Welcome to the PDC Summer School
Introduction to High Performance Computing

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Co-Chair PDC Summer School
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Goal of the School

- Introduce you to high-performance computing

- Give you practical knowledge to apply to your own work

- Discuss practical applications and look into the future

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What is expected of you?

- Attend the classes
  - Sign up attendance sheet

- Read the handouts and material on the web

- Get lab attendance form signed every lab session

- Submit a project abstract before you leave
  - Then complete the project for credits

- Fill in the online feedback form
  - Use the password that is being distributed now

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Various Information

- Certificates will be issued to all successful students

- Tutors will be available for lab sessions
  - Ask them questions
  - But they will also ask you!

- Labs in groups of 2-3people

- Door access code for lab room: **8050**

- Wireless
  - Eduroam
  - If you don't have eduroam you can use KTHOPEN
   - Passwords will be distributed as needed

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Social Program

- Get-together picnic this afternoon at 17.30 at the main building's courtyard (meet in "Ljusgården")

- Possibility to see the PDC computer room tomorrow afternoon

- Summing-up dinner on Thursday, August 25, at 18:00, Jakthornet

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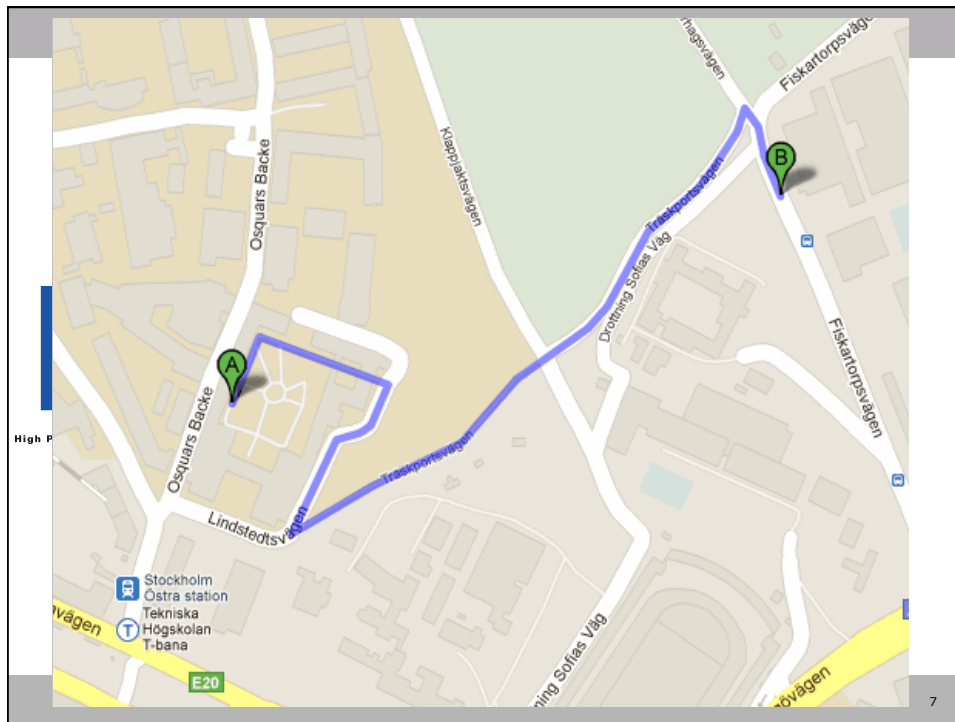
What is PDC

- A major Swedish Supercomputing Center supported by SNIC (Swedish National Infrastructure for Computing)
  - Supporting a wide variety of sciences

- Located at the Royal Institute of Technology (KTH), Stockholm
  - Associated to School of Computer Science and communication (CSC)

- Summerschool run jointly with CSC
  - Since 1996

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PDC's Mission

Research

Conduct world-class research and education in parallel and distributed computing methodologies and tools

Infrastructure (PDC-HPC)

Operation of a world-class ICT infrastructure for Swedish research, including HPC and data services, with associated user support and training

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PDC Computing resources

Ekman - Dell PowerEdge Cluster
Climate and Flow research

Hebb - IBM Blue Gene
Stockholm Brain Institute, Mechanics, and INCF

Povel
Prace Prototype (energy efficiency)
4320 cores (180 4x6core AMD nodes)
36 TF theoretical peak performance
5.76 TByte memory

