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# LUNARC

CENTER FOR SCIENTIFIC AND TECHNICAL COMPUTING



# What is Lunarc?

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Founded by researchers for researchers

from a classical HPC center → *"knowledge based center with HPC experience and resources"*

e-science partner from HPC resource to end-user

*"Everything is not about the number of cores"*

Usability (visualisation, rviz, user interfaces)  
Training (new users, advanced users)  
Outreach (close to research groups)

Supporting Swedish researchers on all levels

# History

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# press meddelande



**LUNDS UNIVERSITET**



**datum**

Informationschef  
Christer Hjort  
046/107008

1987-11-20

## **Lunds universitet och IBM startar centrum för superdatorberäkningar**

Ett internationellt kompetenscentrum för superdatorberäkningar kommer att byggas upp vid Lunds universitet i samarbete med IBM. Här ska man arbeta med utveckling av olika datortillämpningar inom kvantkemi, statistisk mekanik, strukturmekanik (s k FEM) samt datorgrafik. Gästforskarprogram, seminarier, kurser och symposier ingår också i programmet för LUNARC dvs Lund University NIC Applications Research Center (NIC står för "Numerically Intensive Computing" vilket kan översättas till superdatorberäkningar).

Det var Carl-Hugo Bluhme, VD för IBM Svenska AB och Lunds universitets rektor Håkan Westling, som annonserade bildandet av LUNARC vid en presskonferens på fredagen. Den 20 november var samtidigt årsdagen för invigningen av IBMs stordator (3090-150 system med vektorprocessor) i Lund.

# Sveriges starkaste dator finns i Lund



FOTO: BERT OLSSON

Berg 1 till 8 heter de åtta processorer som tillsammans utgör SP1 – Lunarcs nya starka datorsystem, stort som ett kylskåp. Här flankerat av fr v Göran Sandberg, avdelningen för byggnadsmekanik, Bo Jönsson, fysikalisk kemi och Björn Roos från teoretisk kemi.

LUND.

I går invigdes Sveriges kraftfullaste paralleldator som ska betjäna tre forskaravdelningar vid Lunds tekniska högskola.

– Det var väl en väldig tur att vi inte vann kampen om det nationella superdatorcentret. Då hade vi stått här utan att vilja ha det i dag, konstaterar Björn Roos från avdelningen för teoretisk kemi.

I och med att den nya kylskåpsstora SP1-datorn kopplas samman med de arbetsstationer som redan finns på avdelningarna får Lund samma kapacitet som kampens "vinnare" Linköping. När systemet till sommaren kompletteras med SP2 blir kapaciteten dubbelt så stor.

## Nytt prisläge

– Utvecklingen inom datortekniken går nu snabbare än någonsin. 90-talet har inneburit en revolution både vad beträffar beräkningsresurser och prisprestanda, säger Bo Jönsson från avdelningen för fysikalisk kemi.

– 3090-datorn som vi använde 1986–1991 kostade till exempel tio gånger så mycket och hade bara en femtiondedel av den nya datorns kapacitet. Dessutom var den stor som ett helt rum och drog mycket mer ström, påpekar Göran Sandberg vid avdelningen för byggnadsmekanik.

De tre forskaravdelningarna samarbetar i Lunarc (Lund University Numeric Intensive Computing Application Research Center).

## Nya möjligheter

Men vad är då vitsen med ständigt utbyggd kapacitet?

– Om en sak kan göras snabbare kan vi testa av fler saker och göra fantasirikare beräkningar. En stor dator möjliggör mer komplicerade simuleringar och ökar dessutom säkerheten i resultaten, förklarar Göran Sandberg.

Beräkningsvetenskap handlar nämligen om att simulera verkliga processer på datorn. Normala jobb kan ta allt från fem minuter till fyra dygn för

datorn att räkna ut. Med den utbyggda kapaciteten skulle det rentav vara möjligt att simulera nollösningen för vattenflödet vid Öresundsbron – något som tidigare ansetts för jobbigt att genomföra.

## Allt går snabbt

Generationsväxlingen för datorer är snabb – maximalt tre år. Men priserna går ner. För de 100 miljoner kronor i investeringskostnader och 50 miljoner i driftskostnader som från början var tänkt att investeras i ett nationellt superdatorcenter skulle man i dag kunna installera lika starka datorsystem som det i Lund på en massa universitetsfilialer runtom i landet. Bara de 15 miljoner som Linköping lagt på att uppgradera sin superdator skulle räckt till tre stycken SP1-datorer och alltså tredubbelt så stor kapacitet.

I det perspektivet finns det inte längre någon anledning för Lunds tekniska högskola att sörja över att man förlorade kampen mot Linköping.

ELISABET HALLENCREUTZ

# History

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- Started 1986 as a collaboration between
  - Theoretical Chemistry
  - Physical Chemistry
  - Structural Mechanics
- Introduced the first academic super computer in Sweden
- In 1996, Lunarc was reorganised as a formal centre at Lund University
- Member of SNIC since 2003



# Organisation

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# Organisation

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- Board
  - Göran Sandberg, Chairman
  - Sine Larsen, University of Copenhagen, formerly Director MAXLAB
  - Sofia Feltzing, Astronomi
  - Jakob Donner, Medicinska Fakulteten
  - Stefan Wallin, Astronomi och teoretisk fysik
  - Johan Revstedt, Energivetenskaper
  - Maria Sandsten, Matematisk statistik
  - Fredrik Andersson, Ekonomihögskolan
- Operation
  - Jonas Lindemann, Director
  - Anders Follin, Technical Director



# Application experts

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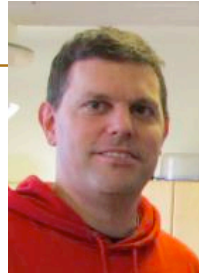
- SNIC Parallel expert – **Joachim Hein**
  - Provides advice to users with parallel codes
  - Helps users apply for PRACE time
  - Gives regular courses in OpenMP and MPI
  - Coordinates the SNIC training program
- Federated computing / Development – **Jonas Lindemann**
  - Provide support for grid-usage
  - Improving grid usability
  - Federated computing / Workflows
  - Development projects



# Application experts

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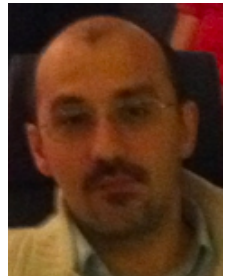
- GPU expert / Support – **Anders Sjöström**
  - Provides advice to users with GPU codes
  - Evaluates GPU architectures
  - Support coordinator
- Chemistry – **Magnus Ullner**
  - Extensive knowledge in chemistry workflows
  - Extensive knowledge in scheduling/queuing systems
- eScience – **Anders Follin (Tech. Director)**
  - Develops and implements enhanced workflows and infrastructures for research communities
  - Scientific Visualization, computer graphics



# System experts / Developers

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- **Robert Grabowski**
  - Teamleader system group
  - Center storage and operations
- **Alex Contis**
  - Security expert
  - National storage maintainer / Grid operations
- **Tore Sundqvist**
  - System expert
- **Roger Larsson**
  - Developer for potential SNIC and LU projects (C++/Java and more...)



# Lunarc resources

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# Resources

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- Provides HPC resources for local and national users
- Provides an efficient and easy to use HPC environment
  - Documentation
  - Optimised libraries
  - Compilers
  - Remote Desktop environment
- Provides support to users
  - User registration, quota and queue issues
  - Advanced user support (Application experts)
- Designs and implements state-of-the-art resources

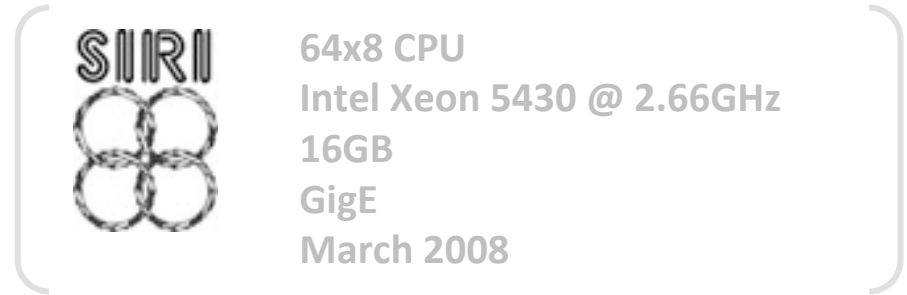


# Current resources

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216 x 8 CPU  
Intel Xeon e5520 @ 2.26GHz  
24GB  
Infiniband QDR/DDR  
November 2009



64x8 CPU  
Intel Xeon 5430 @ 2.66GHz  
16GB  
GigE  
March 2008



208x16 CPU  
AMD 6220 @ 3.0 GHz  
32-64 GB  
Dec 2011



(16+8) x 16 CPU  
Intel Xeon  
68 GPU:s Kepler + 1 Xeon Phi  
Fall 2012

Alarik

Erik

Tier-3 Resource for High Energy Physics in Lund (hosting)



# Visualisation resources

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- Remote visualization
  - Attached to compute cluster (i.e. a node)
  - Hardware accelerated remote visualization
    - » Nvidia Quadro 5000
    - » Teradici HBA (compression and encryption)
    - » Teradici zero state client portal
  - Software based solution with HW OpenGL acceleration
  - Remote desktop access "Lunarc HPC Desktop"
  - Provides a unified HPC "desktop" experience





