



**PDC Center for  
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**National Supercomputer Centre  
at Linköping University**

# NSC & PDC

## Resource and Technology Providers for SeRC

Erwin Laure  
Director PDC-HPC

Bengt Persson  
Director NSC

## NSC & PDC



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- Two leading Swedish HPC centers within the Swedish National Infrastructure for Computing (SNIC)
- Founded in 1989 (NSC) and 1990 (PDC)

# Resources and Technologies for eScience



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- eScience is critically dependent on the provision of excellent resource for
  - Networking (by SUNET)
  - Computing (by NSC & PDC)
  - Storage (by NSC & PDC)
  - Visualization (by LiU and KTH)
- To make efficient use of these resource expert support and advanced technologies are needed
  - Advanced algorithms
  - Parallelization
  - Distributed computing
  - Data storage and management
- Task of “core eScience” together with NSC & PDC

# NSC & PDC inside SeRC



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- Major resource and technology providers
- Swedish bridgehead for European e-Infrastructures (EGI, DEISA/PRACE)
- Thanks to SeRC NSC and PDC are in the process of better aligning their strategies and support
  - Complementary competences
  - Harmonized user environment
  - Joint application support on major systems
  - MoU signed by KTH and LiU rektors



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# System News

# Lindgren - PDC's latest HPC system



- Cray XE6
- 2 12core AMD Opteron CPUs 2.1 GHz, 32 GB RAM per node
- 1516 compute nodes (36,384 cores), 305 TF TPP, 237 TF sustained
- Gemini 3D torus network
- SNIC PRACE system
- Would be Nr. 8 in Europe and Nr. 28 worldwide on the November 2010 Top500 list





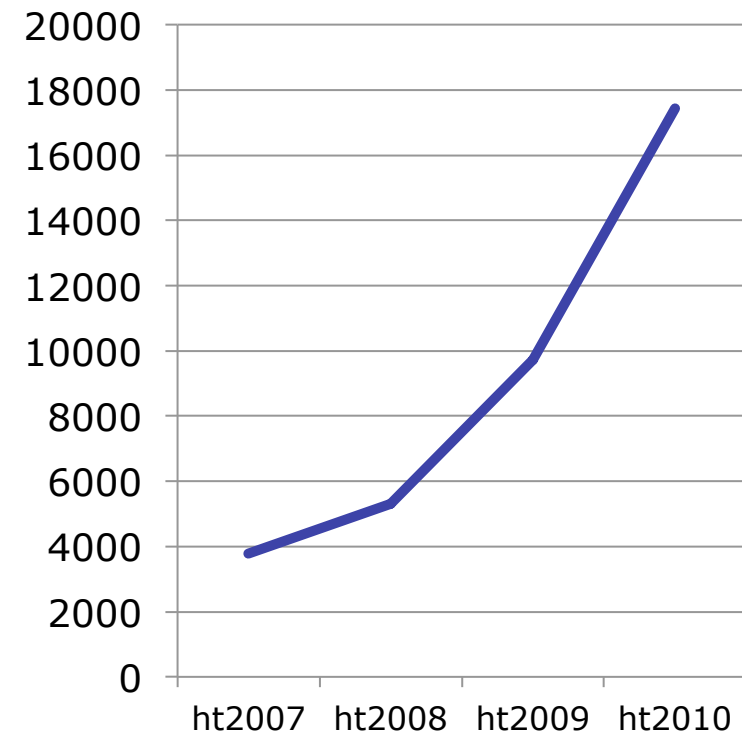
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## Triolith at NSC

- Successor of Neolith
- 2012Q1
- Size still to be decided



- Swedish needs for ht2012 are estimated to 52 million core hours per month => about **104 million core hours** per month on annual basis
- Current SNIC resources in 2012 provide 59 million
- Triolith need to provide **~45 million core hours/month**

# Compute Infrastructure Summary



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System	Cores	TPP
Cray	36,384	305 TF
Ekman	10,144	89 TF
Ferlin	5,360	58 TF
SweGrid PDC	744	8 TF
Hebb	2,048	6 TF
Povel	4,320	36 TF
Neolith	6,440	60 TF
Kappa	2,912	26 TF
Matter	4,096	37 TF
Byvind	1,120	12 TF
Bore/Gimle	2,152	22 TF
Skylord	456	5 TF
Smokerings	448	6 TF
<b>Total</b>	<b>76,633</b>	<b>670 TF</b>



# New computer hall ...



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- ... at NSC
- providing 4 MW
- extension to 20 MW if needed
- ready early 2012

