

SURFsara HPC services



UNESCO-IHE symposium, 30 & 31 March 2017



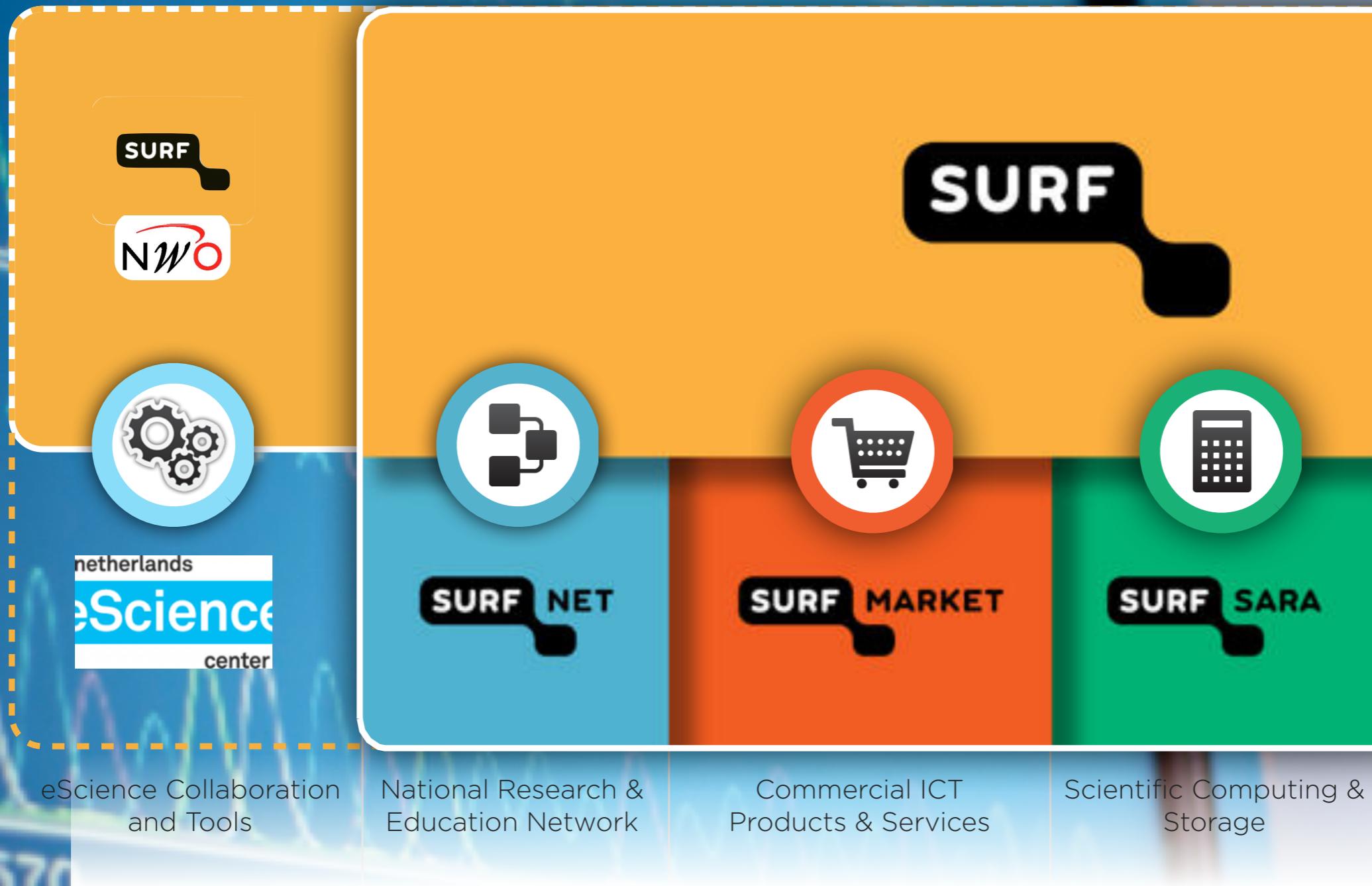
Natalie Danezi, Ander Astudillo



Outline

- Introduction to SURFsara
- High Performance Computing (HPC) in Research
- HPC applications in practice
 - Scaling up vs. scaling out
 - Interactive mode vs. jobs
- SURFsara HPC services
- Getting access to HPC systems

SURF family



UNESCO-IHE symposium



SURF SARA

Our history

- 1971: SARA
 - Stichting Academisch Rekencentrum Amsterdam
 - founded by UvA, VU, CWI
- 1984: National Supercomputing Center
- 2013: SURFsara