10,144 cores (1268 nodes, 2 quad core AMD)
89 TF theoretical peak performance
20 TByte memory

1024 nodes
6 TF theoretical peak performance

Key - HP SMP
32 Cores, 256 GB memory

Ferlin and SweGrid - Dell Cluster
SNIC Foundation Level Service
32 nodes with Infiniband

6120 cores (765 nodes, 2 quad core Intel)
7 TByte memory
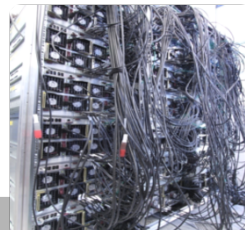
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Lindgren - PDC's latest HPC system

You will be running your exercises on Lindgren's Test and Development System **summer-cray**

- 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
- Nr. 9 in Europe and Nr. 31 worldwide on the June 2011 Top500 list

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PDC's Computational Resources

System	Cores	TPP
Lindgren	36,384	305 TF
Ekman	10,144	89 TF
Ferlin	5,360	58 TF
SweGrid	744	8 TF
Hebb	2,048	6 TF
Povel	4,320	36 TF
Total	**59,000**	**502 TF**

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Heat Reuse Project

- Background: today around 1.3 MW 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

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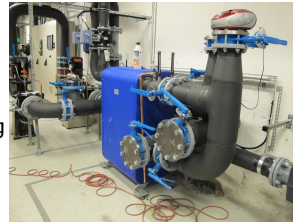
Storage

- ~20 TB disk
  - Accessible via AFS

- ~900 TB disk
  - Currently attached to individual systems
  - Lustre parallel file system
    - Site wide configuration planned

- IBM tape robot
  (~2900 slots, ~2.3 PB)
  - Accessible via HSM, TSM, and dCache
    (planned via NDGF)

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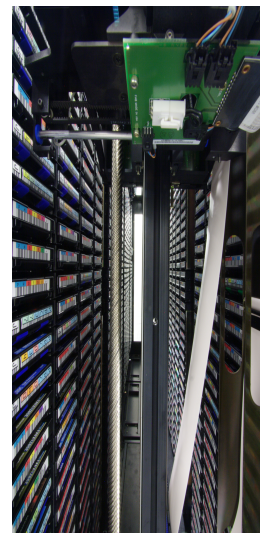
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Software

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- Commercial/Community codes
  Gaussian
  Jaguar
  Gromacs
  VASP
  Fluent
  Blast
  Edge
  Starcd
  Dalton
  Charmm
  Numerical libraries

- User codes
  CFD
  Ab initio
  Monte Carlo
  Bioinformatics

- Programming
  MPI, OpenMP
  Fortran/C/C++ compilers
  Tools
  – acumem
  – totalview
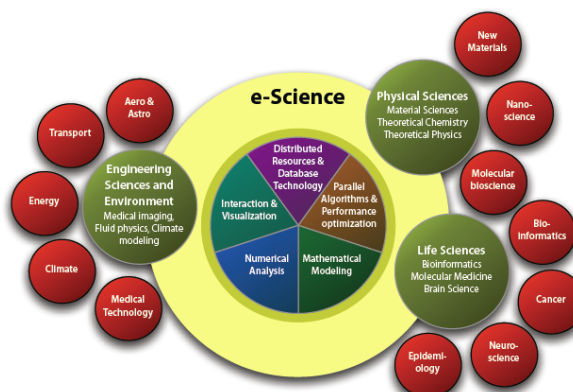 – papi, papiex
  – jumpshot
  – hpctoolkit
  – Paraver

SeRC - Swedish eScience Research Center

- Collaboration of KTH, SU, KI, and LiU

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Other Activities

- Prace - Partnership for Advanced Computing in Europe
  Design of future European supercomputing landscape
  - Prototype
    - Focus on energy efficiency and high density packing
  - Tier-1 system
    - Cray

- Integration in DEISA - Distributed European Infrastructure for Supercomputing Applications

- Windows HPC prototype

- Cloud computing
  - Nordic cloud study (NEON)
  - Cloud infrastructure project (Venus-C)

- Advanced software support
  - SeRC
  - Scalable Software Services for Life Sciences (ScalaLife)

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Have interesting,
challenging,
fun
two weeks!

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