# Heat Reuse Project



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- Background: today around XXX kW used at PDC
- Project started 2009 to re-use this energy
- Goals:
  - Save cooling water for PDC
  - Save heating costs for KTH
  - Save the environment
- Use district cooling pipes for heating when no cooling is required
- No heat pumps
- Starting with Cray
- First phase of Cray will heat the KTH Chemistry building



# Application Support



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- NSC and PDC provide advanced application support
  - Installation and tuning of application software
  - Advice on efficient resource usage
  - Hardware selection
  - Performance tuning and code optimization

# Application expertise



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- Domain-specific
  - Bioinformatics
    - Joel Hedlund (NSC)*
  - Comp. Chemistry
    - Torben Rasmussen (NSC)*
    - Olav Vahtras (PDC)*
  - Materials sciences
    - Peter Larsson (NSC)*
    - Weine Olovsson (NSC)*
  - Climate
    - Chandan Basu (NSC)*
  - Neuroinformatics
    - Mikael Djurfeldt (PDC)*
  - Molecular Dynamics
    - Rossen Apostolov (PDC)*
  - CFD
    - Mattias Chevalier (PDC)*
- Code optimisation
  - Chandan Basu (NSC)*
  - Soon-Heum Ku (Jeff, NSC)*
  - Jonathan Vincent (PDC)*
- Software development
  - Henrik Wiberg (NSC)*
  - Per Lundqvist (NSC)*
  - Daneil Johanssoon (NSC)*
- PRACE
  - Lilit Axner (PDC)*
- Clouds
  - Zeeshan Ali Shah (PDC)*

# Selected New Activities



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- Cloud tested @ PDC
  - Develop and test cloud services
  - Started with complex disease community
- VIC GPU testbed @ PDC
  - Operated for VIC-Stockholm
  - Proposal to SNIC to extend it towards a national pilot together with NSC that will host an experimental system with new hardware
- Exascale Research @ PDC
  - EC Project "CRESTA" will start in autumn

# International Dimension



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- Swedish bridgehead for European e-Infrastructures
  - Provide resources to European e-Infrastructures under the coordination of SNIC
  - Support Swedish users in gaining access to them



 [www.swegrid.se](http://www.swegrid.se)  
SweGrid



ELIXIR

EUROPEAN LIFE SCIENCES INFRASTRUCTURE FOR BIOLOGICAL INFORMATION



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## Swedish DECI6 projects that run on other EU Tier-1 systems from July 2010 – April 2011

- 1. Department of Computational Biology (KTH), project BRAINCOR, 700 000 CPU = 525 000 CPU(Jugene - FZJ) and 175 000 CPU (Genius - RZJ). Both machines are in Germany
- 2. Department of Theoretical Physics (KTH), project SIVE 4 200 000 CPU = 4 200 000 CPU(HeCTOR-EPCC) in Edinburg, Scotland
- 3. Department of Mechanics (KTH), project WALLPART 2 100 000 CPU = 2 100 000 CPU (HeCTOR-EPCC) in Edinburg, Scotland
- Total of 7 000 000 CPU hours have been exchanged
- Plus Swedish participation to Euforia Virtual Community



## **DECI-6 Project that run on Ekman from July 2010 – April 2011**



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- DFT-COH from IDRIS, France – 660.000 CPU
- FREESA from CINECA, Italy – 1.560.000 CPU
- GAME from RZG, Germany-Cyprus – 2.400.000 CPU
- HoSAM from CSC, Finland – 1.600.000 CPU
- HPQCD3 from EPCC, Scotland – 768.000 CPU
- Total of 7 000 000 CPU hours have been exchanged





## **PRACE 2nd Regular Call – access to Tier-0 systems**



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- **REFIT - Rotation effects on flow instabilities and turbulence**
- **Project leader:** Arne Johansson, KTH  
Department of Mechanics, Sweeden  
**Collaborators:** Dr. Geert Brethouwer, KTH  
Stockholm, Sweeden / Prof. Dan Henningson,  
KTH Stockholm, Sweeden/ Prof. Rebecca  
Lingwood, University of Cambridge, United  
Kingdom / Prof. Martin Oberlack, Technische  
Universität Darmstadt, Germany / Dr. Philipp  
Schlatter, KTH Stockholm, Sweeden
- **Computer system:** JUGENE, GAUSS/FZJ  
**Resource awarded:** 46 000 000 core-hours



## PRACE Internal Call for Community Codes



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- **Gromacs** application from SNIC/KTH/PDC – Collaborative project between SNIC/KTH/PDC, CINECA (Italy) and NCSA(Bulgaria)
- **Dalton** application from SNIC/KTH/PDC – Collaborative project between SNIC/KTH/PDC, SIGMA-UiO from Norway, BSC from Spain, STFC from UK