Our location - Ams Science Park



Our users



Our mission

- High Performance Computing
(HPC)
in Research

Bridging the gap between *research* and advanced ICT services

- Compute
- Storage
- Visualisation
- Network
- Communities
- Consultancy

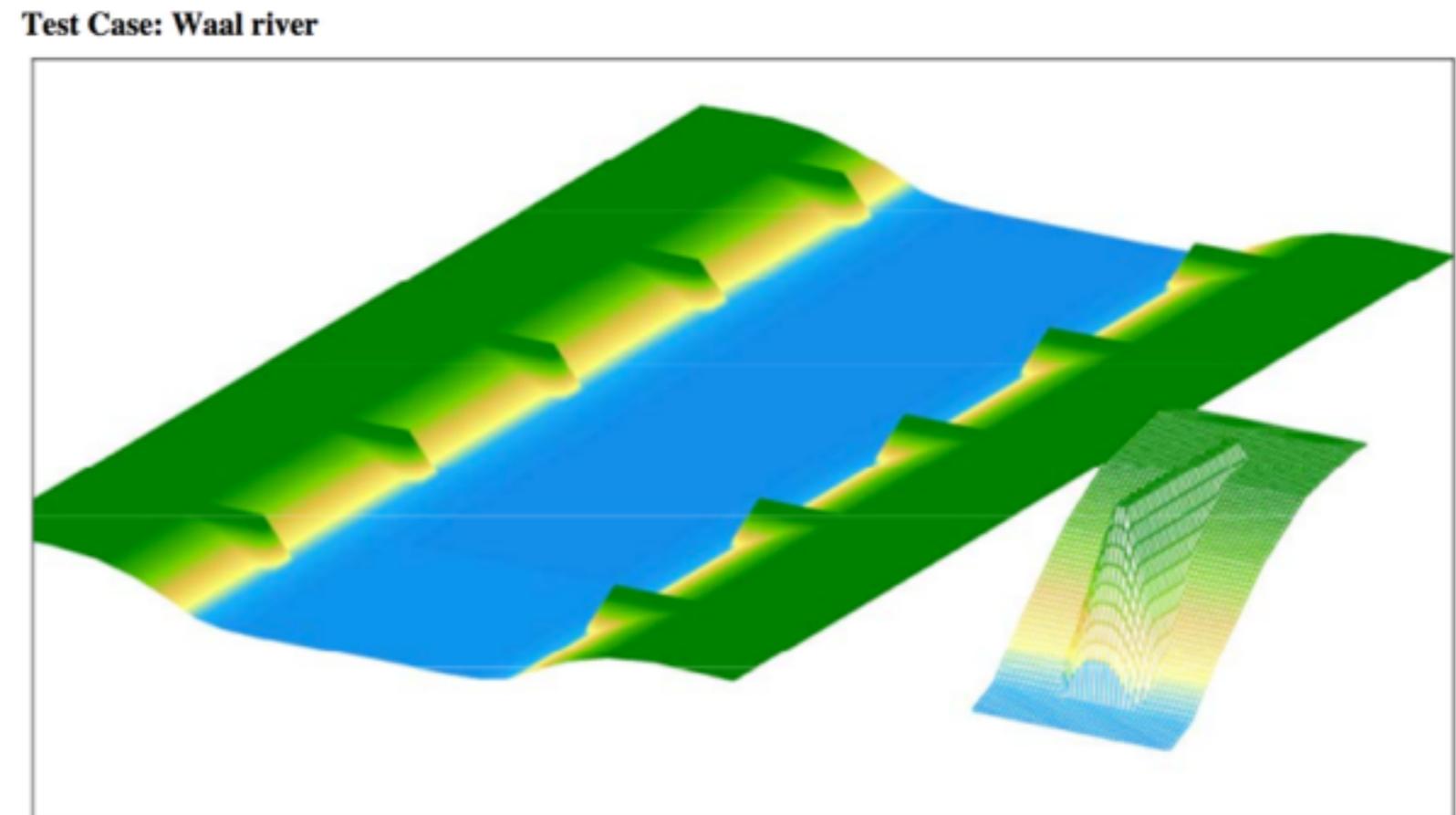
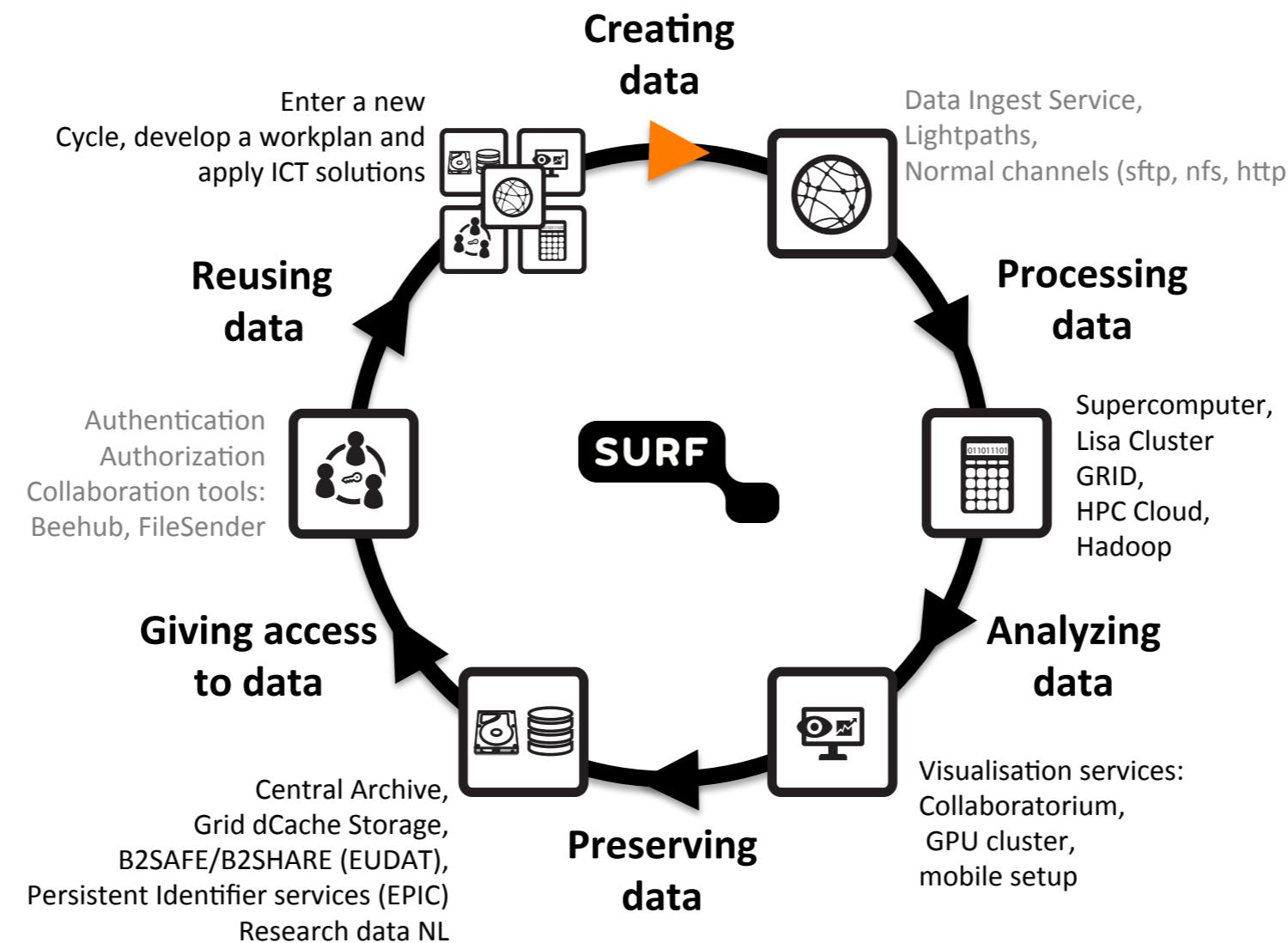


