CSC's services for researchers

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HPC support

Non-profit state organization with special tasks

Turn over in 2019

51 M€

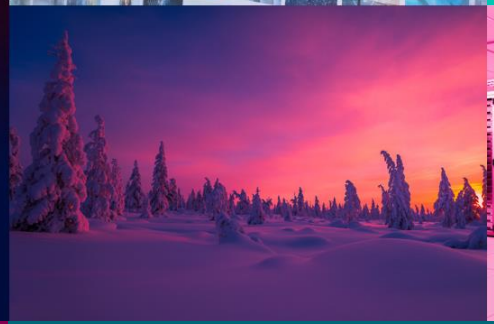
Headquarters in Espoo, datacenter in Kajaani

Owned by state (70%)

and all Finnish higher education institutions **(30%)**

Circa **430** employees

Thanks to our agreement
with the Ministry of Education and Culture,
our services targeted at researchers
are largely free of charge!



CSC's solutions

Computing and software

Data management and analytics for research

Support and training for research

Research administration

Solutions for managing and organizing education

Solutions for learners and teachers

Solutions for educational and teaching cooperation

Hosting services tailored to customers' needs

Identity and authorisation

Management and use of data

ICT platforms, Funet network and data center functions are the base for our solutions

Our customers

Researchers,
research institutes and
organizations

Organizations providing
education

Memory organizations,
state and public
organizations

Support in all of the phases of a research process

Scientific drivers for CSC infrastructure

New challenges

Large scale simulations

- For example climate change, space weather, fusion reactors, astronomical phenomena, particle physics

Mid-scale simulations

- For example materials science, energy technology, GIS

Data-intensive computing

- For example computational econometrics, bioinformatics, language research

Data-intensive computing for sensitive data

- For example medical research, register research

Artificial intelligence

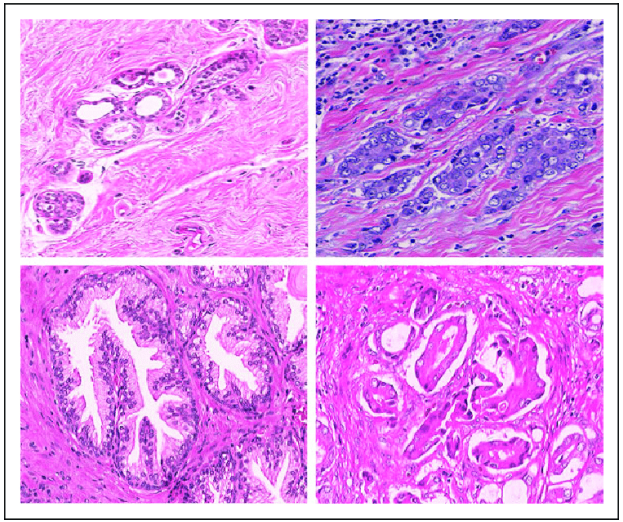
- For example natural language research, business applications, computer vision

Internet of Things (IoT) and data streams

- For example satellites, weather stations, sensor networks

Real-world examples – artificial intelligence

- Prediction of molecular phenotypes for cancer diagnosis
  - Molecular phenotyping can make diagnosis of breast cancer more precise and comprehensive
  - Deep neural networks are utilized for classification of histopathology image data
  - Large data volumes and optimized computational pipeline using both CPU and GPU computation
  - PI: Pekka Ruusuvuori, Tampere University



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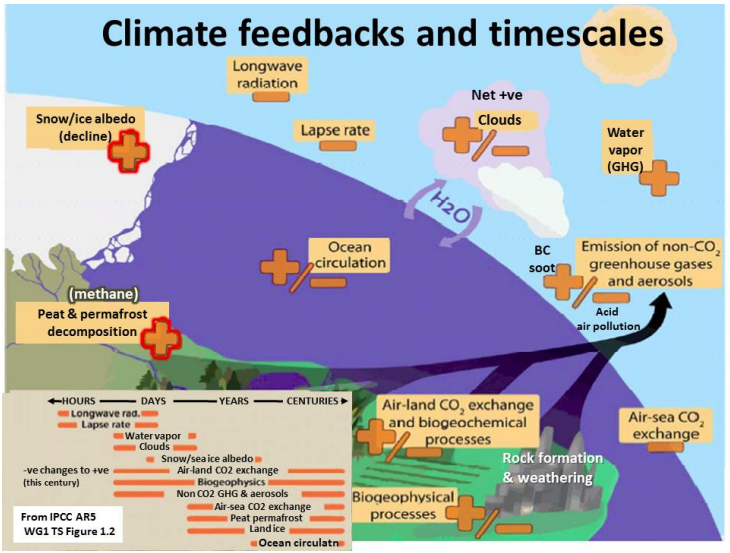
Real-world examples - medium-scale simulations & data-intensive computing & data streams