# Computer room

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- 2 computer rooms (125+75) m<sup>2</sup>
  - Upper room used for HPC resources
  - Lower room used for Storage
- Water cooled racks (HP MCS and APC)
- 2 x 10 GigE connections to SUNET



# Storage resources

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# SweStore – National Storage

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- Lunarc maintains 600 TB for the national storage initiative
- 40 servers connected directly to the internet with approximately 20-40 TB storage each



# Center Storage

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- Filesystem shared on all Lunarc resources
  - /lunarc/users/...
- Currently 75 TB
  - Can be expanded
- Implemented using a HP X9000 storage system
- Needs an urgent upgrade ...
- Proposal for new Lustre-based center storage sent to SNIC



# Cluster storage

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- File systems provided by a specific resource
- Lustre filesystem on Platon
  - /platon/users/...
  - Lustre with 4 servers (2 MDS and 2 OSS)



# Grid cache

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- 100 TB of storage on Alarik-grid
- Caches downloaded input files for grid jobs
- Reduces downloads



# Lunarc training

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# Courses given by Lunarc

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- **Joachim Hein** responsible for our training curriculum for Lunarc and SNIC
- Teaching by
  - Joachim Hein (MPI, OpenMP, Intro)
  - Jonas Lindemann (Python, Fortran, Grid, Intro)
  - Magnus Ullner (Intro)
  - Rickard Nilsson (MPI, OpenMP, Intro)
  - Anders Sjöström (Intro)
  - Anders Follin (Intro)





# Courses given by Lunarc

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- **Message Passing with MPI (JH)**
  - Three day course, incl. lectures and practicals
  - Has been given several times since 2011
    - » Lund
    - » Göteborg
    - » Linköping
    - » Uppsala
  - Registration open: 29 - 31 October 2014 in Lund
  - Very popular!



# Courses given by Lunarc

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- **Shared Memory Programming with OpenMP (JH)**
  - 2½ day course, incl. lectures and practicals
  - Offered in the past in Lund and Linköping
  - Planned for December 2014 in Lund
- **Introduction to HPC (ALL)**
  - Lectures on:
    - » UNIX
    - » Systems and services offered by Lunarc and SNIC
    - » Accessing and using the Lunarc clusters
  - ½ day of practical exercises
  - Registration open for 2 October 2014



# Courses given by Lunarc

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- **Programming in Science and Technology (JL)**
  - SeSE course
  - Given 4 times. 5 year 2012
  - Python/Fortran/Object-orientation
- **Advanced programming in Science and Technology (JL)**
  - New course given in fall 2012
  - C++/Fortran/Object-orientation
  - Teacher: Jonas Lindemann
- **Introduction to Grid Computing (JL)**
  - New course given in 2 times in 2011
  - Introduction to the ARC Middleware



# Courses given by Lunarc

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- **Efficient programming of modern HPC architectures (JH/JL)**
  - Postgraduate course (7.5 ECT)
  - COMPUTE research school in the science faculty
  - Given twice (HT12 and VT14)
  - Course content
    - » Fortran, Python, build systems
    - » OpenMP, MPI
  - Exercises and Project require accessing Lunarc systems



# Application experts

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# Joachim Hein

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- HPC Training
  - Coordinates and provides training within SNIC
  - MPI / OpenMP
- Application install and optimisation
- Grant application support (PRACE)
- Consultancy
- Machine studies
- European project
  - PRACE
  - European Exascale Software Initiative (EESI)
- Winner of HPC Innovation Excellence Award, June 2014
  - Work on Plasma turbulence code – GS2



# Anders Follin

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- Visualisation expert
- PRACE
  - Participated in WP10.3 Remote visualisation
  - Leading role in group
  - Hardware based solutions for remote visualisation
- e-science workflows
  - coordinator for national 7T project and SBI biomedical archive
- Application expert in Sensor and Storage
  - Currently MAX IV and ICOS



# Anders Sjöström

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- MATLAB / R / Python expert
- GPU Programming
- System expert on the GPU resource Erik





# Jonas Lindemann

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- Expertise in distributed and federated computing
  - Experience in ARC middleware development
- User interface design and development
- Programming in Science and Technology
  - Dynamic languages
  - Numpy / Scipy
  - Mixed-language programming



# Strategic Alliances

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# Strategic Alliances

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- **Lund Bio Imaging Center – LBIC**
  - National 7-Tesla MRI installation (LBIC)
- **SBI - Swedish Bioimaging Network**
  - Workflow integration
- **MAX IV –**
  - Scientific Data Management
- **ICOS / MERGE**
  - Workflow integration
- **HUMLAB**
  - Research infrastructure development



# Projects

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# SNIC coordinated training

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- SNIC HPC training program coordinated by J. Hein
- Established regular Skype and F2F meetings with contacts from all SNIC centres
- Conducted a user survey
- Coordinated training activity plan for 2014 with training activities at all centres (courses and online material)
- Announcement of training activities to users and staff
  - centralised SNIC training web page (live)
  - SUPR generated SNIC mailing lists (to be activated)





Page **Discussion**

Read [View source](#) [View history](#)

## Training

This page provides an overview on high performance computed related training available to users and personnel of the SNIC.

**Contents** [hide]

- 1 Training events offered or supported by SNIC
- 2 Training offered by other providers
- 3 Community specific training
- 4 Links

### Training events offered or supported by SNIC

<input type="checkbox"/>	<input type="checkbox"/> Start date	<input type="checkbox"/> End date	<input type="checkbox"/> Event type	<input type="checkbox"/> Location	<input type="checkbox"/> Description
<a href="#">Introduction to PDC (September 2014)</a>	16 September 2014	16 September 2014	Course	Stockholm	Introduction to PDC
<a href="#">DDT (PDC September 2014)</a>	25 September 2014	25 September 2014	Course	Stockholm	Debugging applications using DDT
<a href="#">Introduction to HPC (Lunarc October 2014)</a>	2 October 2014	2 October 2014	Course	Lund	Introduction course for new users of high performance computing
<a href="#">Uppmax Intro Course (October 2014)</a>	20 October 2014	24 October 2014	Course	Uppsala	Introduction course for new users of Uppmax systems
<a href="#">MPI (Lunarc October 2014)</a>	29 October 2014	31 October 2014	Course	Lund	An introduction to parallel programming using MPI
<a href="#">MPI (PDC November 2014)</a>	25 November 2014	27 November 2014	Course	Stockholm	Writing parallel applications using MPI

An overview on training events offered in the past is available from the [past training events page](#).

### Training offered by other providers

- [SeSE](#) provides courses in the field of e-Science for PhD-students within the Swedish academia.
- The [Prace training portal](#) provides an overview on the training offers available from PRACE. These include course, tutorials and slide sets from past events.

### Community specific training

- The [Science for Life Laboratory](#) (SciLifeLab) provides [training courses](#) focused on molecular biosciences.

### Links

- [SNIC coordinated training project page](#).

- Main page
- Research areas
- Centres
- Software
- Resources
- Training
- SweGrid
- SNIC storage
- Projects
- Support

- People
- Application experts
- Systems experts

For Staff

- Editing policies
- Management
- Internal

Toolbox

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This page was last modified on 27 August 2014, at 12:28.

This page has been accessed 1,246 times.



# SNIC Emerging Technologies

- Focus areas defined by TC during spring
  - Access-methods and remote visualisation
  - Future HPC and Accelerators
  - Storage Technologies
- Project officially started in May
- Some areas have already started
- Project plans due september-october

Document type	Proposal	Title	Access-methods and remote visualisation
Document status	DRAFT		
SNIC Emerging Technologies		2014-05-19	DNR

## Access-methods and remote visualisation

Project partners: LUNARC, UPPMAX  
Project start: 1H2014  
Project end: 2H2014/1H2015

Document type	Proposal	Title	Future HPC and Accelerators
Document status	DRAFT		
SNIC Emerging Technologies		2014-05-19	DNR

## Future HPC and Accelerators

Project partners: LUNARC, PDC, HPC2N  
Project start: 1H2014  
Project end: 2H2014/1H2015

### 1 Description

Document type	Proposal	Title	Storage Technologies
Document status	DRAFT		
SNIC Emerging Technologies		2014-05-19	DNR

## Storage technologies

Project partners: C3SE, HPC2N  
Project start: 1H2014  
Project end: 2H2014/1H2015

### 1 Description

There are many storage technologies employed within SNIC. To be able to deploy solutions that are suitable for different usage scenarios, it is important that there is a continuous evaluation of available storage technologies. It is also important that prototype solutions are evaluated closely to users and facilities. Typical projects within this focus area could be:

- File systems for different I/O patterns.
- New storage hardware.
- Higher-level file services.
- Client tools for accessing available resources.
- Integration services.