Figure 1: Overview of part of the simulation domain. The grid representation of a groin can be seen at the bottom right.

SURFsara services

- **Lisa** national compute cluster
- **Cartesius** national Supercomputer
- The **Grid**: interconnected clusters across NL
- **Oort** HPC Cloud cluster
- Central Archive, Beehub, SURFdrive, PIDs, Ingest Service for Data Services
- ..., SDA, Visualisation, Networking, Consultancy, Innovation

HPC project lifecycle



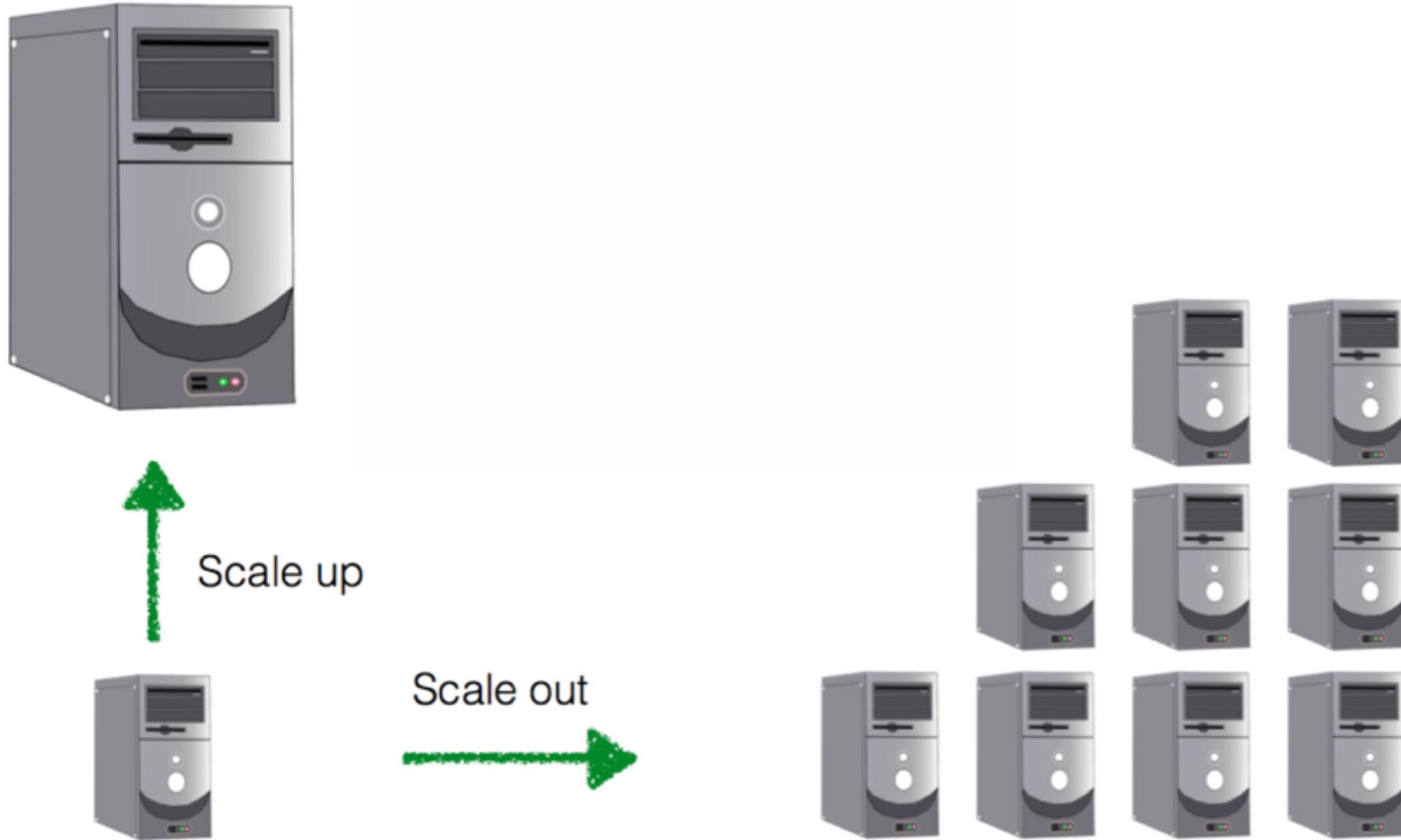
How HPC can benefit research

- Faster results
- Task repetition
- Higher accuracy
- Larger computational domains
- Larger volume of data

<http://www.advancedgwt.com/groundwater-software/data-management-and-visualization/groundwater-desktop.html>

HPC in practice - Scalability

Delft3D: Modelling suite for integral water solutions



HPC in practice - Interactive mode vs. jobs

Delft3D: Modelling suite for integral water solutions

- Interactive mode:
 - Example:
 - Go to the example directory: `$ cd mysimulation/Delft3D-WAVE`
 - Start the calculation on the same computer: `$. run_flow2d3d.sh`
 - The calculation will be executed on this computer
- Non-Interactive mode or **jobs**:
 - Example:
 - Wrap your application (`run_flow2d3d.sh`) in a ‘digital envelope’, called **job**
 - Submit the job to a cluster: `$ qsub wrapper.sh`
 - The job will start your calculation on a remote computer