- Atmospheric feedback mechanisms
  - In study of climate change, understanding feedback mechanisms is crucial for because they may either amplify or diminish the effect. Therefore these are key for determining the climate sensitivity and future climate.
  - This research involves various environmental measurements, satellite data and multiscale modelling. The multiscale models research start from nanoscale (quantum chemistry), reaching out towards global atmospheric models.
  - PI: Prof. Markku Kulmala, University of Helsinki

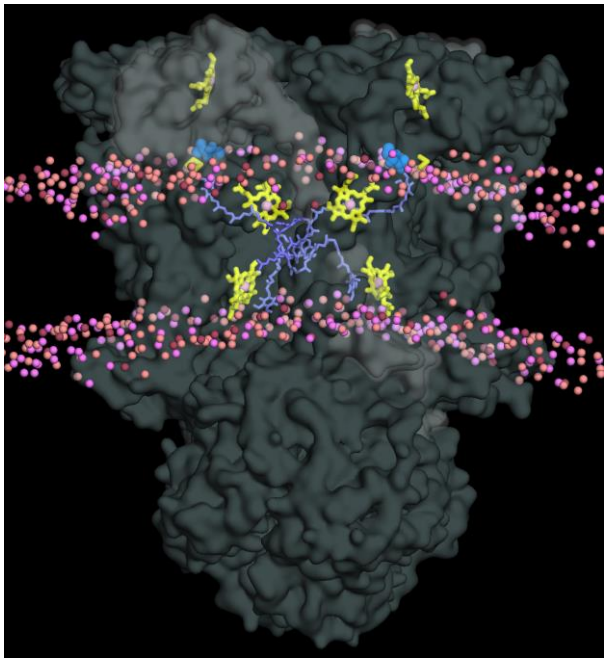


Real-world examples – medium scale simulations

- Spreading of aerosol particles in air
  - Computational fluid dynamics modelling of airborne transmission of coronavirus
  - Medium scale simulations with few hundred CPU cores
  - PI Ville Vuorinen, Aalto University

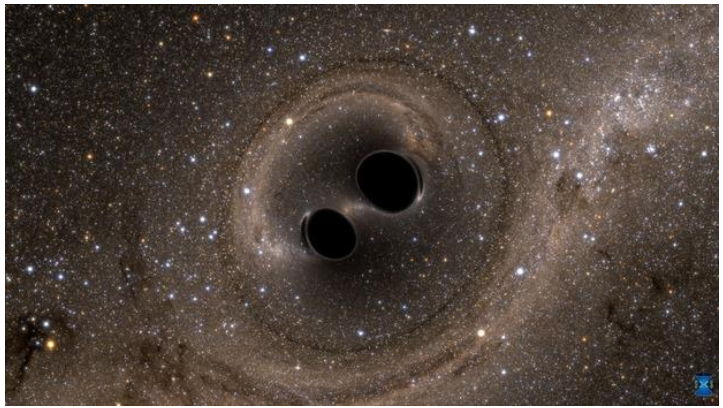
Real-world examples - medium-scale simulations

- Atomic level simulations of mitochondrial mutations
  - Molecular dynamic simulations of amino acid change and electron transfer during cellular respiration
  - New insight into GRACILE syndrome
  - Medium scale simulations with hundreds of CPU cores
  - PI: Vivek Sharma, University of Helsinki



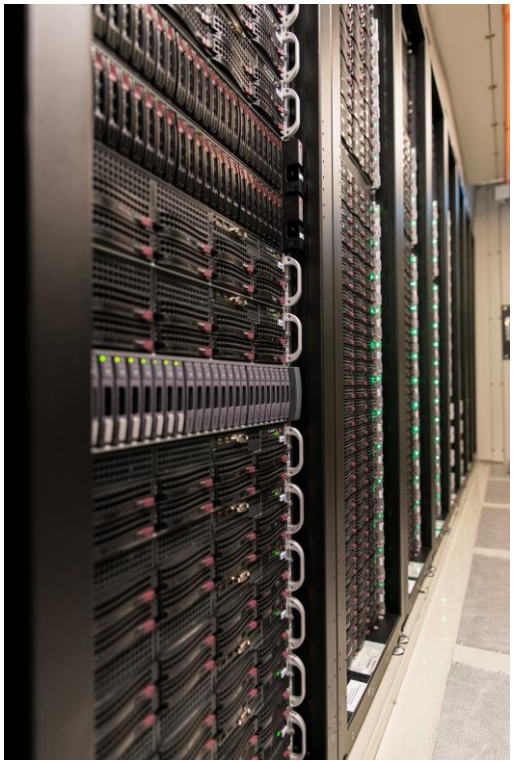
Real-world examples - large-scale simulations