## Other Contributions: PRACE Internal Call for community codes



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- **EC-Earth** application from SARA, The Netherlands - SNIC/LiU/NSC is one of the contributing partners
- **GPAW** application from CSC, Finland-SNIC/UmU/HPC2N and SNIC/Chalmers are two of the contributing partners



## **PRACE Preparatory Access Call & DECI-7**



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- *Tier-0 access application:*  
[http://www.prace-ri.eu/IMG/pdf/PRACE\\_third\\_regular\\_call.pdf](http://www.prace-ri.eu/IMG/pdf/PRACE_third_regular_call.pdf)  
(Application deadline June 22)
- *Tier-1 access Pilot DECI call:*  
<http://www.prace-ri.eu/IMG/doc/PRACE-DECI7-ACRONYM.doc> (Application deadline June 22)
- *Preparatory Access call:*  
[http://www.prace-ri.eu/IMG/pdf/prace\\_preparatory\\_access\\_call.pdf](http://www.prace-ri.eu/IMG/pdf/prace_preparatory_access_call.pdf)  
(No deadline – constantly open)

## Other Major Projects



**SAAB**



**SCANIA**

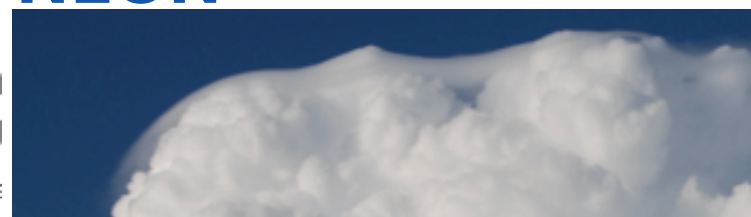
**NEON**



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Virtual multidisciplinary EnviroNments USing Cloud infrastructures



International Neuroinformatics  
Coordinating Facility



**GRDI 2020**

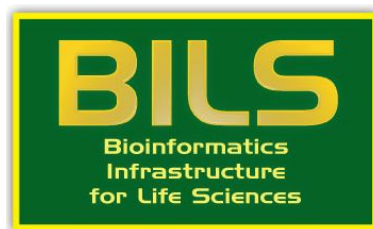
A Vision for Global Research Data Infrastructures



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**SMHI**

**SND-KM**



**Windows® HPC Server 2008**

**Scalable Software Services  
for Life Science**



# Summary



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- NSC and PDC are the major resource and technology providers for SeRC
- Increased collaboration and harmonization thanks to SeRC
- Ensure efficient access to European e-Infrastructures

Skip slides beyond this ...



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# Grid computing

## What is the grid good for?



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- Bioinformatics
- other scientific areas

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SweGrid

- Burst computing
  - High demand for short periods of time
    - high during development / production / analysis of new datasets
    - low during analysis / writing papers

Share resources to enable more efficient use

- Database accessibility
- Availability
- Unified interface





# What is NDGF?

- Nordic Data Grid Facility
- A WLCG Tier1 facility

Worldwide LHC Computational Grid

Stores and processes data from LHC at CERN

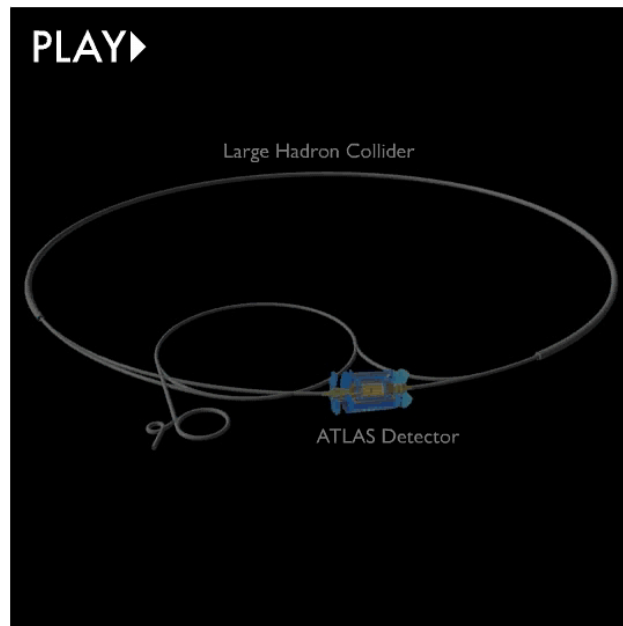
- peak rate  $\approx 1.6\text{Gb/s}$ , when the accelerator is running  
(and that's after most of the data have been filtered away)



