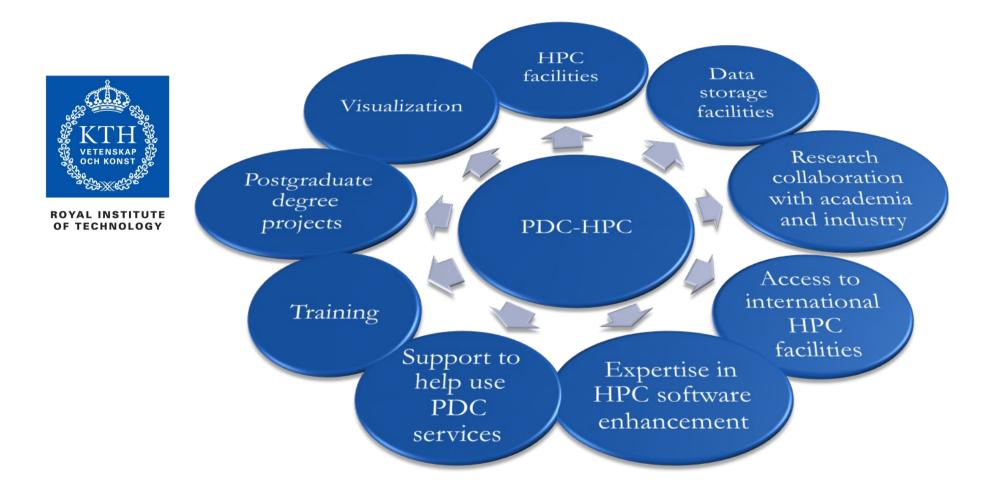
Introduction to the PDC environment



ROYAL INSTITUTE OF TECHNOLOGY PDC Center for High Performance Computing KTH, Sweden

> Rossen Apostolov (rossen@kth.se) Application expert at PDC

PDC Offers...



PDC for Academic Users

 Access to PDC computing and data storage facilities via the Swedish National Infrastructure for Computing (SNIC)



- Advanced and introductory user training including workshops, seminars and courses
- User support
- Application expert help



- Access to European computing facilities via PRACE Infrastructure calls
- Access to application experts at other European centers for help with scientific applications via PRACE Infrastructure calls

PDC Key Assets: First-Line Support and System Staff

First-line support



ROYAL INSTITUTE OF TECHNOLOGY Helps you have a smooth start to using PDC's resources and provides assistance if you need help while using our facilities

System staff: System managers/administrators



January 2014



Ensure that PDC's HPC and storage facilities run smoothly and securely

PDC Center for High Performance Computing

KTH VETENSKAP OCH KONST

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PDC-HPC application experts hold PhD degrees in different scientific fields and are experts in HPC.

Together with researchers, they optimize, scale and enhance scientific codes for the next generation supercomputers.



Jonathan Vincent Computational Physics





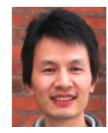
Rossen ApostolovMichael DjurfeldtComputational ChemistryComputational Neuroscience



Henric Zazzi Bioinformatics/Genetics



Radovan Bast Computational Chemistry



Jing Gong Scientific Computing

PDC Center for High Performance Computing

PDC Key Assets: Broad Range of Training

PDC Summer School every year: Introduction to HPC



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- Specific courses: Programming with GPGPU, RecentAdvances in Distributed and Parallel Computing,Software Development Tools, Recent Advances inCloud Computing, and many many more....
- PDC user days, PDC Open House and Pub Afternoon



PDC Center for High Performance Computing

PDC Key Assets: Access to EU Facilities and Experts



ROYAL INSTITUTE OF TECHNOLOGY PDC is an active partner in many international and national projects.



PDC Center for High Performance Computing

PDC and Industry

PDC is working with industrial researchers and developers on major international projects that push high-performance computing to the next level.



ROYAL INSTITUTE OF TECHNOLOGY PDC recently established a business development unit that provides consultancy and HPC services to industries.