- Gravitational waves from early universe
  - Computational modeling of sources of gravitational waves
  - Phase transitions at Higgs boson "turning on" (10 picoseconds after Big Bang)
  - Large simulations with over ten thousand CPU cores
  - PI: David Weir, University of Helsinki



CSC's Computing services

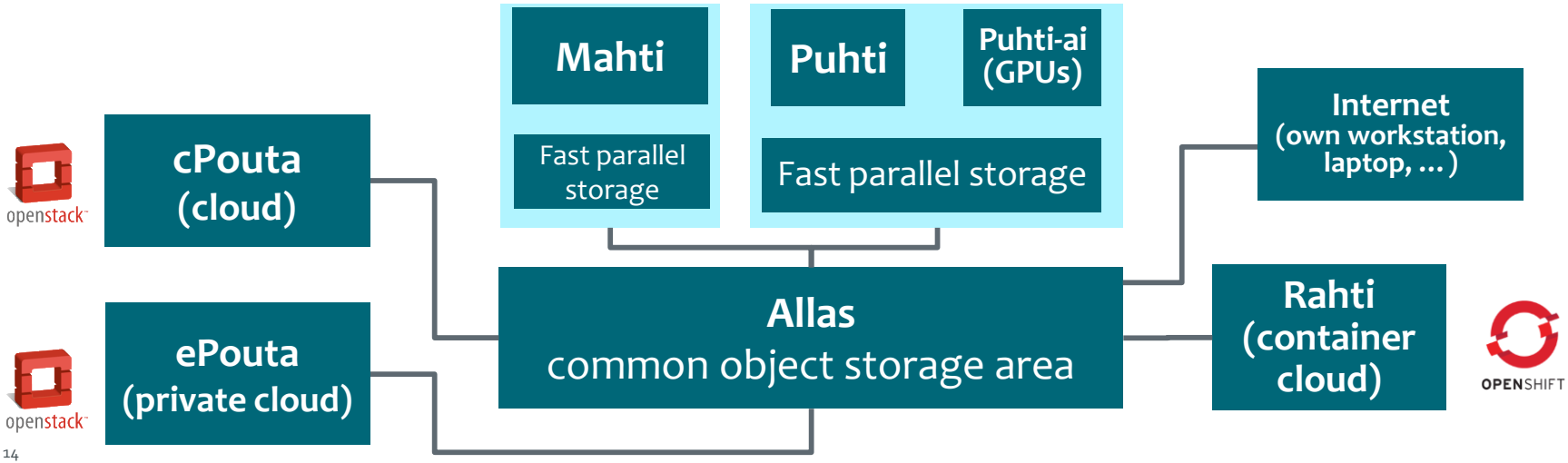
- **Supercomputers: Puhti and Mahti**
  - **Puhti** - Supercomputer with Intel CPUs (2019)
  - **Puhti-ai** – Supercomputer with GPUs (2019)
  - **Mahti** - Supercomputer with AMD CPUs (2020)
- **Cloud services**
  - **Pouta** and **Rahti**
- **Object storage service: Allas**
  - New service for computing and cloud services, data can be shared to Internet
- **When you need even more**
  - PRACE research infrastructure



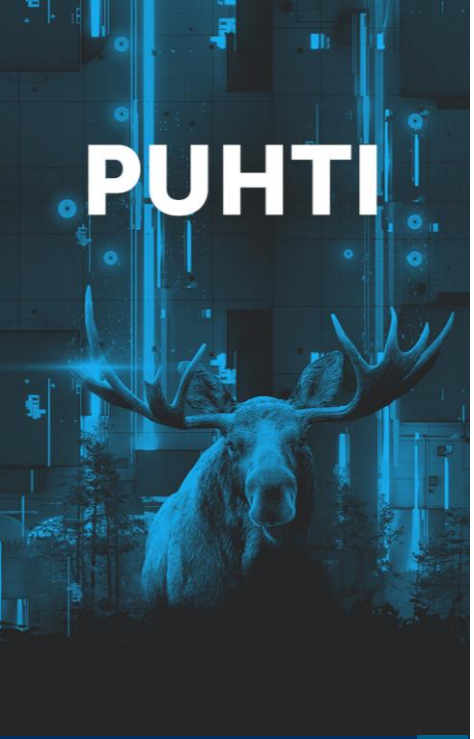
The new Finnish research infrastructure for data management and computing