### 2 Objective and deliverables

- Investigate how existing resources can be facilitated in new ways and how new approaches for users on how to use existing solutions can be facilitated to provide better support for I/O-intensive simulations and work-flows. (C3SE)
- Investigate how the RobinHood service of Lustre v2+ filesystems can be used in conjunction with Tivoli TSM to speed up incremental backups. (C3SE, HPC2N)
- Investigate how the RobinHood service of Lustre v2+ filesystems can be used to provide more fine-grained quotas, ex. for project storage etc. (C3SE)
- One solution that has been used in SNIC for a number of years for long-term storage of research data is dCache in combination with TSM for archiving to tape. There are several alternatives to using TSM for archiving to tape, which should be further studied both from a performance and cost effectiveness. One example is LTFS [3]. To look at various options for long-term storage is also something that connects well to activities within WLCG and EISCAT\_3D for which HPC2N are involved in. (HPC2N)



# MAX IV

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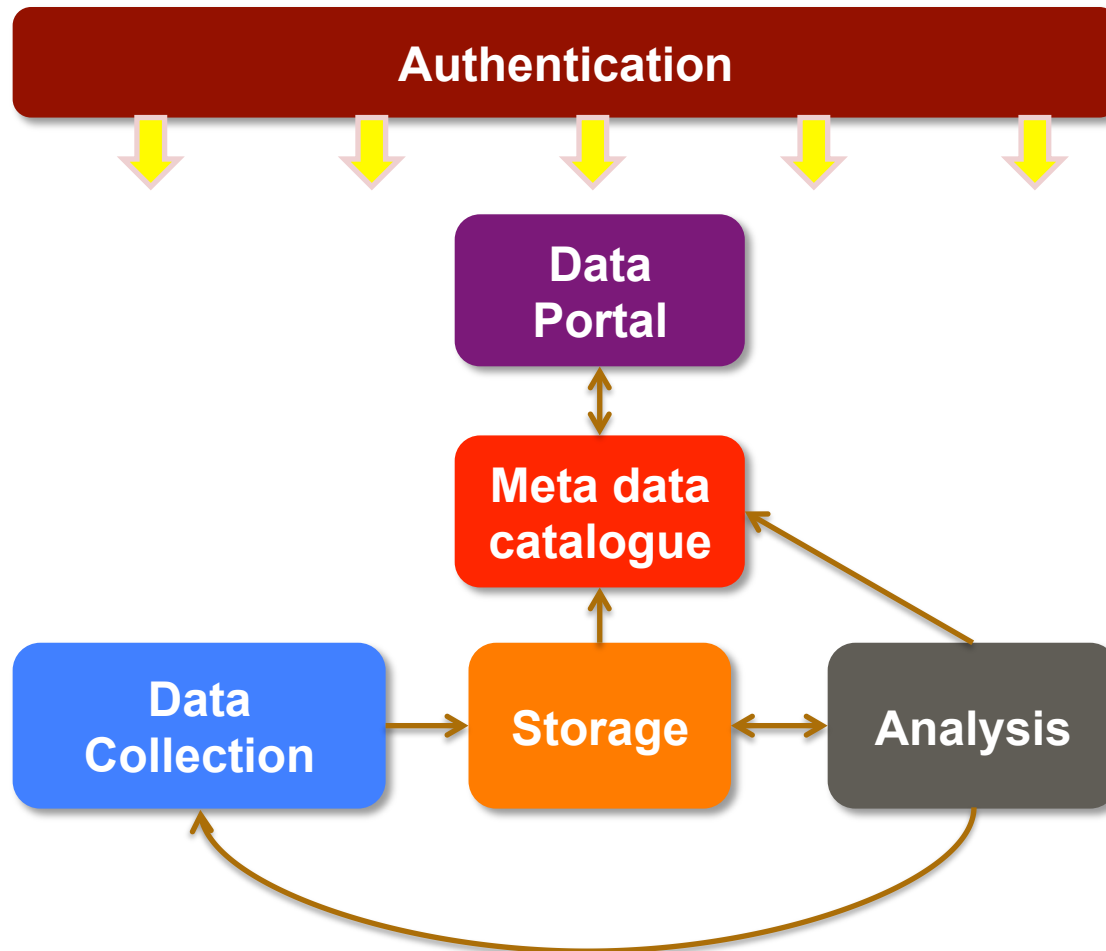
- Lunarc has worked together with MAX IV during late fall 2013 and spring 2014 to define a scientific data management infrastructure
- A prototype setup has been implemented in a virtual environment
  - Ensures that the proposed infrastructure is viable and services interoperating
- A remote analysis desktop solution has been developed based on the same tools as in "Lunarc HPC Desktop"
- Users have been able to evaluate the setup with regards to storage and analysis tools



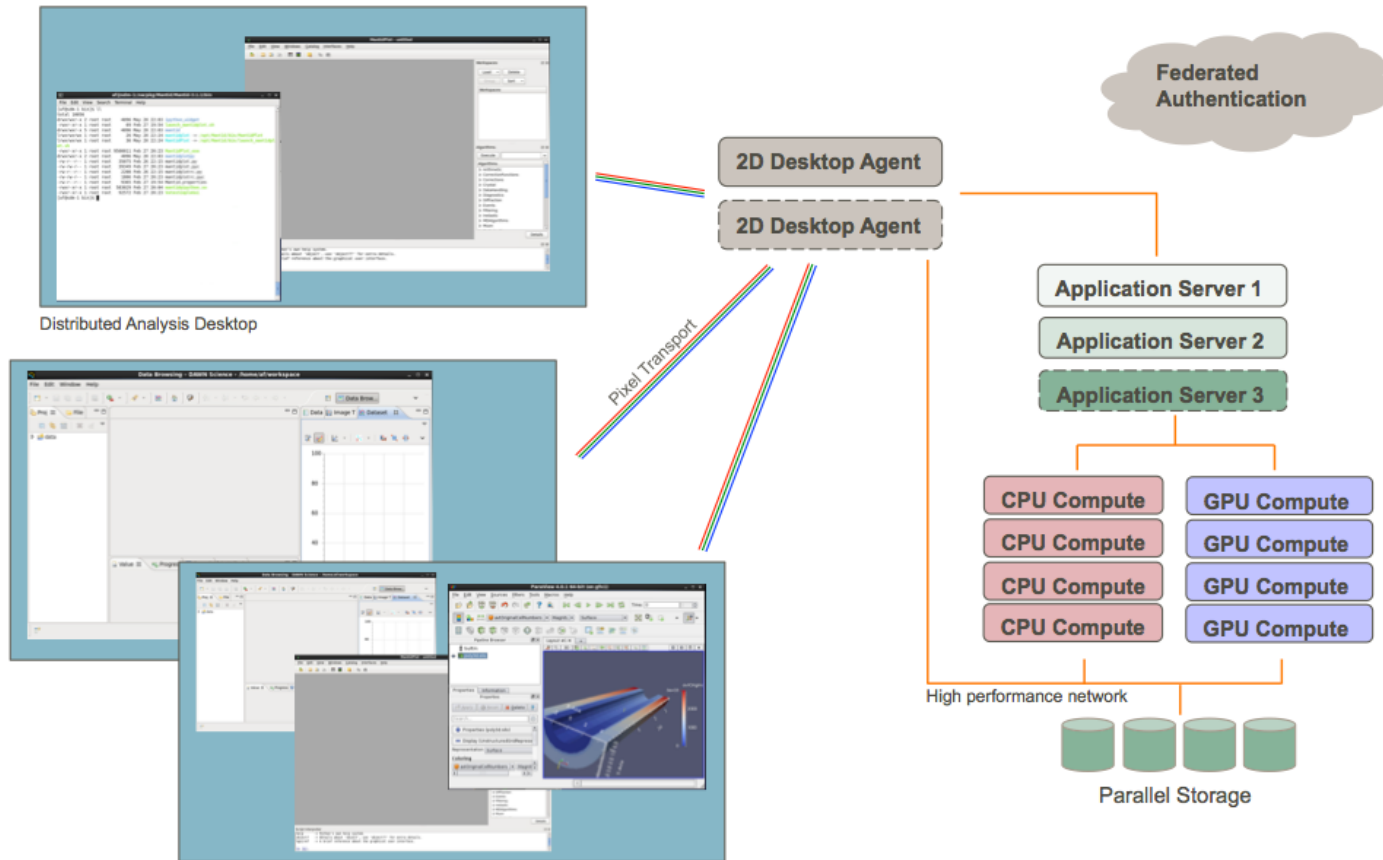


# Data Management Prototype

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# Data Analysis "Desktop"