Access to PDC resources

User account



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- Time allocation (CAC)
 - Which clusters you can access
 - How many jobs you can run per month
- Time allocation requirements
 - Can be personal or shared within a group
 - Every user must belong to at least one time allocation

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Time allocations

- Applicant must be a senior scientist in swedish academia
- Need evidence of successful work at a medium level
- Evaluated on a technical and scientific level
- Decided by SNAC twice a year
- No formal limits
- Applicant must be a senior scientist in swedish academia
 - Evaluated on a technical level only
 - Limits depend on machine
 - Lindgren: 200 kcorehours/month
- Applicant can be a PhD student or higher
- Evaluated on a technical level only
- Limits is 5000 corehours/month



_arge

Medium

Sma



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Computers at PDC

Lindgren

Hardware 1516 nodes 24 cores/node 2.1 GHz AMD Magny-Cours cores 32 GB RAM



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- Intended for very large jobs (>512 core/job)
- Queue limit is 24 hours
- Runs the Moab/Torque queue system
- Partially reserved for PRACE, SCANIA, INCF
 - Large allocations: 75%
 - Medium allocations: 20%
 - Small allocations: 5%
- Lifetime: Q4 2014

Povel

Hardware 170 nodes 24 cores/node AMD Opteron 2.2 GHz CPUs 32 GB RAM (P nodes) 64 Gb RAM (Q nodes)



- Intended for Lindgren pre/post processing
- Not allocated through SNIC
- Runs the EASY queue system
- Lifetime: Q4 2014

Ferlin

Hardware 512 nodes 8 cores/node AMD Opteron 2.2 GHz CPUs 16 GB RAM

- Intended for small/long duration jobs
- Funded by KTH
 - Not allocated through SNIC
 - Only available to Stockholm affiliated PIs
- Runs the EASY queue system
- Only for small or medium allocations
- Lifetime: Q4 2014



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Hardware single node 64 cores Xeon E7-4830 X CPUs 1 TB RAM



- Intended for large memory jobs
- No proper time allocation
 - No queue system installed
 - Users book part of the machine
 - Access/time is given out sparingly



Hardware 8 node GPU cluster 3 nVIDIA Tesla M2090 60 GB RAM



- Intended for GPU testing
- Medium allocations in general
- Runs the Moab/Torque queue system
- Can be applied for through SUPR
- Lifetime: Q1 2015

Summary of PDC resources



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Computers	Ellen	Ferlin	Lindgren	Povel	Zorn
Core/node	32	8	24	24	8
Nodes	1	512	1516	170 P 20 Q	
RAM (Gb)	1000	16	32	32 P 64 Q	60
Small allocations (corehours/node)	1000	5000	5000	5000	1000
Medium allocations (corehours/node)	3000	80000	200000	80000	3000
Large Allocations (corehours/month)			>200000		
Allocation via SNIC			yes		yes
Allocation via RT	yes	yes		yes	
Lifetime		Q4 2014	Q4 2014	Q4 2014	Q1 2015
Queue software		EASY	MOAB Torque	EASY	MOAB Torque
OS	CentOS6	CentOS5	SUSE/ CNL	CentOS5	CentOS6
AFS	yes	yes	Not on compute nodes	yes	yes
Lustre	yes		yes	yes	yes

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And many more...

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Cloud computing





Cloud Computing: Advantages

Less maintenance

Hardware, applications and bandwidth are managed by PDC.

Continuous availability

Public cloud services are available wherever you are located.



The OS, applications and data storage you need is allocated in a flexible way.

Elasticity

Clouds can be scaled to meet your changing IT system demands and more hardware can easily be added

Expert service

Expedient's cloud computing services are continuously monitored and maintained by PDC.



Cloud Computing: Disadvantages

More elasticity means less control



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Not everything fits into the cloud

Depending on the cloud provider, you may face restrictions on available applications, operating systems, and infrastructure options. Complicating matters more is the simple fact that not all platforms can live in the cloud.