Balanced HPC ecosystem for various workloads

Heterogeneous, workload-optimized node architecture, support for complex workflows, datasets-as-a-service and containerization



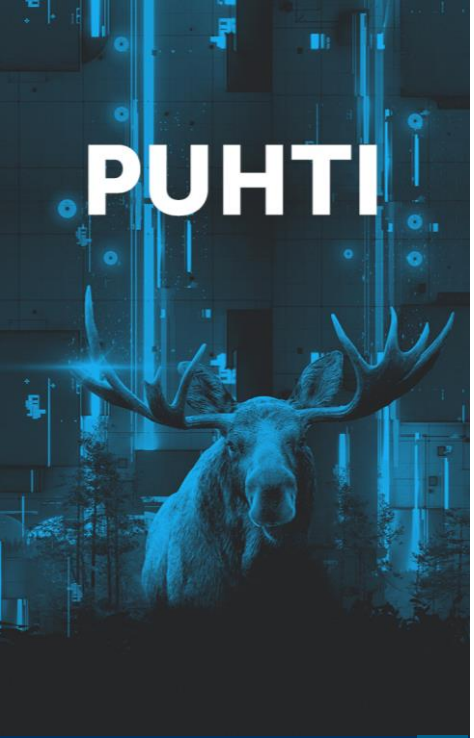
Computing services



In customer use since September / 2019

Puhti Supercomputer

- Supports wide range of use cases
- Powerful CPU partition with ~700 nodes
  - Range of memory sizes and storage options
  - Fast interconnect between nodes
- Workloads from interactive single core data processing to medium scale multiple node simulations
- 80 GPU nodes with total of 320 GPUs
  - AI and other workloads with GPUs
  - Also heavy AI models spanning multiple nodes
- 4 Petabytes work disk for data under active use



In customer use since September 2019

Technical specifications

	CPU	CPU cores	Memory	Number of nodes
Puhti CPU parition	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	192 GB	532
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	384 GB	92
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	384 GB + 3.2 TB NVMe	40
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	768 GB	12
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	1.5TB	6
Puhti-AI GPU partition	Xeon Gold 6230 4 x V100 32 GB	2 x 20 cores @ 2.1 GHz	384 GB (Host) 128 GB (GPUs) 3.2 TB NVMe	80

- Infiniband HDR interconnect between nodes
  - 100 Gb/s in CPU partition, 200 Gb/s in GPU partition

In customer use in Q3 / 2020

Coming soon: Mahti Supercomputer

- Massively parallel jobs requiring large floating point performance and capable interconnect
  - In principle jobs can scale across full system
  - Also smaller parallel workloads
- Jobs use always full nodes for maximum performance
- Over 8 petabytes of work disk for data under active use

In customer use in Q3 / 2020

Technical specifications

- 1404 compute nodes with next generation AMD Rome CPUs
  - Two 64 core AMD EPYC 7H12 processors per node
  - 2.6 GHz base frequency (maximum boost 3.3 GHz)
  - 256 GB of memory per node
  - About 180 000 cores in total
- Infiniband HDR interconnect between nodes
  - 200 GB/s bandwidth
- Theoretical peak performance 7.5 Pflop/s

CSC's Cloud Services

- IaaS Cloud
  - User supplies a virtual machine (VM) image
  - Services accessible over internet
- WebUI, CLI & Rest APIs supported

cPouta

openstack™

- IaaS Cloud for Sensitive Data Processing
  - Services accessible only from customer network
- WebUI, CLI & Rest APIs supported

ePouta

openstack™

- PaaS Cloud
  - User supplies Docker container
  - Services accessible over internet
- In Closed Beta Phase
- WebUI, CLI & Rest APIs supported

Rahti

OPENSHIFT

- Different hardware flavours (hpc, GPU, I/O, ...) available for all cloud services