Using a remote machine

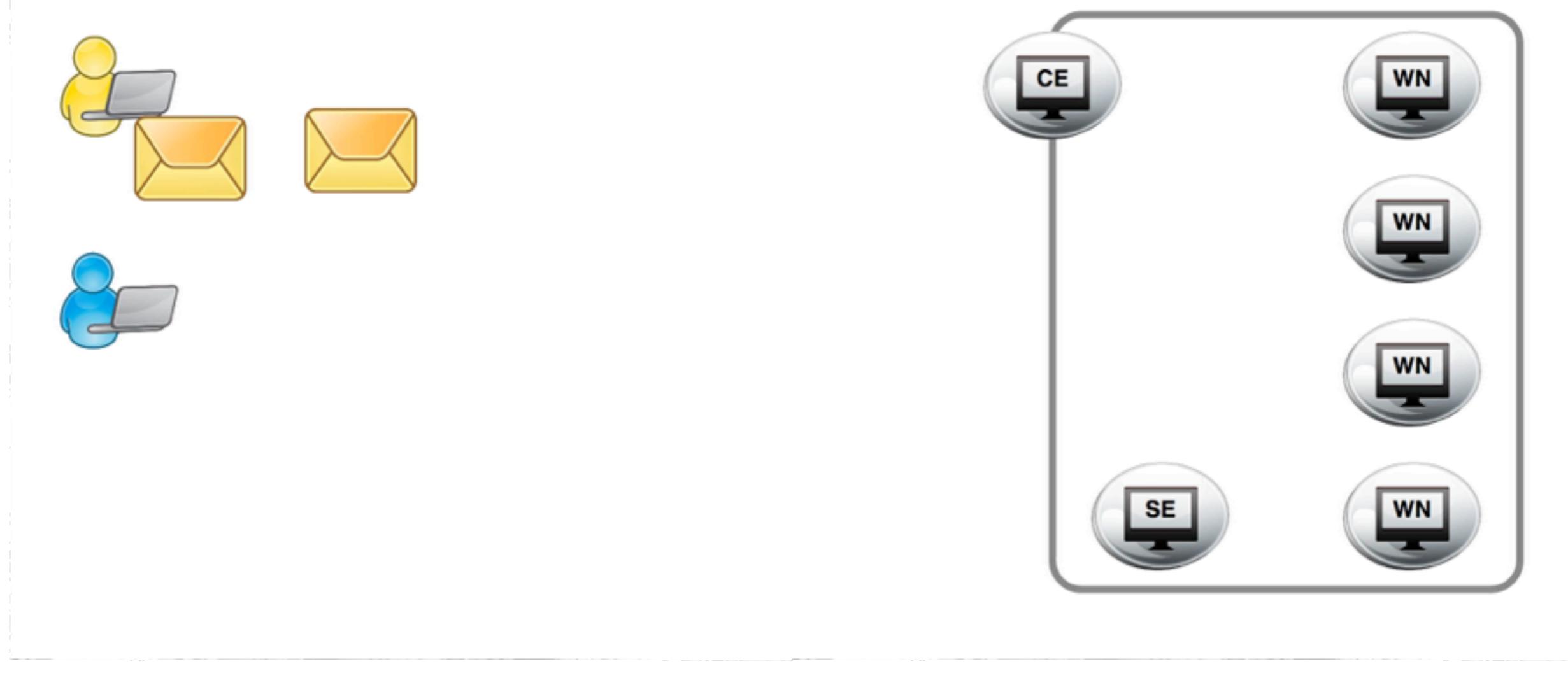


http://web.grid.sara.nl/mooc/animations/single_user.html Animation: EGI - SURFsara MOOC 2014

Lisa cluster: job scheduling system

- Compute intensive applications
- Not data intensive applications
- Well supported software stack
- Relatively easy to start

Using a cluster



<http://web.grid.sara.nl/mooc/animations/cluster.html> Animation: EGI - SURFsara MOOC 2014

