases higher-level workflow engines and languages can be used to abstract some of this complexity away (e.g., Dask, Spark, openEO, CWL/Toil, Galaxy, Pegasus, …)

↓

e.g., https://medium.com/pangeo/dask-jobqueue-d7754e42ca53

EESSI (software compilation, packaging, distribution)

Software packaging

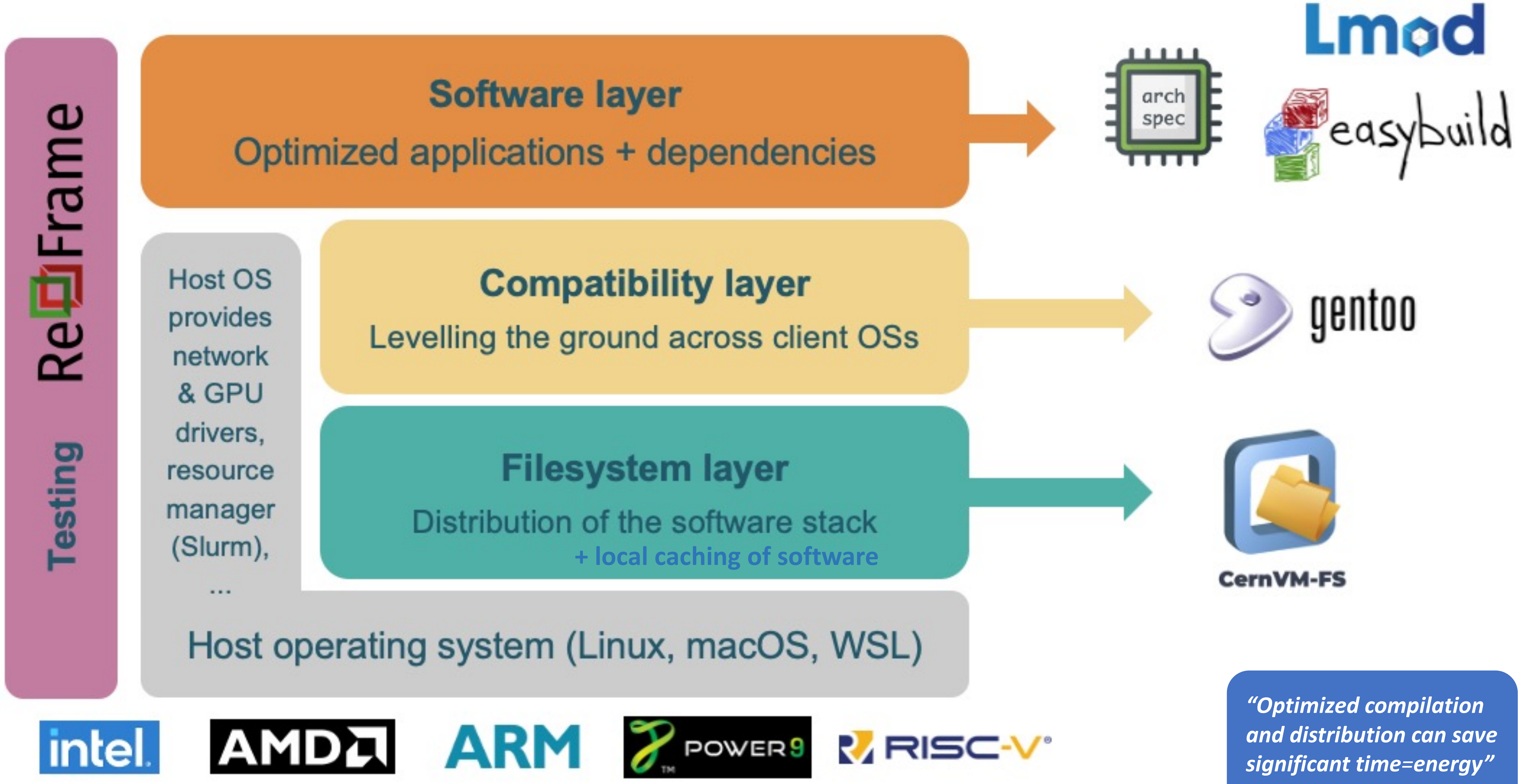
Some popular software packaging methods,