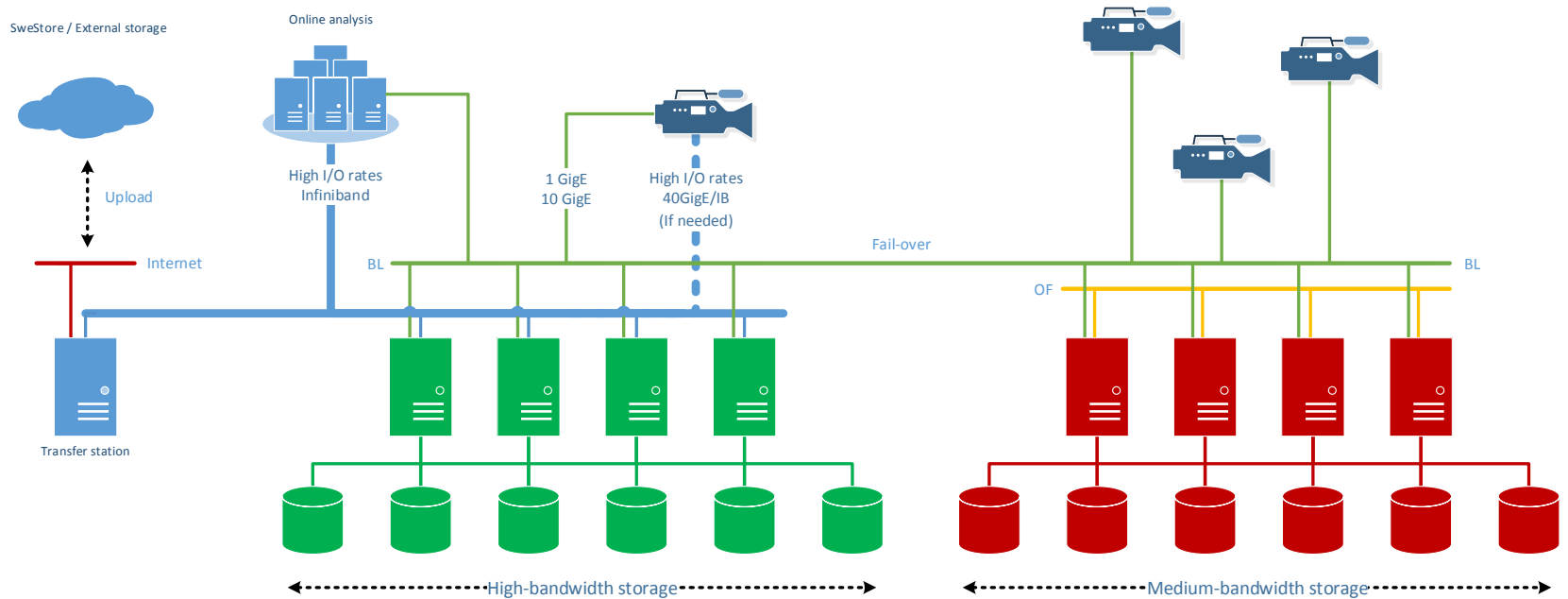


AF 2014-06-03

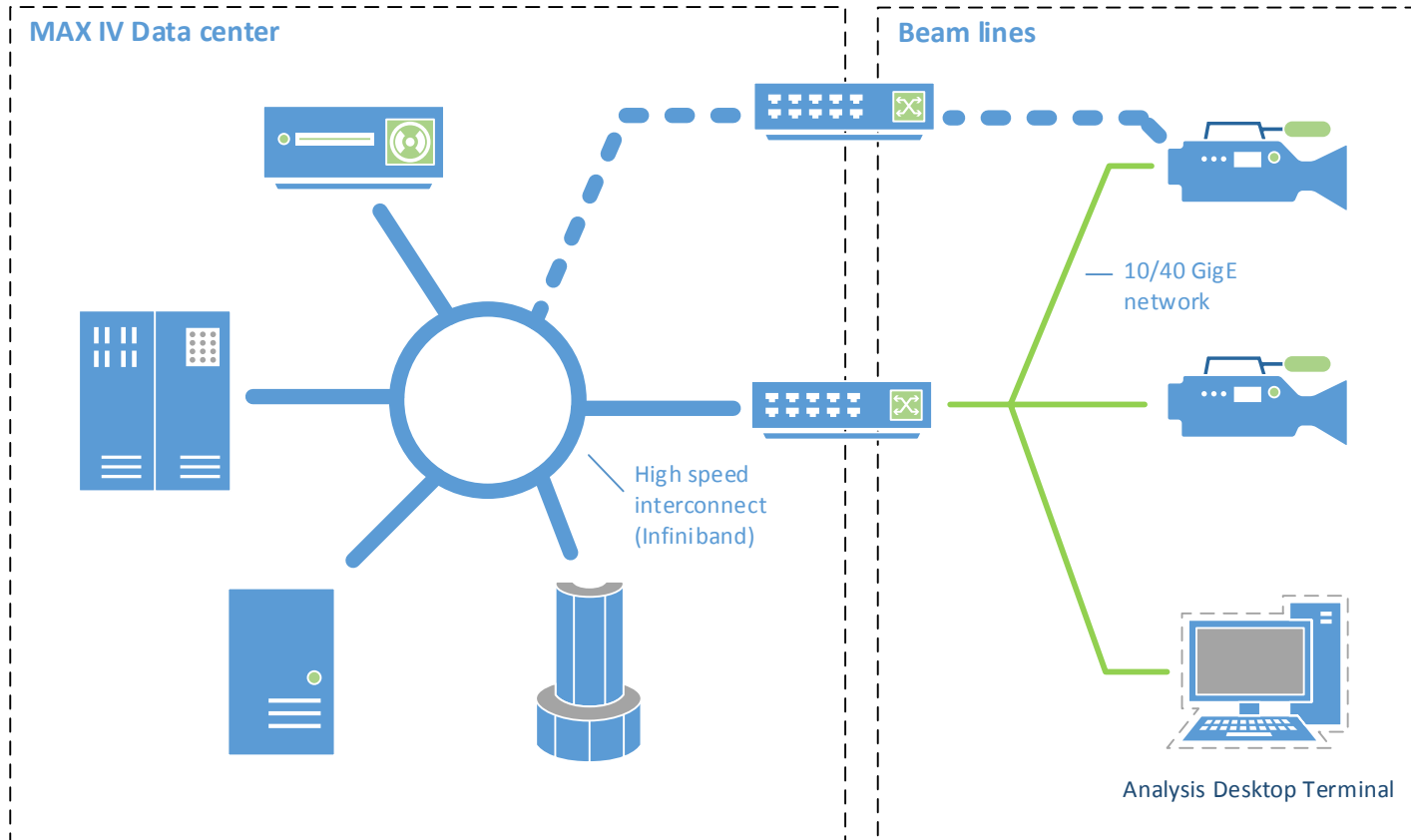


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# Proposed Storage Architecture



# Network Architecture



# ICOS – Integrated Carbon Observatory

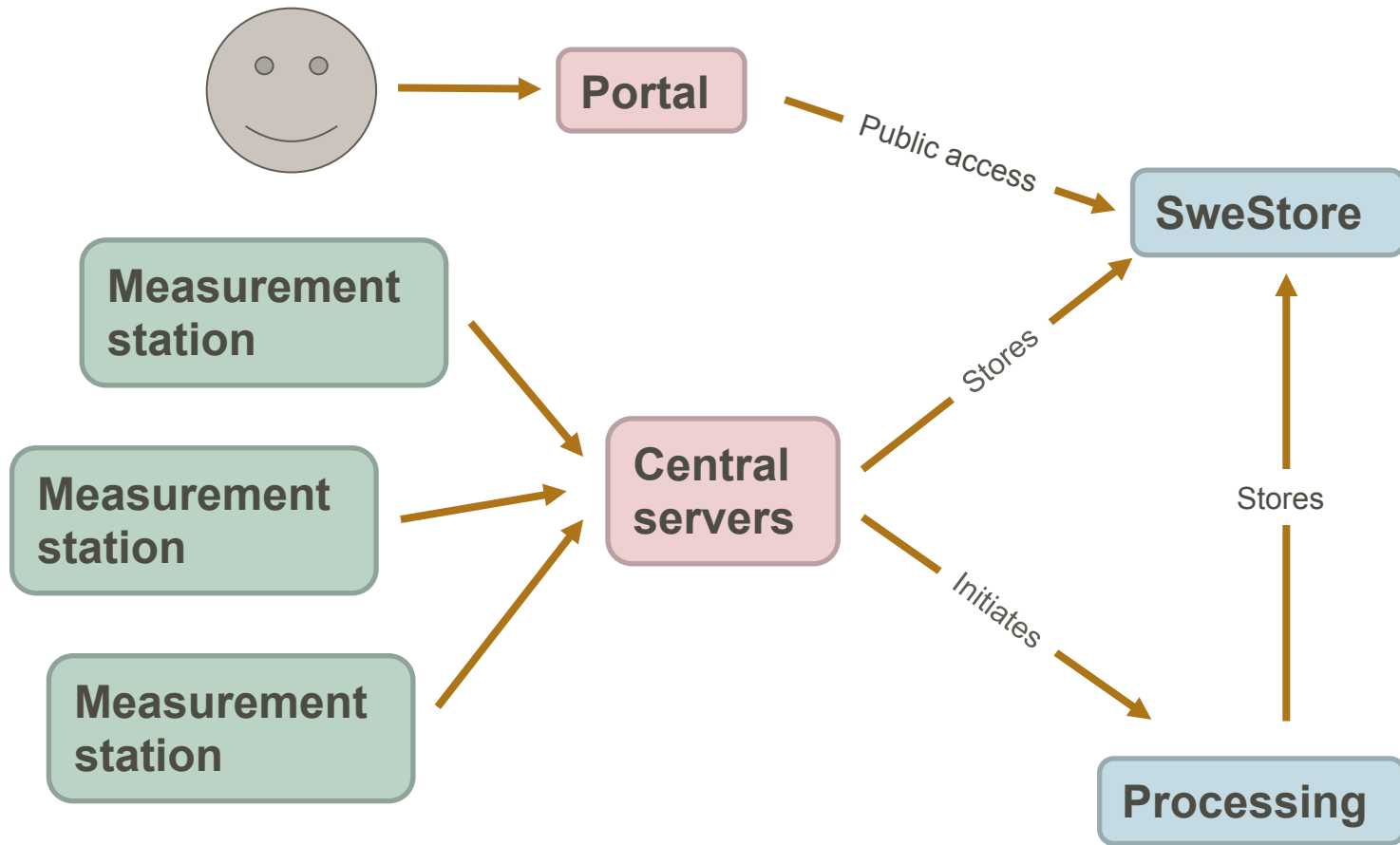
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- We have been working together with ICOS in LU to defined a workflow from sensors to the national storage infrastructure
  - Initial problems due to lack of dCache / ARC Windows support
- iRODS access is being evaluated as a solution
  - Command line Windows clients is not fully supported by iRODS
  - Lunarc has built "beta" versions of the iRODS clients, but a more long-term commitment is needed