Cartesius Supercomputer

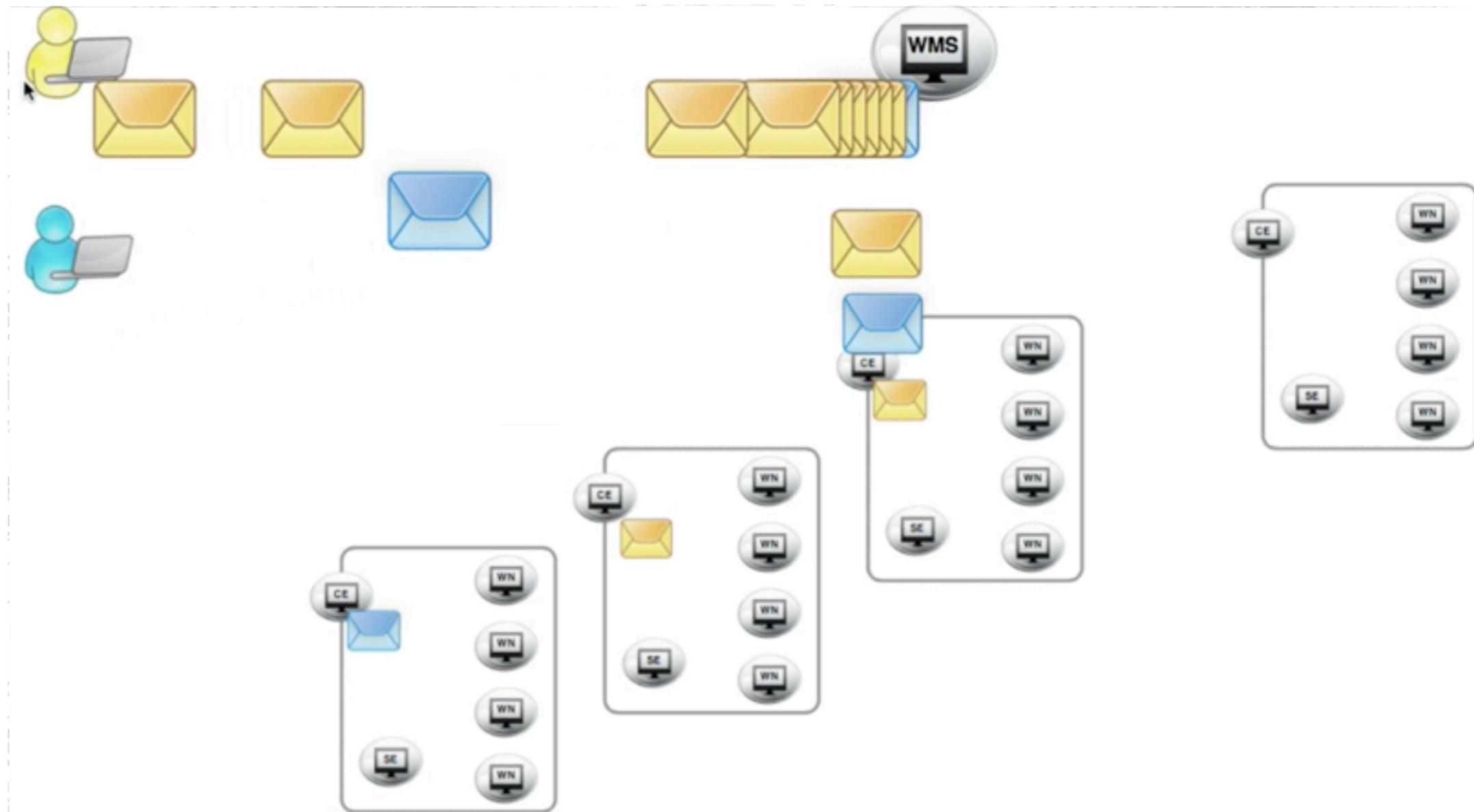
- Bigger than Lisa
- Large memory, fast interconnect, fast and large I/O
- European collaborations: PRACE, HPC-Europa
- Climate models, cell simulations
- Programming experience required

Grid: cluster of clusters

- Independent tasks: Parameter sweeps, Monte-Carlo, ..
- High volume of compute and data
- Capacity: +/- 12 000 cpu cores, peta bytes of storage
- Linux experience required