1) Modules
2) Containers (packed and unpacked)
3) Python environments [a]

[a] On LSCS systems with a shared filesystem (e.g., CephFS on Spider for /home , /project) we advise not to use python environments due to the large load (large number of files) they create on the file system. Some information can be found at https://docs.lumi-supercomputer.eu/software/installing/python/

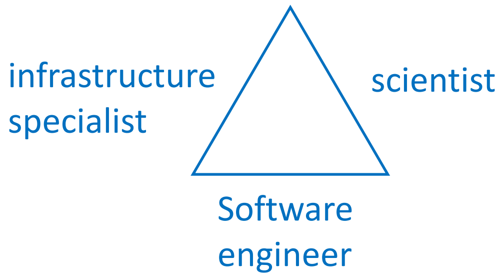
Introduction EESSI: Architecture

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



"Optimized compilation and distribution can save significant time=energy"

What can I / SURF do for you this week ?



1) Support for your work on “Spider” this week
2) As an advisor I can help investigate whether your research problem may be suitable for acceleration via large-scale computer services. ***This requires a dialogue and hence please approach me*** ☺
3) SURF can collaborate with you in European Commission funded projects
4) SURF can innovate with NL researchers and their international collaborators (e.g., we have expertise in *high performance machine learning*, *emerging technologies*, *data management* and *scalable workflows*)
5) SURF is the Dutch national infrastructure for research IT and can provide free ICT resources for NL researchers and their collaborators (https://www.nwo.nl/en/calls/computing-time-on-national-computing-facilities)
6) SURF is the Dutch mandated member in several European e-infrastructures

PRACE egi GÉANT EUDAT EuroHPC Joint Undertaking EUROPEAN OPEN SCIENCE CLOUD gaia-x

EXTRA TALK EESSI UPON REQUEST

SURF

THANK YOU FOR YOUR ATTENTION

Raymond Oonk

raymond.oonk@surf.nl

https://servicedesk.surf.nl/wiki/display/WIKI

Driving research together

SURF

Services for LSCS

Example: SURF Research IT services

High bandwidth network
Dedicated light paths
Encrypted transfers
Cyber Security
AAI / SSO
> 800 Gbps

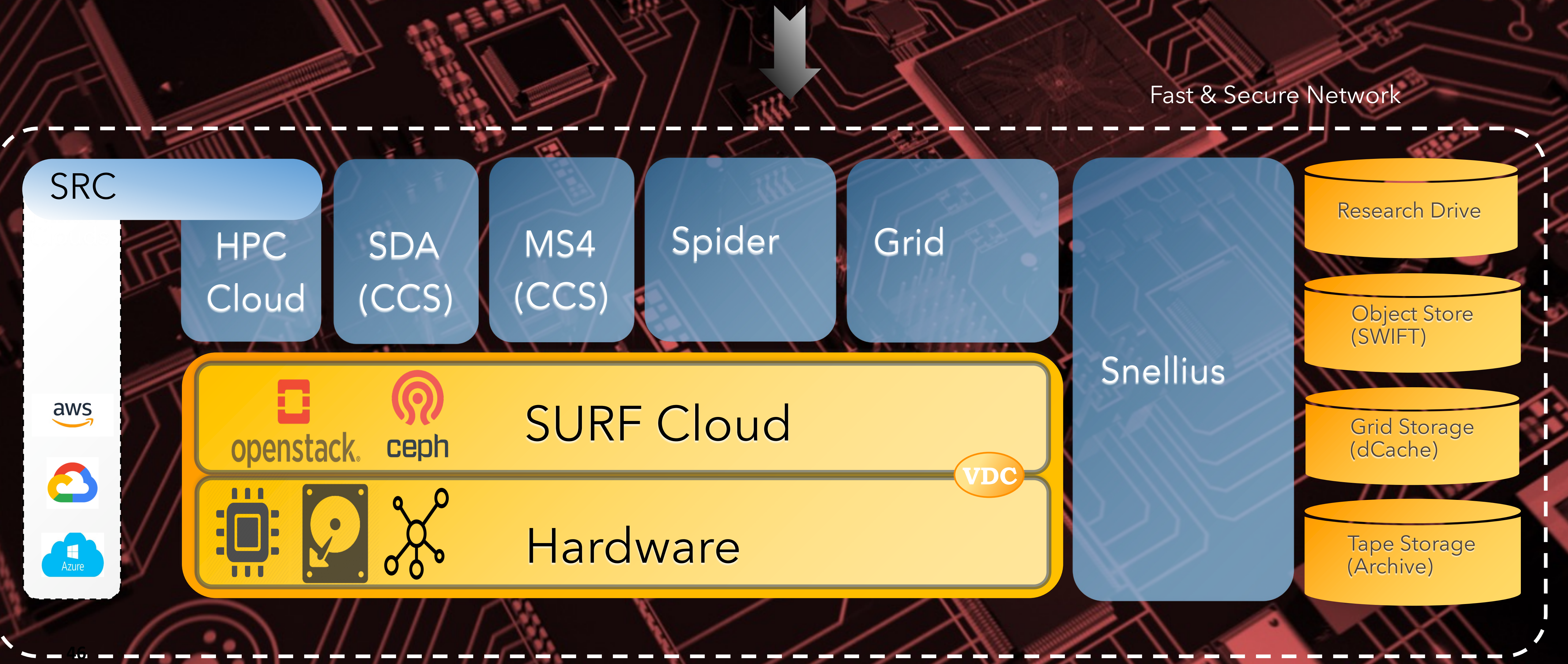
Snellius
Spider (DP)
Grid (DP)
Custom Cloud Solutions
SURF Research Cloud
Public Cloud
Experimental zone
> 100.000 cores