# Very simplified ICOS setup

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# Outreach projects

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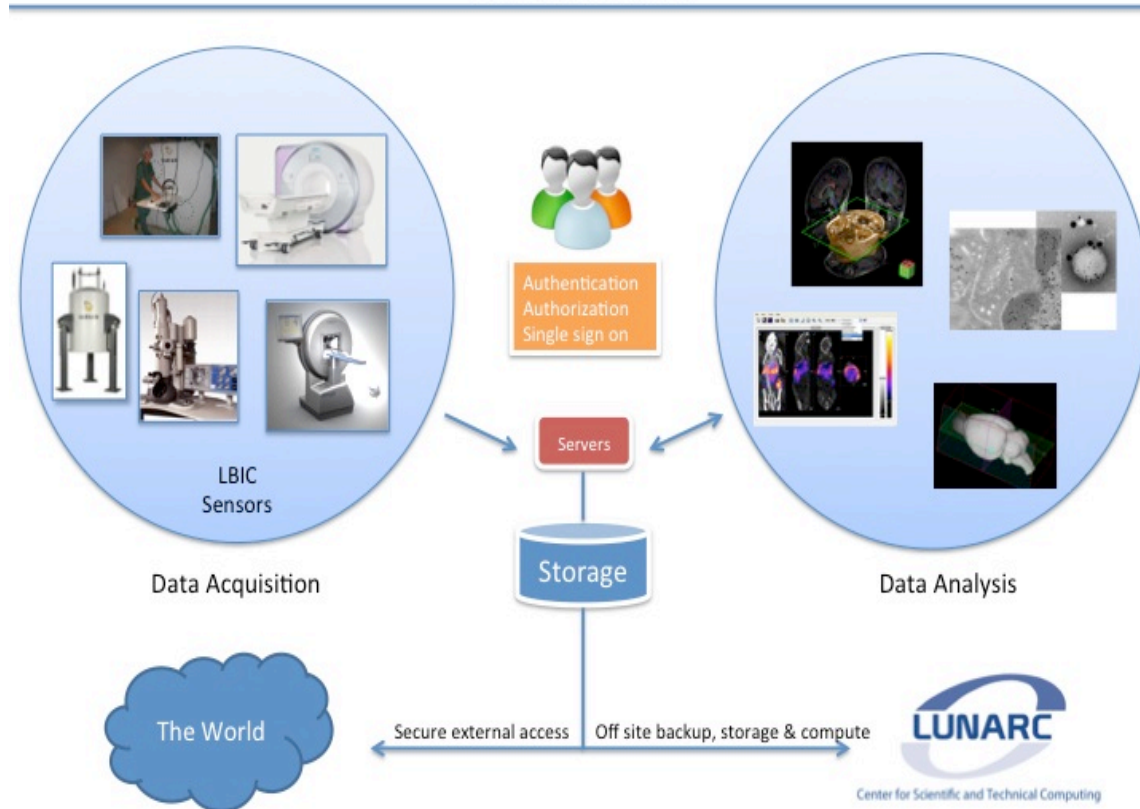
- Lunarc works together with research groups to develop an optimized scientific **e-infrastructure**
  - Develop and implement compute, storage and visualization infrastructure for research data
  - Develop and implement virtual environments for supporting sensor equipment
  - Develop research group e-science workflows



# Lund Bioimaging Center

## LBIC Data Management & Imaging Workflow

-- General workflow --

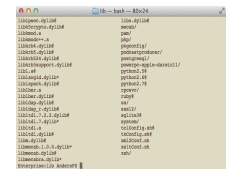
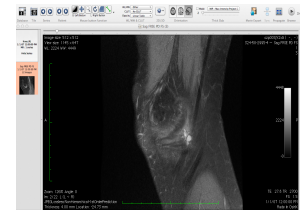
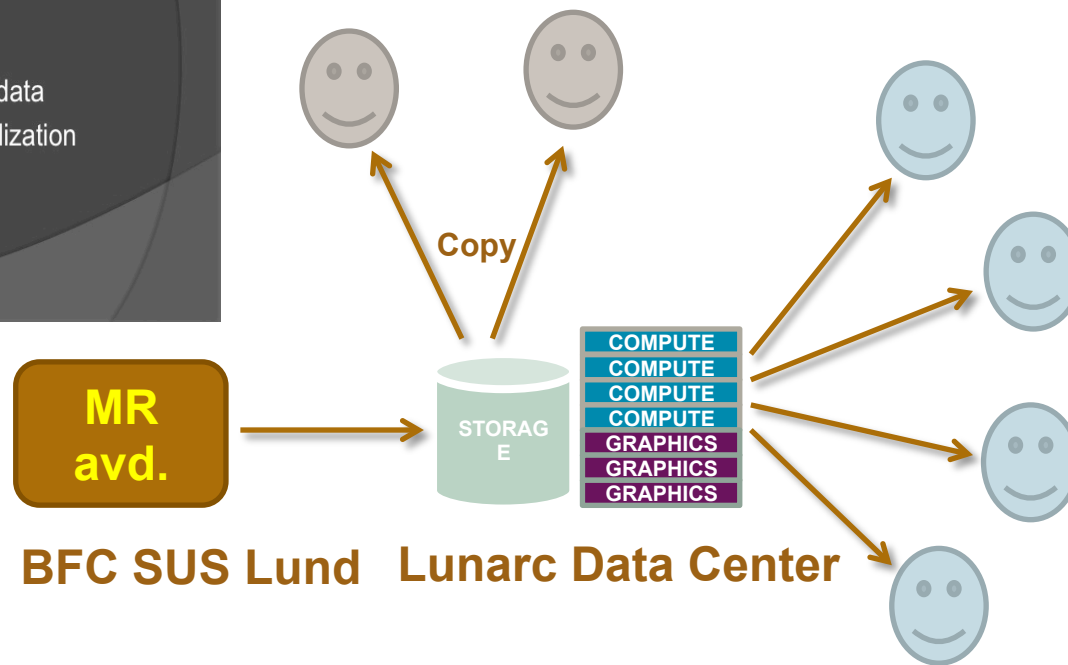




# LBIC National 7-Tesla MRI

## 7T challenges

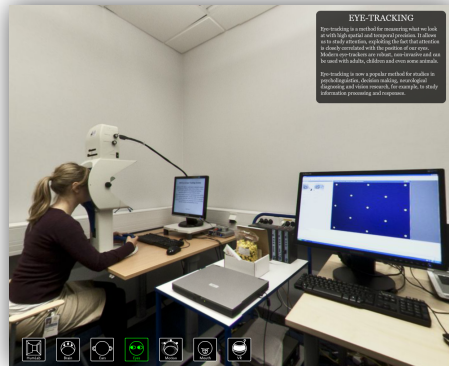
- Data is acquired behind the Hospital Firewall
- Human data
- Data integrity and security
- National access to acquired data
- Compute and (remote) visualization needs



# HUMLAB

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- Work on defining their future local e-infrastructure
- Integration of a multitude of sensors with storage infrastructures.
- Will probably need national storage with publishing capabilities (persistent identifiers)



# Skissernas museum

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- Sweden:s largest repro-camera for aquiring paintings in very high resolutions
- Working on a storage solution with integrated backup.
- Will probably need national storage with publishing capabilities (persistent identifiers)