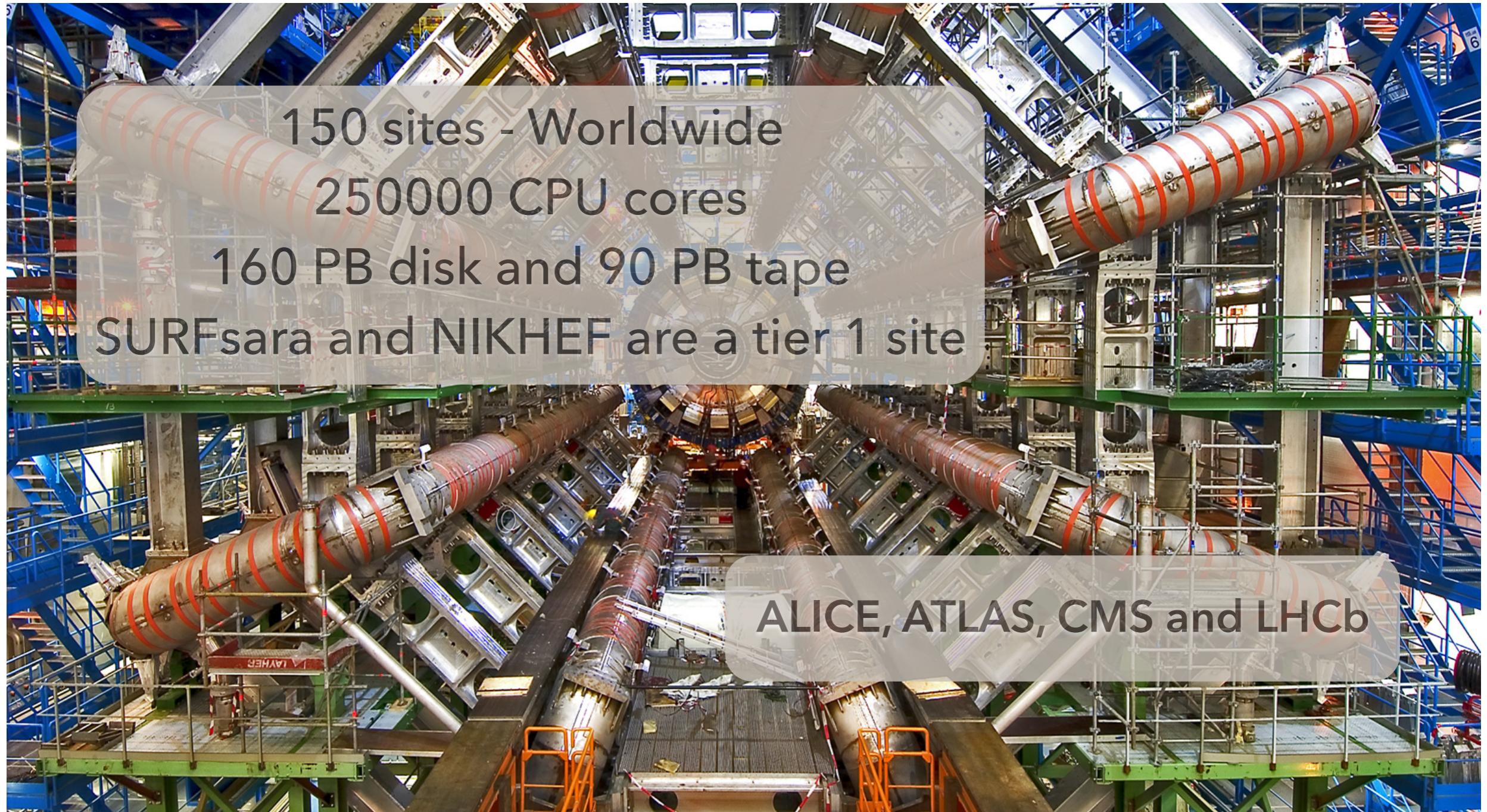
Using a cluster of clusters



<http://web.grid.sara.nl/mooc/animations/wms.html>

Animation: EGI - SURFsara MOOC 2014

Large Hadron Collider at CERN



HPC Cloud

- No jobs, but own computers or Virtual Machines (VMs)
- Not only for Linux fans (Windows is supported)
- You get an account and access to a pool of resources to build your own computer (VM)
- Several Unesco-IHE projects using XBeach, Delft3D, D-Flow FM, Mike, ...
- More? *Hands-on today!*