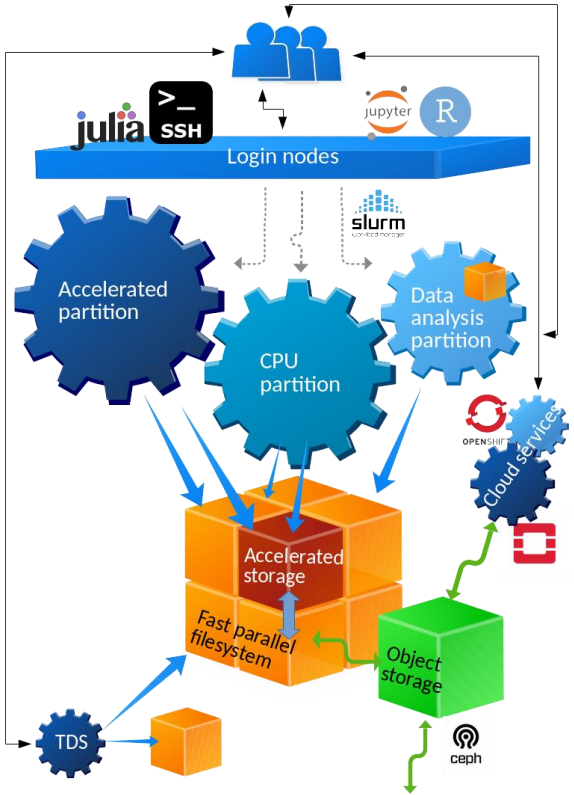
Programming for CSC supercomputers

- **Fortran, C++/C, Python, R, Julia, …**
- Parallel programming with MPI and OpenMP
  - Hybrid MPI + OpenMP becoming more important in Mahti
- Vectorization important for single CPU performance
- High performance libraries
  - BLAS, LAPACK, ScaLAPACK, FFTW, …
- GPU programming with OpenACC and CUDA
- Various frameworks for machine learning workloads
  - Keras, Tensorflow, PyTorch, …

EuroHPC system of the North

LUMI – world leading pre-exascale system

- Consortium lead by CSC
  - Belgium, Czech Republic, Denmark, Estonia, Norway, Poland, Sweden and Switzerland
- 200+ Pflop/s of peak performance
  - 1-2 CPU + 4 (AMD or Nvidia) GPUs per node
  - Highly capable I/O system
  - Supporting Tier-1 CPU partition
- 25 % of the resource dedicated to Finnish users
- To be hosted in Kajaani datacenter
- Available for customers in 2021



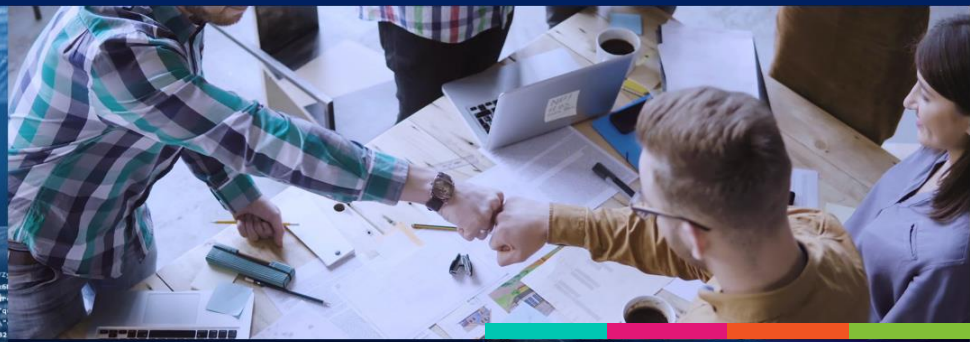
How to prepare for Lumi?

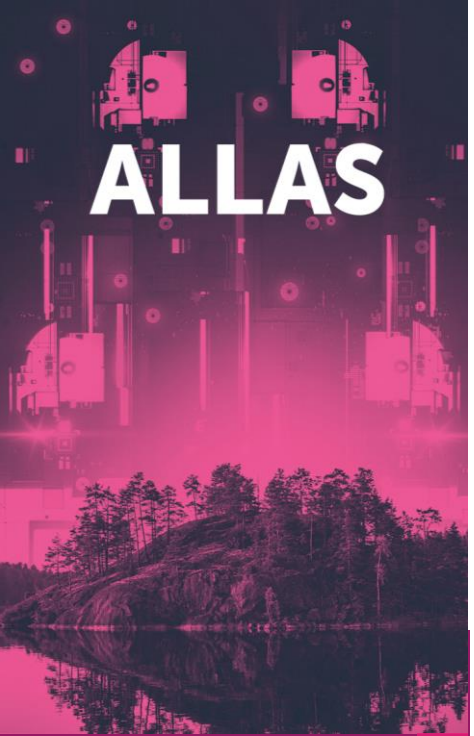
- LUMI is both huge possibility and huge challenge
  - Order of magnitude larger performance increase than normally with new CSC supercomputers (Mahti ~ 4 x Sisu, LUMI ~ 30 x Mahti)
  - Paradigm shift: fully accelerated system
- Thinking projects and use cases for Lumi
  - Cases for Tier-0 grand challenges
  - Existing GPU enabled applications
  - Combining simulation and AI methods within the same workflow
- Modernizing applications and GPU-enabling them
  - "even if it works, fix it"