**SKISSERNAS MUSEUM**  
MUSEUM OF PUBLIC ART

CURRENT  
EXHIBITIONS  
CALENDAR

EDUCATION  
ARCHIVES  
COLLECTION

ABOUT  
VISIT  
CONTACT



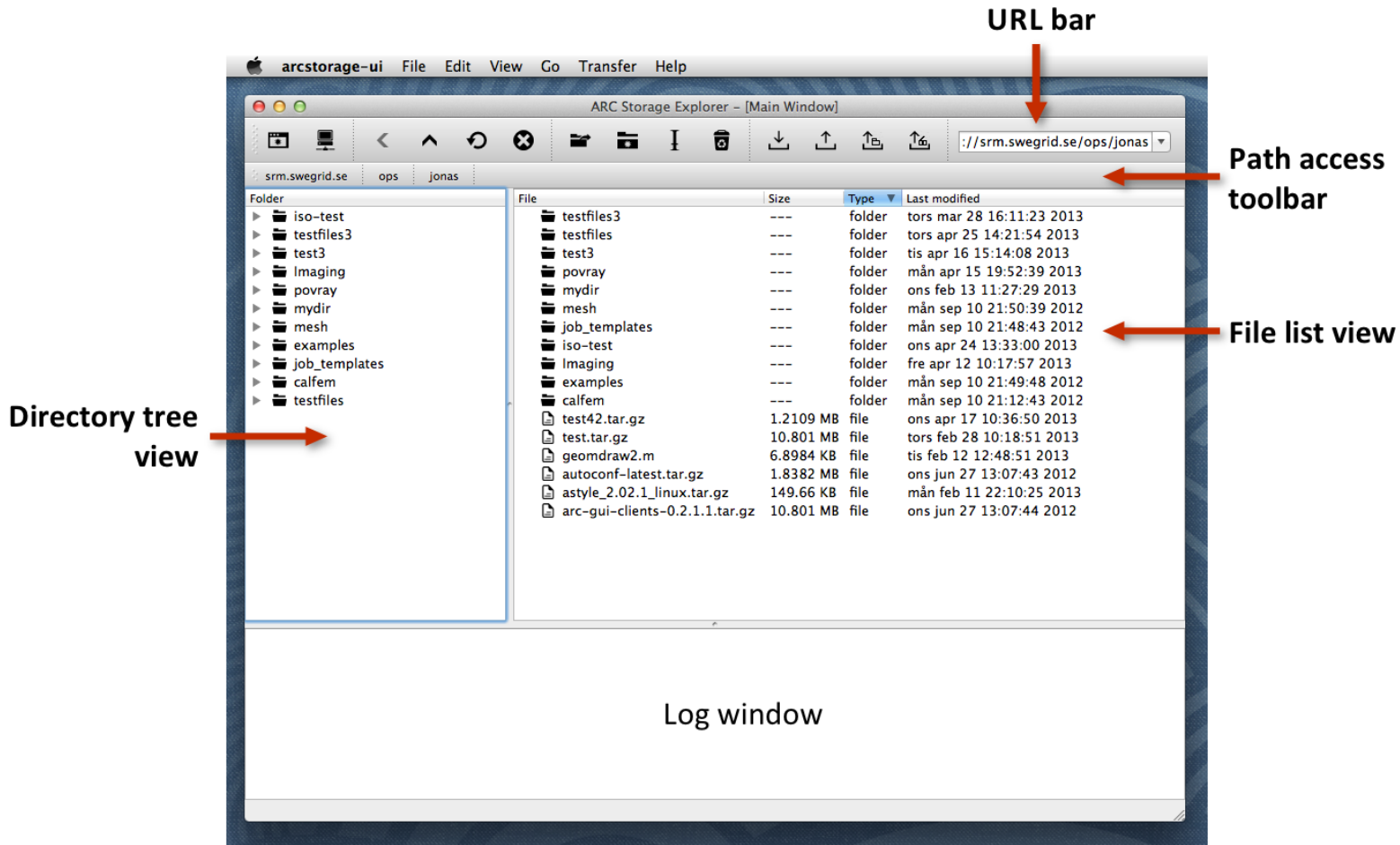
# Development efforts (ongoing)

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- **ARC Storage Explorer**
  - Graphical user interface to dCache
  - Enables easy access to SweStore
  - Available on the Lunard HPC Desktop
- **The Lunarc-Box**
  - SweStore "Appliance"
  - Creates a "Dropbox" solution for Windows and Mac OS X environments
  - Implements smart folders for automatic processing
  - SBI Pilot project implemented at GU

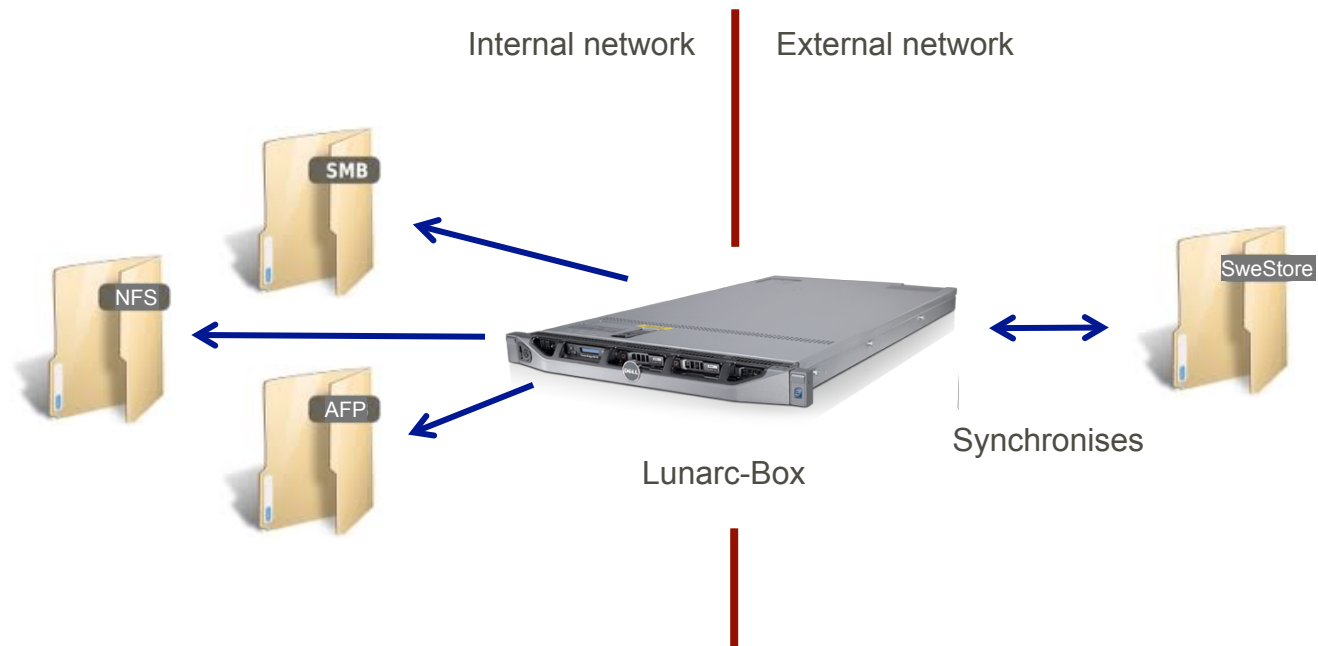


# ARC Storage Explorer

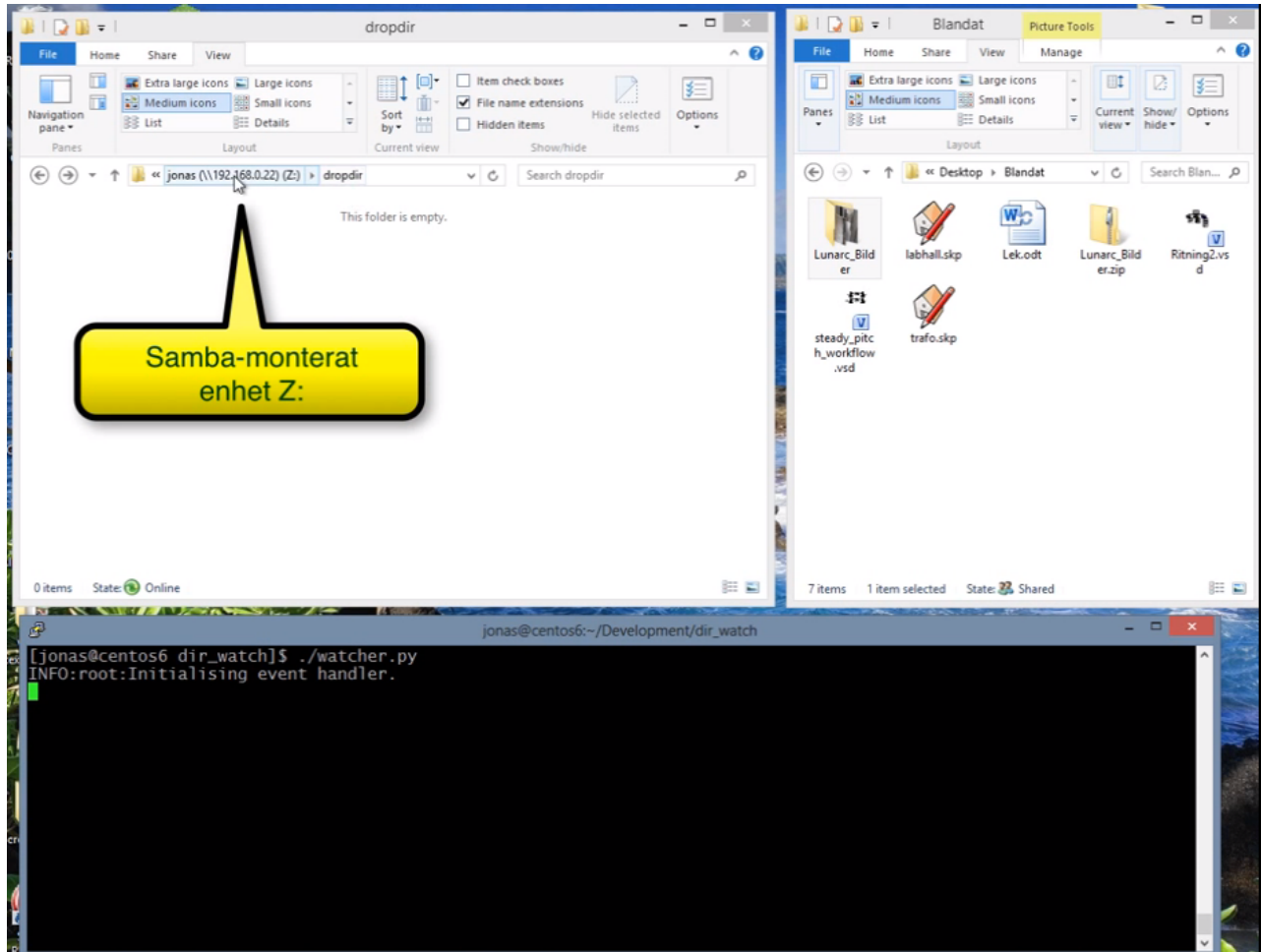


# Lunarc-Box

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# Lunarc-Box



# Security

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- Investigated 2-factor authentication schemes in end of 2008
- A commercial One-Time-Password (OTP) server from NordicEdge (now Intel/McAfee) was chosen
  - Adapted for use with Lunarc infrastructure.
  - Sends SMS with one-time password
  - Easy to integrate in existing PAM-based authentication
- Handles 30000 logins per year.
- Has prevented intrusion attempts.
- Rickard Nilsson has added support for YubiKey