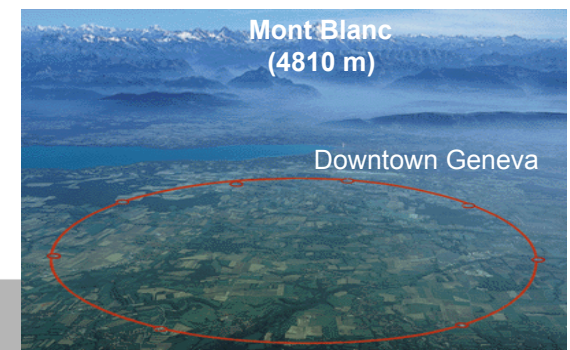
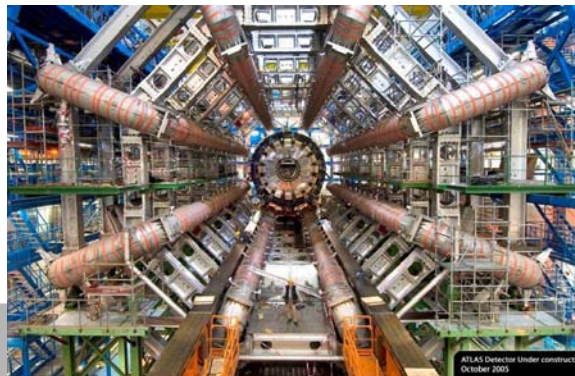