Ceph
dCache
Storage DPU
Object Store
Preservation
EPIC PID
iRODs
> 150 PB

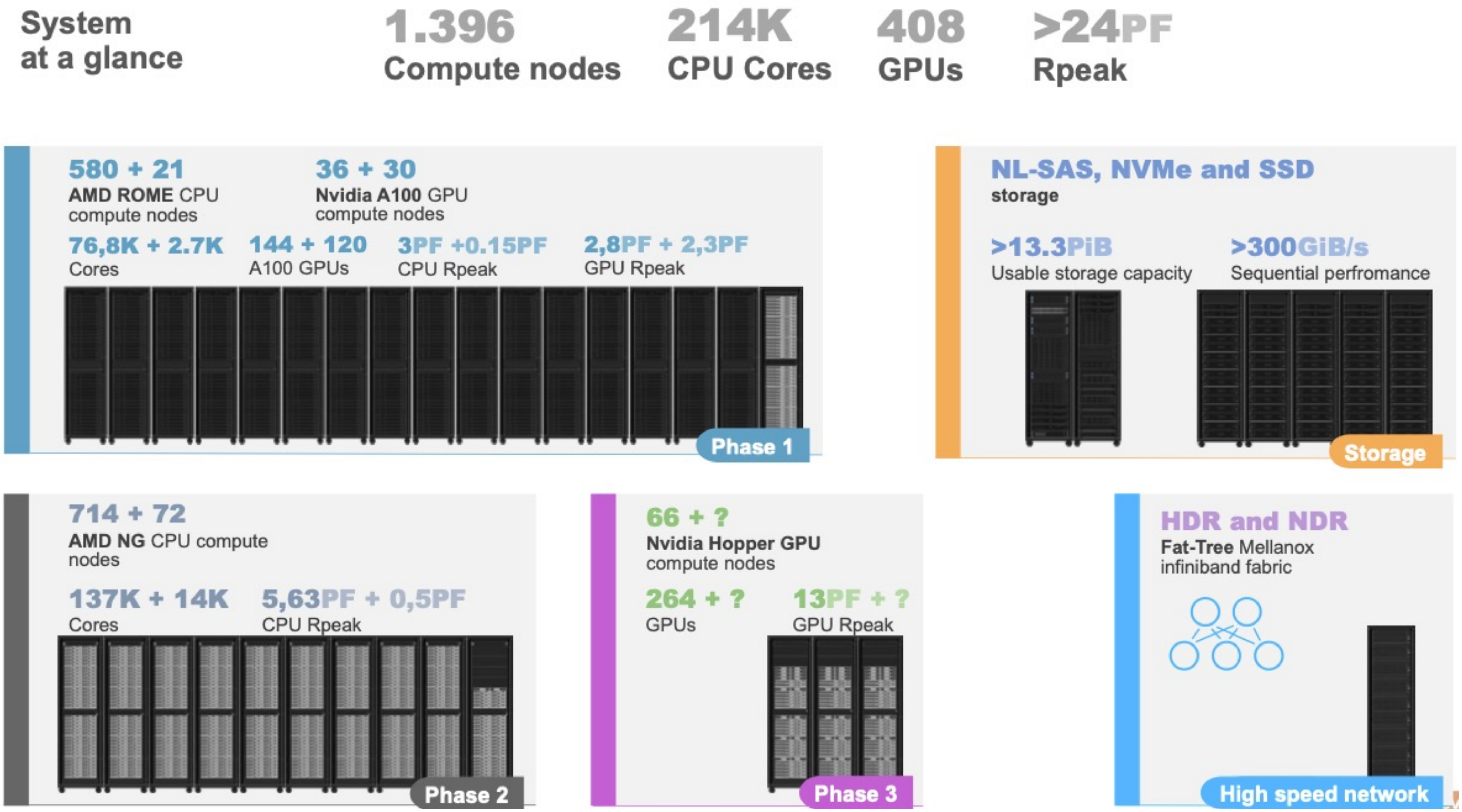
Support
Training
Visualisation
Optimisation
Expertise
Collaboration