# Lunarc HPC Desktop

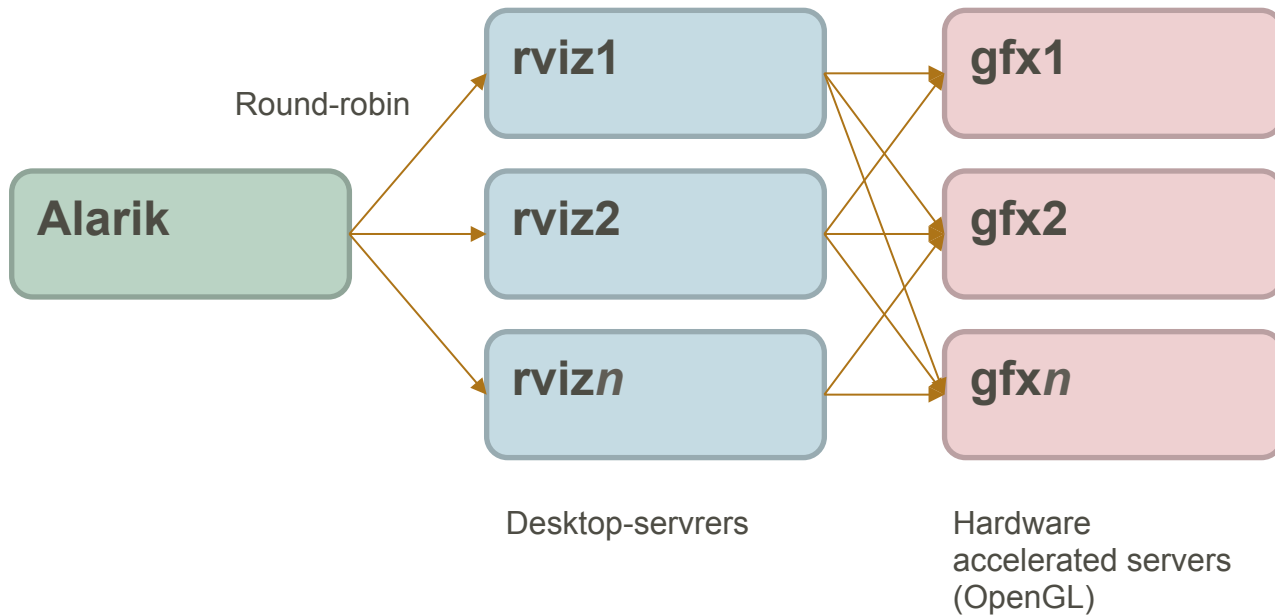
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- Remote desktop environment for users
- Connected directly to file systems and queuing systems
- Provides access to a desktop with common tools such as file browsers, terminals and editors
- A platform for running many graphical environments such as
  - MATLAB, ABAQUS, ParaView, VMD and more
- Desktop session is kept between connections
  - Keep terminals/applications running
- Provide hardware accelerated graphics for some of the installed applications

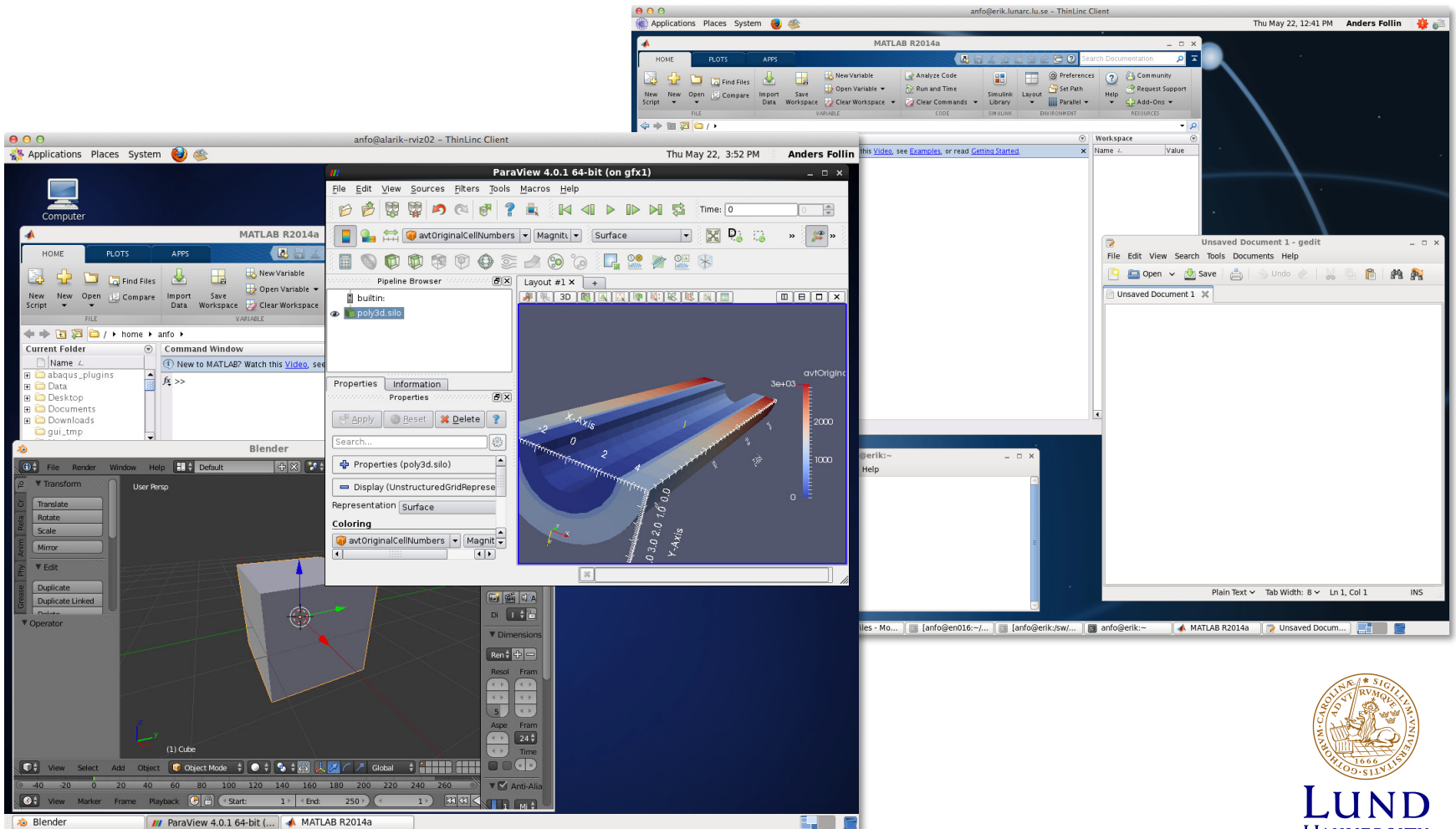


# Lunarc HPC Desktop

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# Lunarc HPC Desktop



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# Benefits using Lunarc HPC Desktop

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- Graphical User Interface
- BIG data stays in data center (e.g. large post processing data)
- Security: No data is transferred across the network
- High performance (parallel) visualization from anywhere
- Desktop state saved between sessions
- Improved workflow



# Lunarc within SNIC

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# Lunarc within SNIC

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- SNIC Partner at Lund University and providing the link between users/communities at Lund University and SNIC.
- Helping users and communities to take advantage of the SNIC resources, as well as providing them with expertise in e-Science.
  - Training and support
  - Integration consultancy. Pragmatically solve real-world e-science workflows for communities
- Provide user-friendly access to computing and storage resources within SNIC
  - Easy to use resources supporting multiple access-methods
  - Provide an path for new users to HPC
- Application scaling support
  - SNIC Parallel expert