Programming models for Lumi

- **Fortran and C++** most important programming languages
  - **Python, R** and **Julia** will likely have a major role in workflow management and as "driver" language
- MPI remains fundamental distributed memory approach
  - OpenMP and various GPU progamming approaches within a node
- GPU programming
  - **CUDA / HIP**
  - **OpenACC / OpenMP5**
  - Language-native GPU support (`std::for_each_n`, `do concurrent`)
  - High-level libraries and frameworks (Kokkos, RAJA,…)

Data services

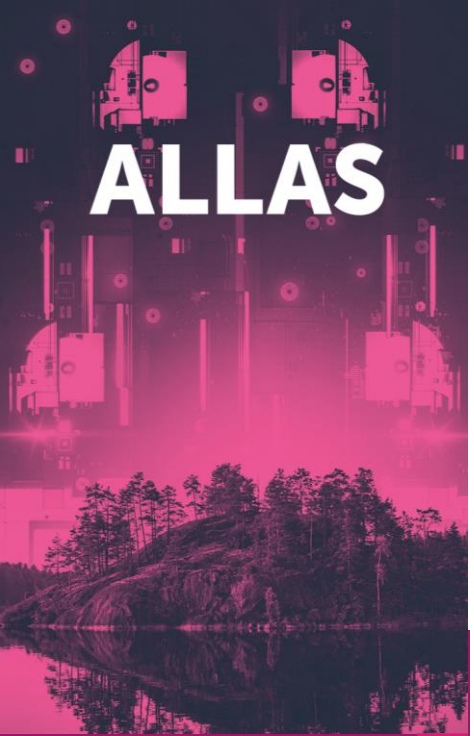




In customer use since October 2019

Allas – object storage: what it is for?

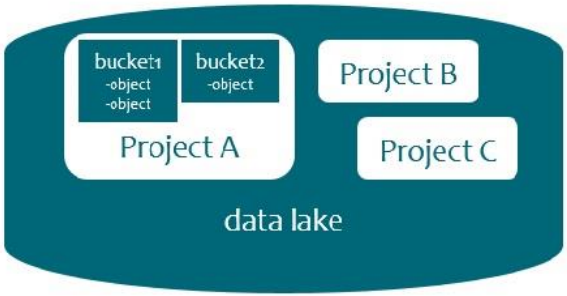
- Allas is new storage service for all computing and cloud services
  - Meant for data during project lifetime
- Data can be stored and retrived directly from anywhere in Internet
  - CSC supercomputers
  - Local workstation
  - Measurement devices
  - …
  - At simplest, web browser is enough
- Easy sharing of data outside project
  - Selected data can be shared publicly to Internet
- Arbitrary metadata can be added to data

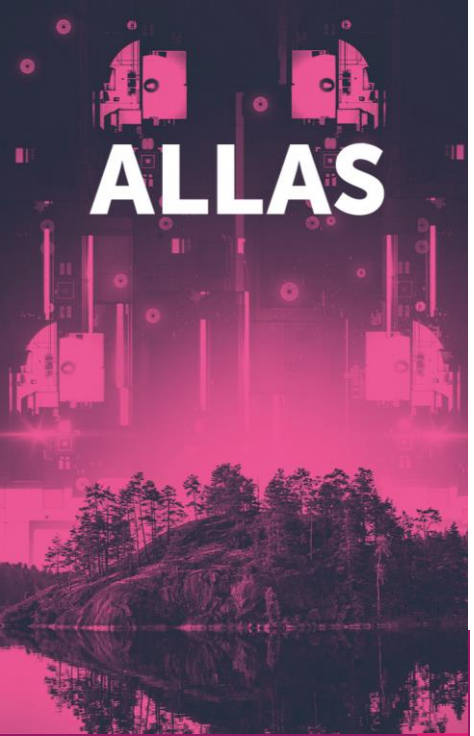


In customer use since October 2019

Allas - storage

- **12 Petabytes** of storage space for data stored over the life-time of a project
  - Storage space is **per CSC project**
- Object storage based on open source CEPH
- Data is stored as **objects** within a **bucket**
  - Blobs of data, can be anything (generally, **object** = file)
  - Project can have multiple **buckets**
  - Name of **bucket** must be unique within Allas
  - Only one level of hierarchy of buckets (no buckets within buckets)
  - Each object can have an URL and accessed over https e.g. with web browser: **https://a3s.fi/my_bucket/my_object**