# Accelerating and colliding particles

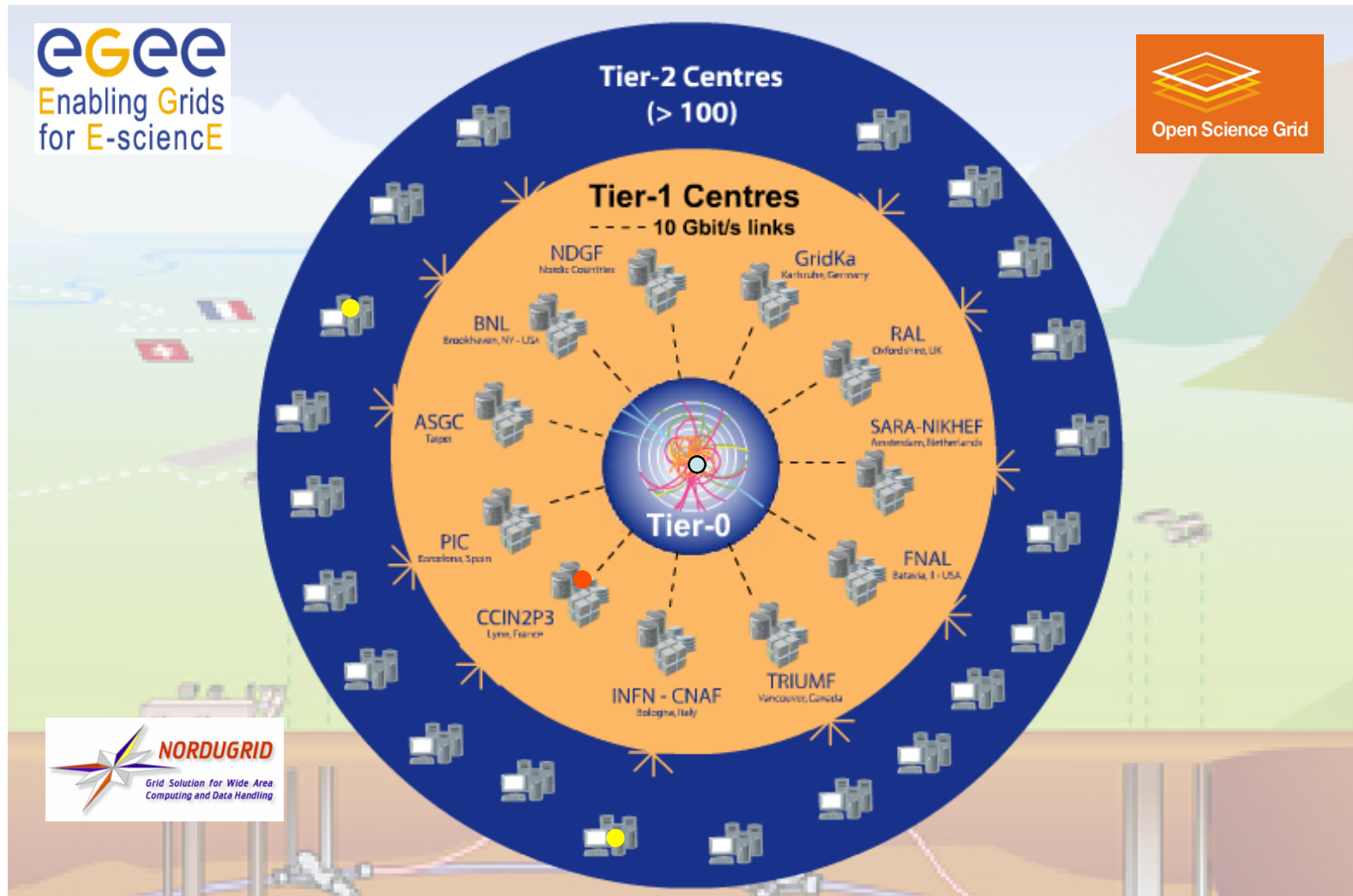
## Large Hadron Collider



- 27 km circumference tunnel
- Start up in 2008
- 40 Million Particle collisions per second
  - Online filter reduces to a few 100 “good” events per second recorded on disk and magnetic tape at 100-1,000 MegaBytes/sec
  - ~15 PetaBytes per year for all four experiments
- Data analyzed by 100s of research groups world wide



# LHC Data Distribution and Access



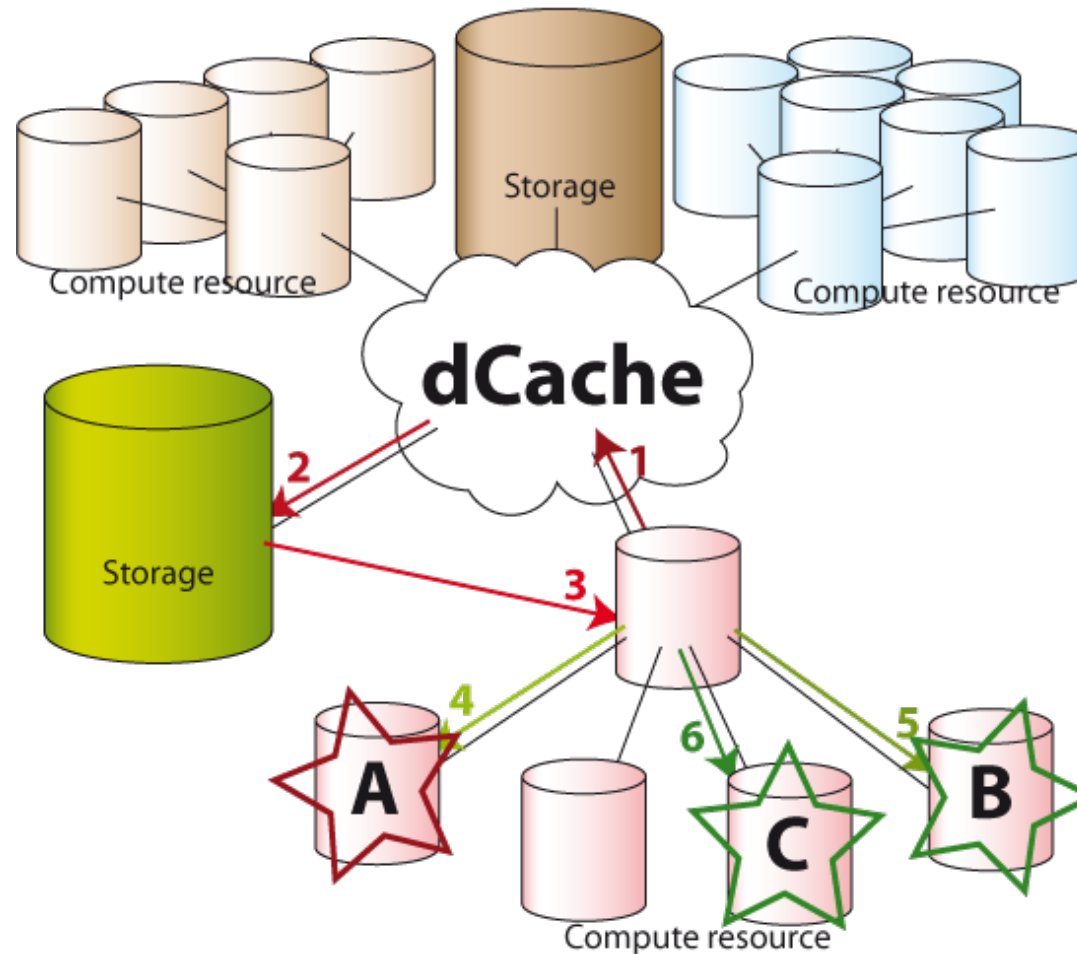
# Cached database access



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Database files are transferred to the cluster at most once per project.