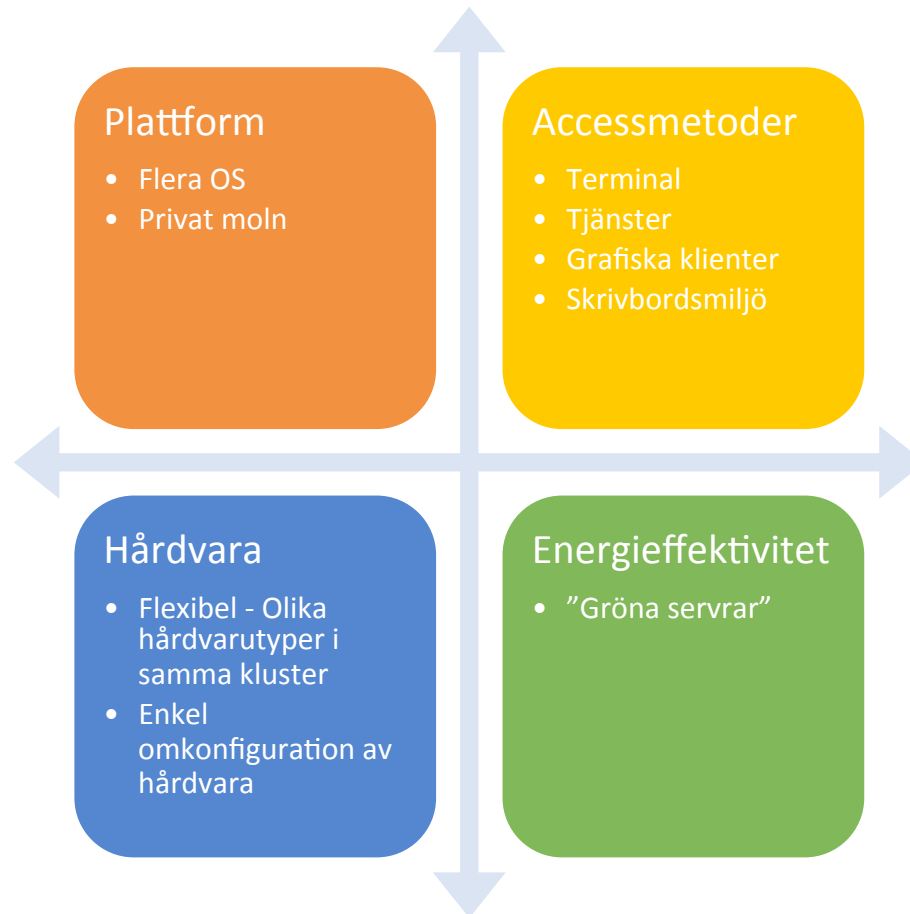
# New Lunarc HPC resource 2015-18

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# Enkelhet och flexibilitet i flera dimensioner

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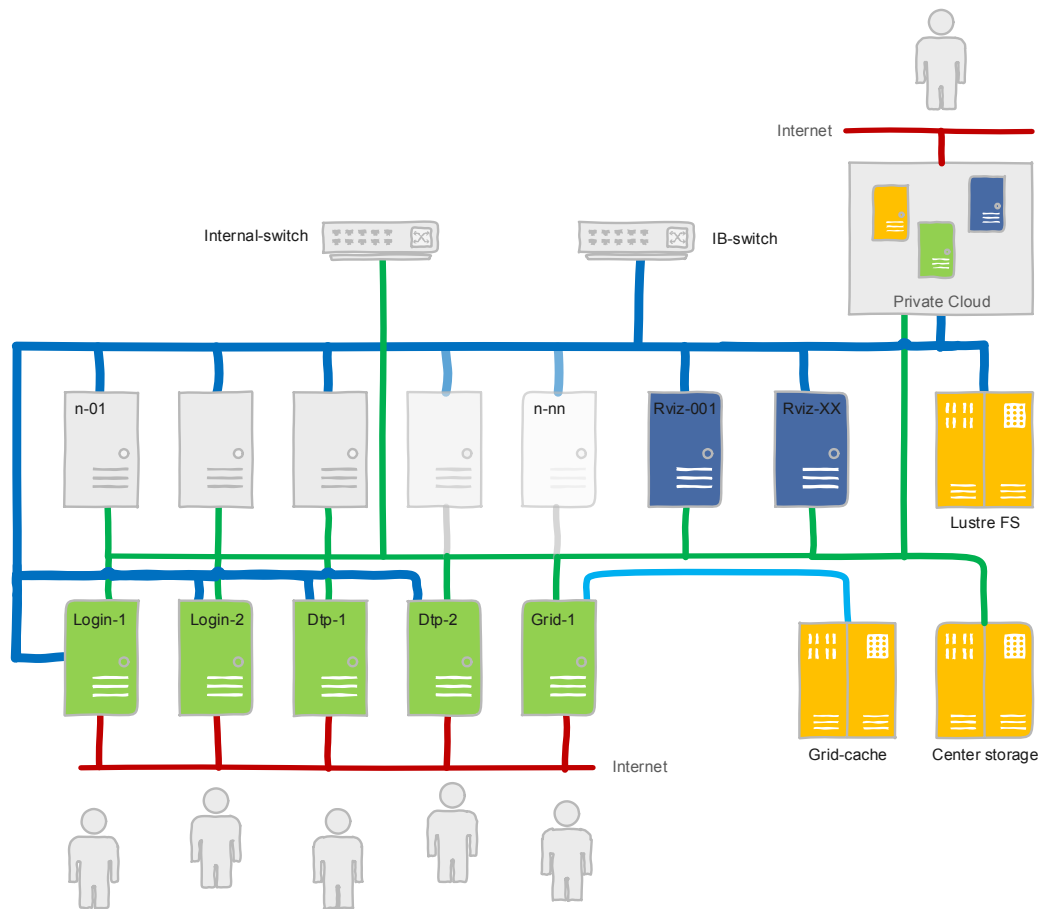
# Flexibel infrastruktur med många tjänster

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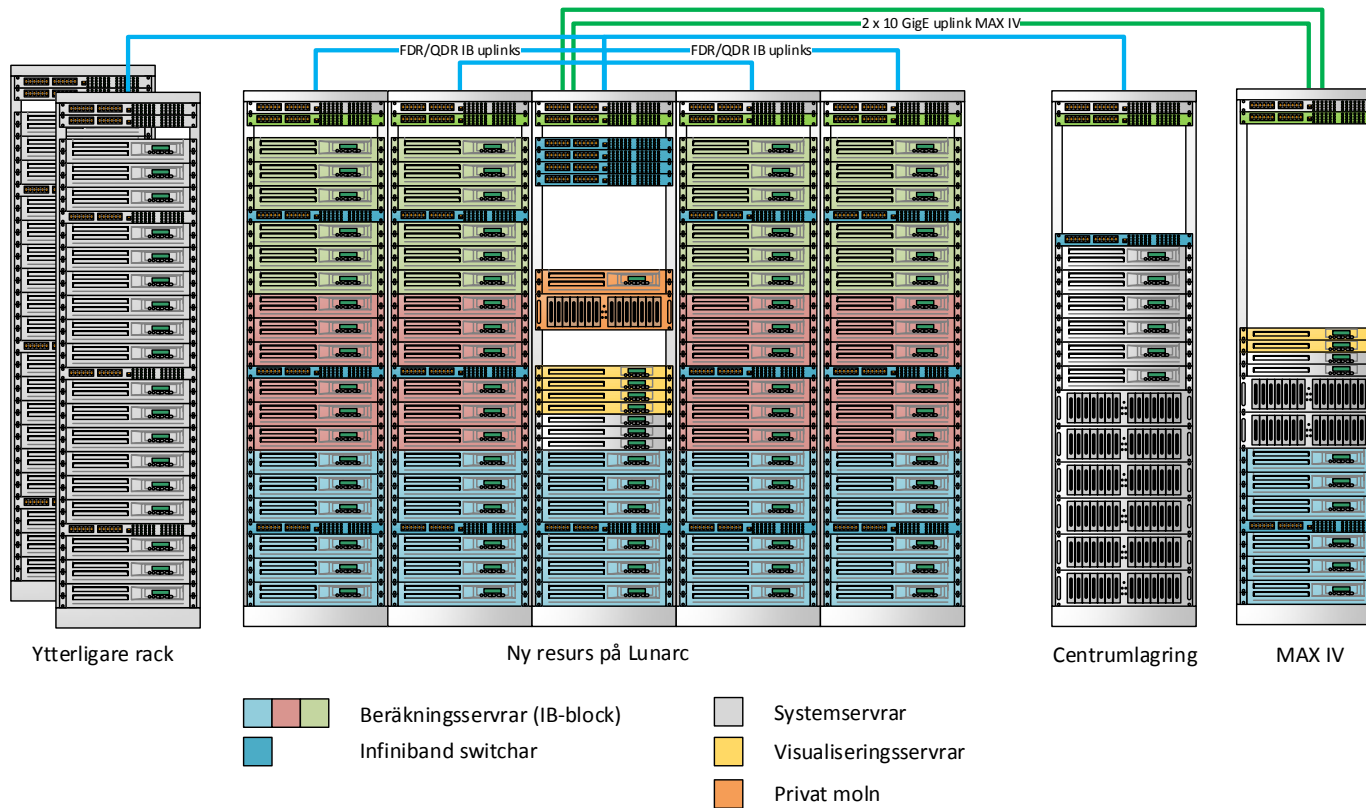
- **Programvaror** nära resurserna med tillgång till filsystem och beräkningsresurser i en tillhörande molnlösning.
- **Nya forskargrupper** kan erbjudas tillgång till en skrivbordsmiljö med grafiska gränssnitt anpassade för deras område.
- **Visualiseringsbehov** med högpresterande hårdvaruaccelererad grafik kopplade direkt till beräkningsresursen
- **Parallell visualisering**
- **Dedikerade lösningar för arbetsflöden** kan dra nytta av molntjänster och grid-teknologi.



# Arkitektur



# Fysisk arkitektur



# MAX IV samarbete

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