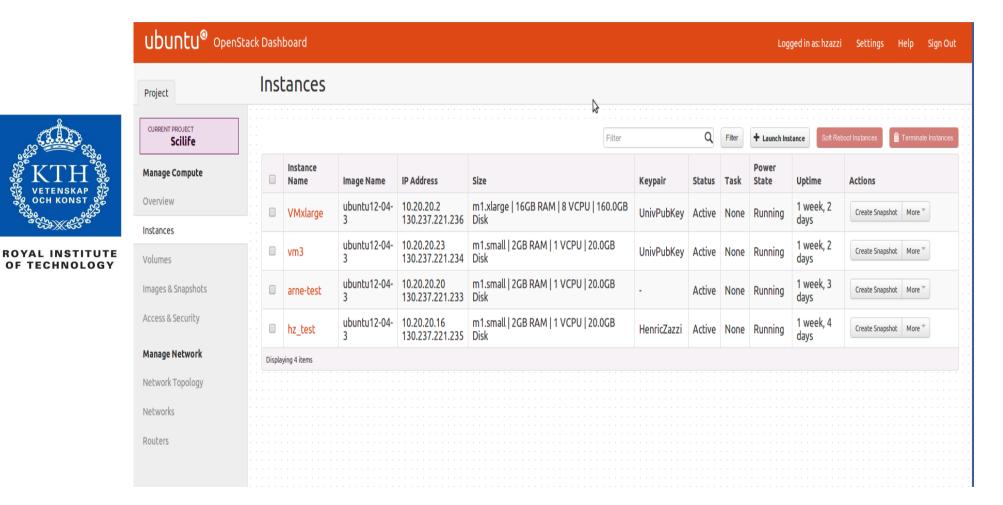
Security and Confidentiality

Cloud computing does pose the risk of increased security threats. While most companies have an up-to-date virus database, this does not make the files and information stored in the cloud immune to hackers.

Decreased performance...

In comparison to cluster computing

PDC OpenStack Cloud



https://www.pdc.kth.se/resources/computers/pdc-cloud

PDC Center for High Performance Computing



How to apply for a PDC account

Apply to a SUPR account

- Needed if you are accessing SNIC resources
 - Lindgren
 - Zorn
- You can apply for a SUPR account at...

supr.snic.se

- Link your SUPR account to PDC
 - Login to SUPR
 - Go to User pages
 - Check centres, if PDC not listed contact PDC support www.pdc.kth.se/about/contact/support-requests



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Apply to a PDC account

- Electronic copy of your passport
- KTH VETENSKAP OCH KONST

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- Examine the computer rules at PDC
- Which postal address the password should be sent
- Which time allocations the users will access
 - Not needed in case the users is applying for a time allocation
- You can apply for a PDC account at...

www.pdc.kth.se/support/accounts/user



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How to login

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Kerberos



- Is an authentication protocol originally developed at MIT
- PDC uses kerberos together with **SSH** for login
- Ticket
 - Proof of users identity
 - Users use password to obtain tickets
 - Tickets are cached on users computer for a specified duration
 - Tickets should be created on your local computer
 - As long as tickets are valid there is no need to enter password
- Realm
 - all resources available to access
 - example: NADA.KTH.SE
- Principal
 - Unique identity to which kerberos can assign tickets.
 - example: username@NADA.KTH.SE



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Kerberos commands

- kinit proves your identity
- klist list your kerberos tickets
- kdestroy destroy your kerberos ticket file
- kpasswd change your kerberos password

```
> kinit -f username@NADA.KTH.SE
> klist -Tf
Credentials cache : FILE:/tmp/krb5cc_500
        Principal: username@NADA.KTH.SE
Issued Expires Flags Principal
Mar 25 09:45 Mar 25 19:45 FI krbtgt/NADA.KTH.SE@NADA.KTH.SE
Mar 25 09:45 Mar 25 19:45 FA afs/pdc.kth.se@NADA.KTH.SE
```





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Login using kerberos tickets

• Get a 7 days forwardable ticket on your local system

kinit -f -l 7d username@NADA.KTH.SE

Forward your ticket via ssh

ssh username@clustername.pdc.kth.se

- Replace *clustername*...
 - Zorn login node: zorn.pdc.kth.se
 - Lindgren login node: lindgren.pdc.kth.se
 - Ferlin interactive nodename
- You will have reached the cluster
- Always create a kerberos ticket on your local system



Login from any computer

You can reach PDC from any computer or network



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- The kerberos implementation heimdal can be installed on most operating systems
 - Linux
 - Windows
 - Mac
- Follow the instructions for your operating system <u>www.pdc.kth.se/resources/software/login-1</u>



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File systems

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• AFS is a global file system accessible everywhere

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ROYAL INSTITUTE OF TECHNOLOGY /afs/pdc.kth.se/home/*username 1st letter/username*

Your home directory is located in AFS

Oldfiles folder contain yesterdays backup of your files

- You cannot run jobs from AFS on Lindgren
- Follow the instructions for your operating system
 <u>www.pdc.kth.se/resources/software/file-transfer/file-transfer-with-afs</u>

Lustre

- Massively parallell distributed file system
- Very high performance
- No backup
- No personal quota. Move your data when finished
- Always start and run your programs in lustre
- Lindgren home directory:

/cfs/klemming/nobackup/username 1st letter/username

Zorn home directory:

/cfs/zorn/nobackup/*username 1st letter/username*



Types of nodes

- Login nodes
 - Do not run computer intensive jobs here
- Shared interactive nodes
 - Only on ferlin
 - Share nodes for running test programs
 - Should be logged into directly and not via the login node
- Exclusive interactive nodes
 - Node will be reserved just for you
 - Should be logged into directly and not via the login node
- Dedicated nodes
 - Reserve using the queue system
 - Node will be reserved just for you