In customer use since October 2019

Allas – usage

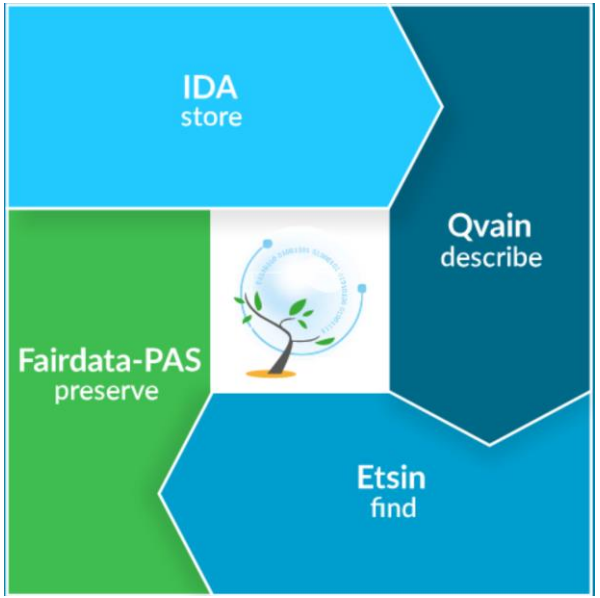
- For computations, data needs to be typically copied to/from supercomputer
- Data cannot with standard Unix commands (ls, cp, mv, etc.) but one needs to use object storage specific tools
  - a-commands
  - CyberDuck (Windows and MacOS)
  - Pouta www-interface (pouta.csc.fi)
  - rclone
  - s3cmd
  - Swifth
  - Python API

Publishing research data

- Research data should be "as open as possible, as closed as necessary"
- Data should include descriptive information (metadata).
- Published data should have a persistent identifier (enables citations).
- Services for storing and publishing stable data
  - Fairdata.fi for Finnish universities and research institutes
  - EUDAT B2SHARE for openly licensed research data in European collaboration

Fairdata.fi

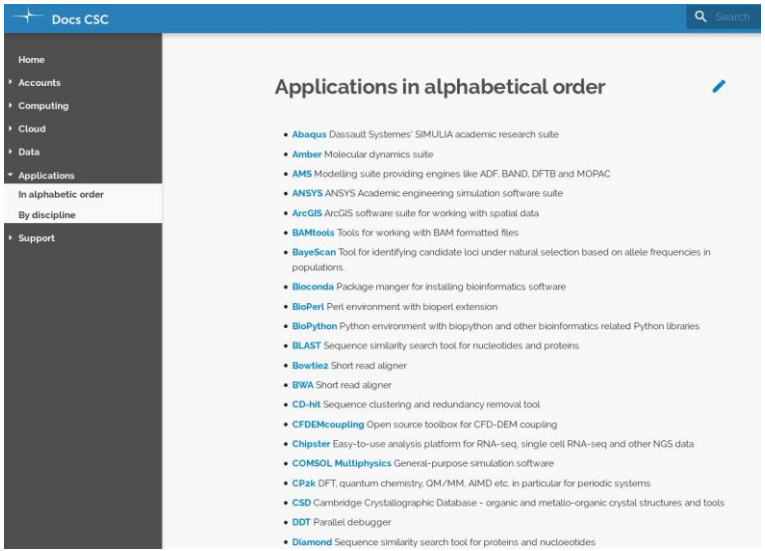
- National integrated services for storing, describing and sharing and preserving research data
- Access is applied via CSC (CSC user account and project are needed), local IDA contact person approves.
- **Make your data safe , documented and citable**
  - **IDA** – Research data storage service
  - **ETSIN** – Research data finder
  - **QVAIN** – Research dataset metadata tool
  - **FAIRDATA-PAS** – Digital preservation for research data
    - A separate contract is needed for PAS service



Support services for researchers

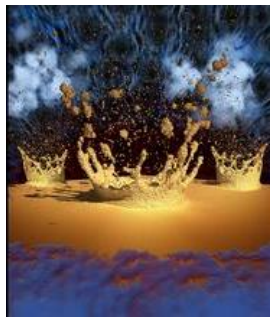
Software

- CSC provides researchers the largest collection of scientific software and databases in Finland.
- The list of pre-installed and supported scientific software packages can be found at: https://research.csc.fi/software
- Users can install also their own applications
  - CSC can provide support