Data center: 100% renewable energy
High information security: ISO 27001

User Applications

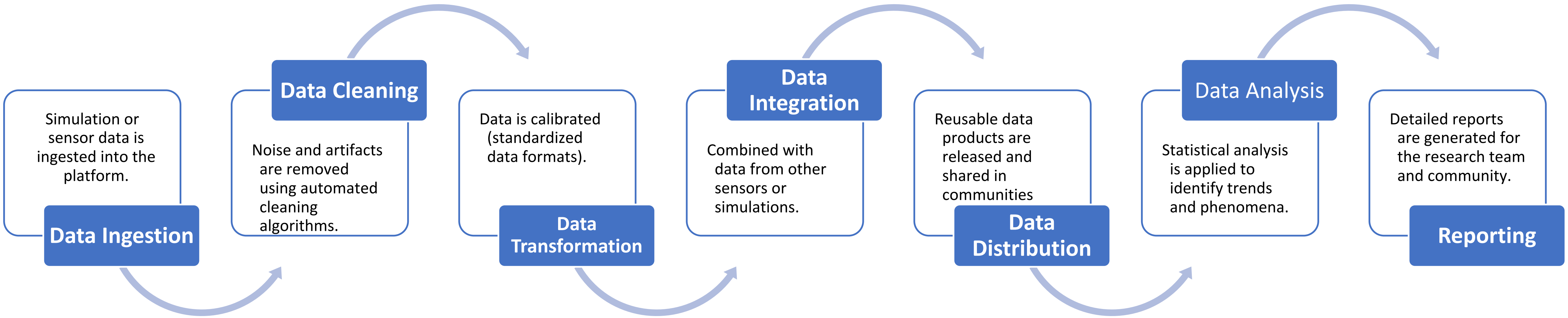


Snellius supercomputer: unavailable this week



SURF: Large-scale computing and Data processing life-cycle

- From project initiation to completion,
we offer **comprehensive support and consulting.**



** Many countries offer large-scale research IT infrastructure and often include IT expertise*

SURF

European (domain agnostic) e-infrastructures for academia

PRACE (https://prace-ri.eu/)

EGI (https://www.egi.eu/)

EUDAT (https://eudat.eu/)

GEANT (https://geant.org/)

EuroHPC JU (https://eurohpc-ju.europa.eu/index_en)

EOSC (https://eosc.eu/)

** Domain specific Research (e-)Infrastructures can a.o., be found in ESFRI (https://landscape2024.esfri.eu/)*