HPC Cloud Dashboard

SURF SARA

Dashboard

s-uihe38 Oort

VMs 1 ACTIVE 1 PENDING 0 FAILED 0

CPU hours

Date	CPU hours
17/03/24	~0.2
17/03/27	~8.0

Memory GB hours

Date	Memory GB hours
17/03/24	~0.2
17/03/27	~8.0

Disk MB hours

Date	Disk MB hours
17/03/24	~50,000
17/03/27	~130,000

Virtual Networks 2 USED IPs 498

Images 2 USED 16.6GB

VMs

Services

Templates

VMs

Services

Storage

Images

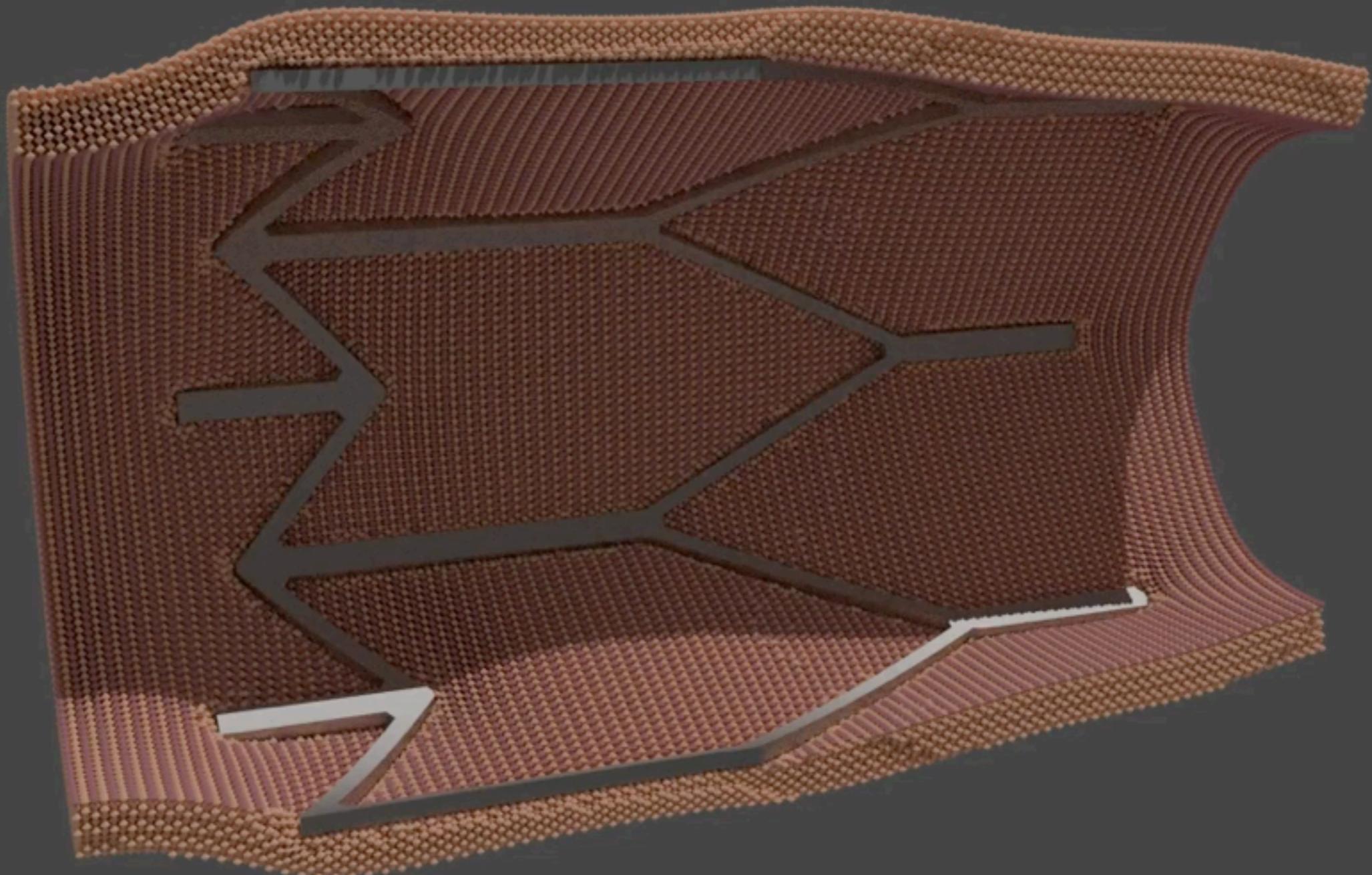
Files

Apps

Network

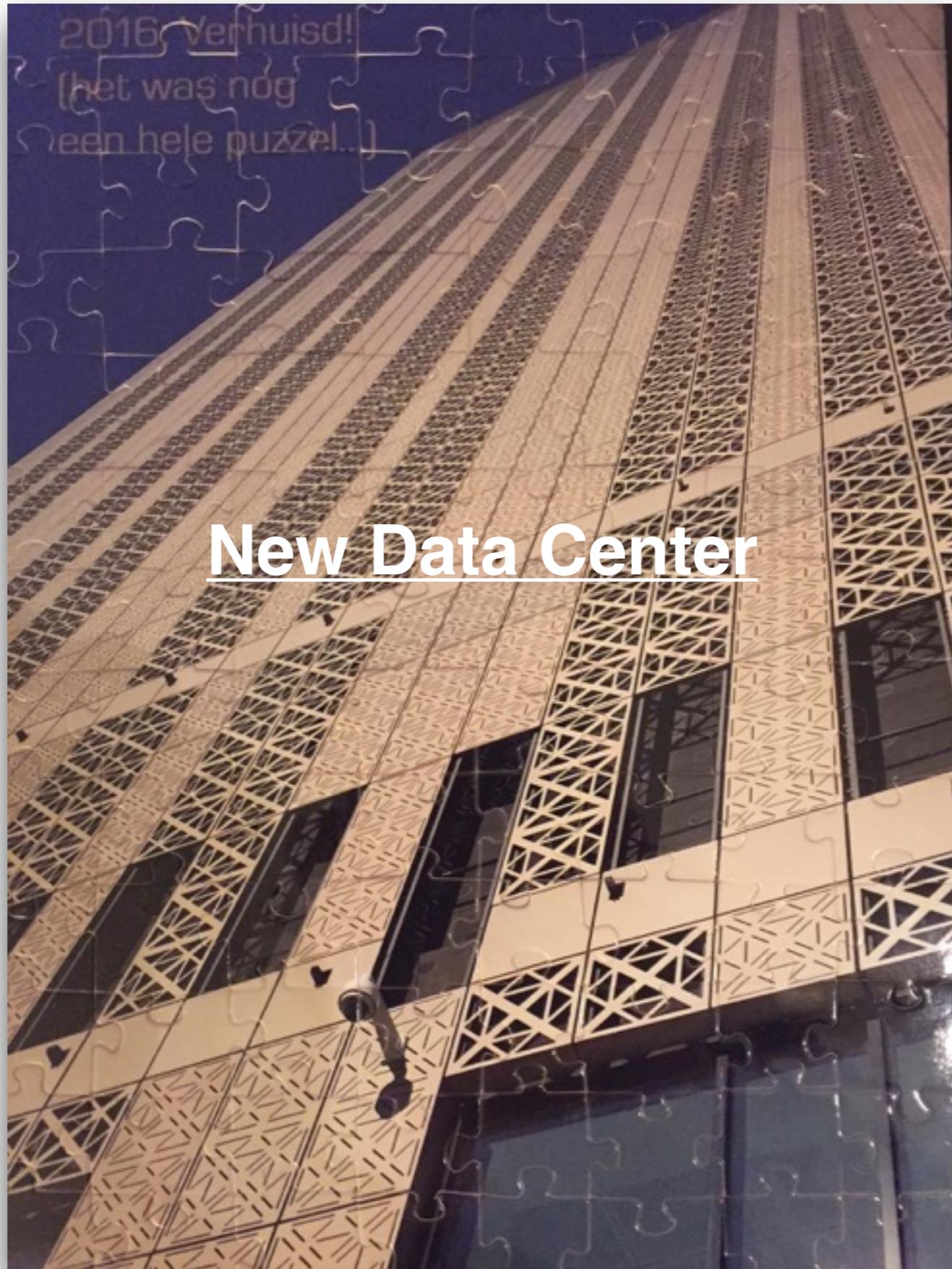
Settings

Visualisation

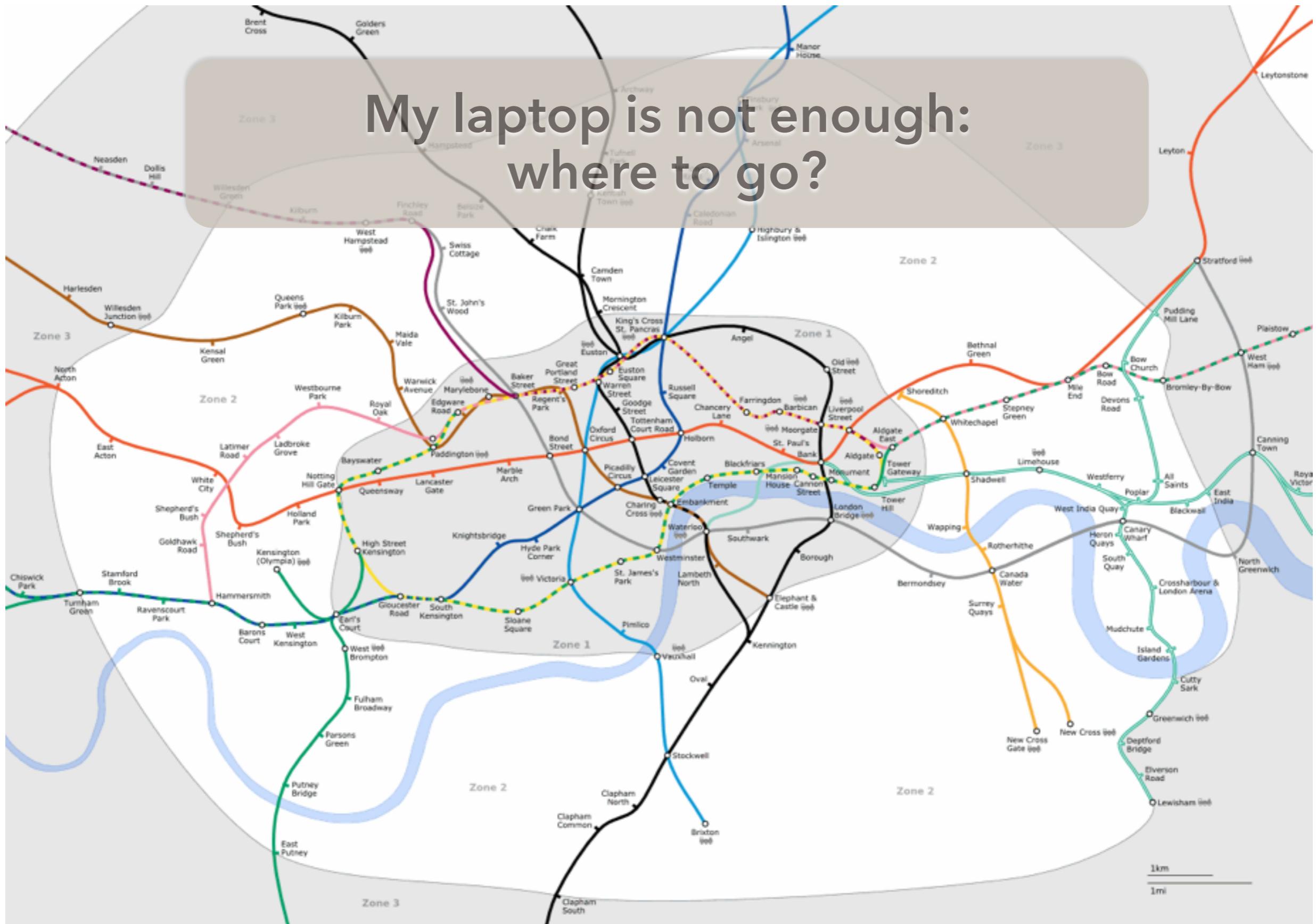


Scalable Data Analytics

- Big Data
- Exploration/mining of data
- Hadoop Map / Reduce
- Spark framework
- ElasticSearch cluster
- Programming experience required



My laptop is not enough: where to go?



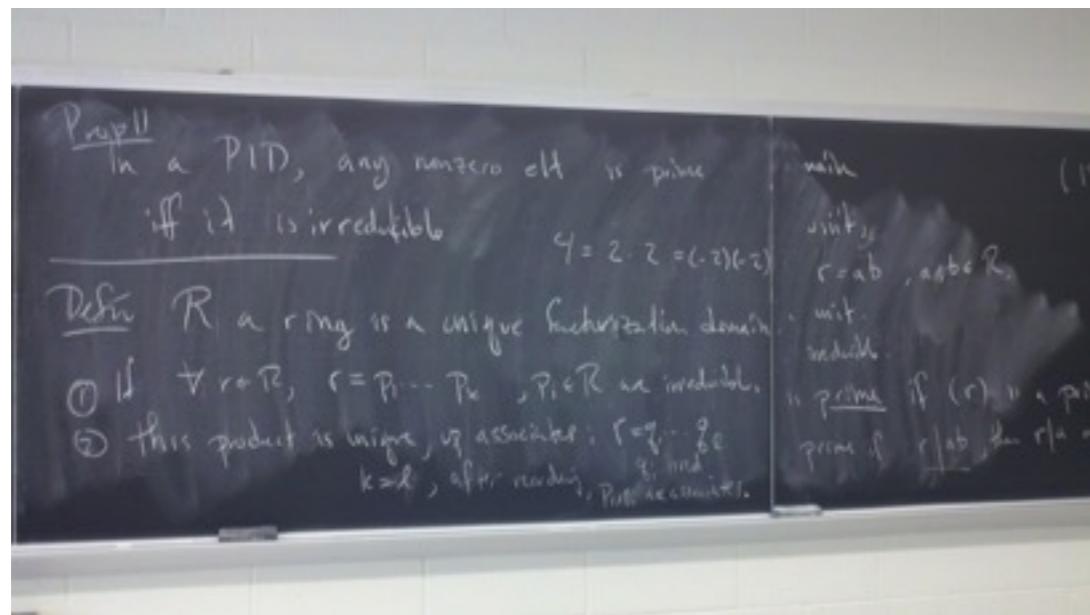
SURFsara services - recap

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Cluster vs. Cloud

Cluster (Lisa/Cartesius)	Cloud (HPC Cloud)
Job scheduling system	One or more Virtual Machine(s)
Access to Linux UI	Access to Web interface from your browser
Calculation submitted via cluster scheduler (job)	Calculation submitted as on user's laptop (interactive mode)
Software installed: <pre>\$ module load delft3d</pre>	User installs/maintains the software
Shared local storage with home account	Scalable storage
Only for Linux apps	Linux & Windows apps supported
No root access, limited walltime	Flexible & Controllable - User is the owner, long-running apps

Standard support



Bring your scientific problem

- We provide advice and support:
 - Getting access
 - Best practices
 - Design & optimisation
 - Integration to large scale



Getting access

- Submit your request here: <https://e-infra.surfsara.nl/>
 - Write a short description of your project
 - Which SURFsara HPC system suits your application
 - ... or, **not sure** what suits you best? We can help!

Trainings, online tutorials

SURFsara and UNESCO-IHE workshop: How water research benefits from HPC Cloud



UNESCO-IHE hosted a RESEARCH workshop last month for research on water engineering and management using HPC systems. SURFsara, as the leading national e-infrastructure provider, delivered a hands-on course on their HPC Cloud and presented its benefits to the water sector.



The slide features a background image of people at a conference. Overlaid text includes:

SURF Research BootCamp

Utrecht, April 21st 2016 During this one-day event researchers are guided through the world of research ICT facilities and provided with the necessary skills to start using them. Participants compose their own mix of workshops to support their research work.

by gera_p 6 months ago 66 Views



Contact



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