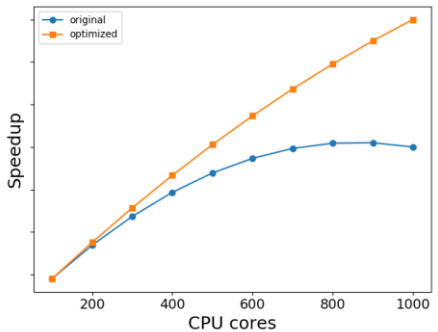
Expert Support in Sciences and Methods

- Help customers to select the most suitable and effective tools and software for each research project
- Advise in the effective use of supercomputers and cloud computation
- Support in optimisation and parallelisation of your own applications
- In-house scientific software development
  - Elmer, Chipster
- Scientific visualization
- Advise in using and applying for international resources
- Ask for support from CSC Service Desk **servicedesk@csc.fi**



Optimization service

- Help CSC's users to improve their HPC software
  - Consulting discourse between an application developer and CSC's specialist
- Suitable development projects
  - Code optimization i.e., improving single-core and parallel efficiency of the application
  - Parallelization of a serial code
  - Reduction of memory and/or I/O requirements of the application
  - Conversion of an MPI application into a hybrid MPI+OpenMP application
  - Enabling the use of the accelerator technologies such as graphic processing units (GPU).
- Send a free-form description of your case to **servicedesk@csc.fi**



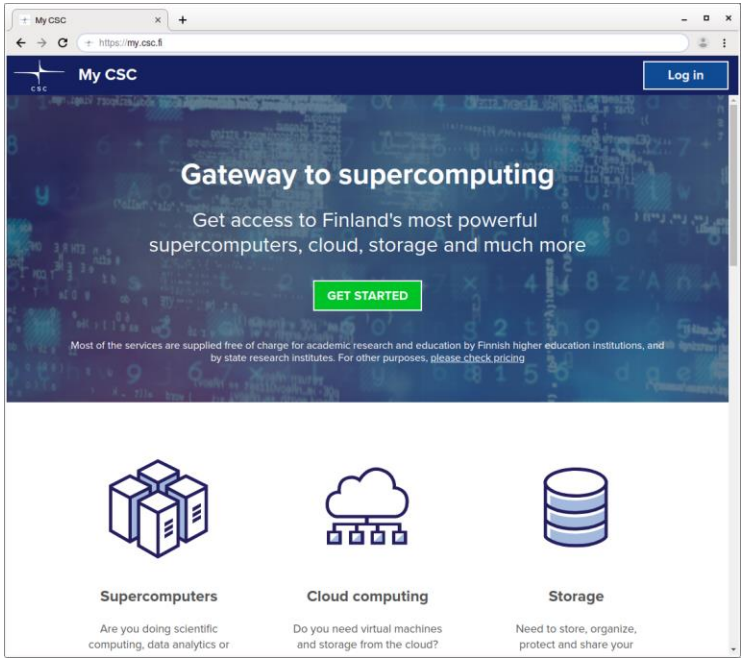
Training services

- Annually about 70 training events for Finnish universities and research institutes: courses, workshops, seminars and webinars
- Lecturers and trainers are leading experts
- Training aimed to familiarize you with the CSC infrastructure and its efficient use
- Courses can be customized according to your needs
- Information and registration for upcoming trainings and learning materials can be found in **CSC's training portal** www.csc.fi/training
- If you have questions related to CSC's training services, contact **courses@csc.fi**

How to get access?

How to get access?

- **Your Haka user ID is your access to more than 160 services.**
  - Web based services ready to use
  - Register at my.csc.fi to get a personal CSC user account
  - If your organization does not have Haka, contact servicedesk@csc.fi
  - Project supervisor applies for resources and services, and can invite other people to projects
  - Instructions https://research.csc.fi/accounts-and-projects
- **Customer service**
  - Support and guidance **servicedesk@csc.fi**
  - Weekdays 8.30–16.00.



When to use CSC services ?

- Single core / single GPU performance not necessarily much different from local workstation or FCGI systems, but added value possibly from:
- Software available in CSC supercomputers
- More memory in CSC supercomputers (up to 1.5 TB)
- Parallel computations with more resources than in local systems
- Moving between different systems should be relatively easy
  - Similar **module** and **batch** system (**Slurm**)

Questions?

Information about CSC in general: www.csc.fi

Information for researchers: research.csc.fi

User documentation: docs.csc.fi

Up-to-date information about the new computing and data environment: research.csc.fi/dl2021-utilization