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Modules

Used to load a specific software into your environment



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module add *software*

loads *software*

module avail

Lists available softwares

module show software

shows information about *software*

module list

Lists currently loaded softwares

- module swap frommodule tomodule
- Swaps *frommodule* to *tomodule*



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How to run jobs

Ferlin, Povel

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Easy queue system

- Queue system to run jobs
 - Installed on ferlin, povel
- Not installed by default

module add easy

• **esubmit** - to submit a job to a dedicated node

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- spusage list available nodes, and some information about them
- **spq** information on what is running in the queue
- sprelease cancel a job
- **spwhen** information on when a job will start
- spattach exports information about number of nodes, name of nodes...
- More information at...

www.pdc.kth.se/resources/computers/ferlin/how-to

How to use Easy to run jobs

To run on interactive node use...



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```
spusage | grep interactive
```

- Login to the interactive node directly from your local system
- You can also book an interactive node for exclusive access

```
esubmit -t minutes -n nodes
```

- You will then receive an e-mail with information about the node in which you can login
- Login to the interactive node directly from your local system
- Submitting a job to a dedicated node

```
esubmit -t minutes -n nodes ./myprogram
```

Prior to starting a job

Get a forwardable kerberos ticket from local computer



ROYAL INSTITUTE OF TECHNOLOGY kinit -f -l 7d *username*@NADA.KTH.SE

Forward your ticket via ssh

ssh username@clustername.pdc.kth.se

Copy your code to your AFS directory

/afs/pdc.kth.se/home/u/username



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Compilers

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GNU Compilation

Compile serial jobs

gfortran -FR -o hello hello.f

gcc -o hello_mpi hello_mpi.c

Compile MPI jobs

ROYAL INSTITUTE OF TECHNOLOGY module add easy openmpi/1.4.3-gcc
mpif90 -FR -fopenmp -o hello_mpi hello_mpi.f
mpicc -fopenmp -o hello_mpi hello_mpi.c

Intel Compilation

- Optimized for computers running intel infrastructure
- Compile serial jobs



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```
module add easy i-compilers
```

```
ifort -FR -o hello hello.f
```

```
icc -o hello_mpi hello_mpi.c
```

Compile MPI jobs

module add easy i-compilers openmpi/1.4.3-intel

```
mpif90 -FR -openmp -o hello_mpi hello_mpi.f
```

```
mpicc -openmp -o hello_mpi hello_mpi.c
```

Portland Compilation

 Closely involved in scientific computation with general purpose GPUs



module add easy pgi

```
pgf90 -FR -o hello hello.f
```

pgcc -o hello_mpi hello_mpi.c

Compile MPI jobs

module add easy pgi openmpi/1.4.3-pgi

mpif90 -FR -mp -o hello_mpi hello_mpi.f

```
mpicc -mp -o hello_mpi hello_mpi.c
```



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Running serial jobs

Interactive node (After logging into it)



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- ./MyPrg
- Dedicated node

esubmit -n 1 -t time min ./MyPrg

- You will receive e-mails about your job
- **time_min** for small jobs usually 5-15 minutes

Running MPI Jobs

spattach



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- Creates the necessary files and variables (\$SP_PROCS, \$SP_HOSTFILE)
- These files and variables can be constructed manually
- Remember to add the EASY module
- Interactive nodes

```
spattach -i -p number_of_nodes myUserCAC
```

Dedicated nodes

```
spattach -t time_min -p number of nodes myUserCAC
```

mpirun -np \$SP PROCS -machinefile \$SP HOSTFILE ./MyPrg

More information about running jobs



ROYAL INSTITUTE OF TECHNOLOGY http://www.pdc.kth.se/resources/computers/ferlin/how-to

Running Matlab

Should normally be run in batch mode



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module add matlab/latest

matlab -nojvm -nosplash -nodesktop < mycode.m > output.out

- This will take mycode.m and write the output to output.out
- More information about matlab

www.pdc.kth.se/resources/software/installed-software/restricted-software/matlab

Example Matlab script



ROYAL INSTITUTE OF TECHNOLOGY #!/bin/bash
Add the matlab software version
module add matlab/latest

#by default EASY job scripts start in the same directory #you submited the script from

#start matlab
matlab -nojvm -nosplash -nodesktop <
mycode.m > output.out



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How to run jobs

Lindgren, Zorn

PDC Center for High Performance Computing

January 2014

Torque/MOAB queue system

- Queue system to run jobs
- Installed on Lindgren and Zorn
- Installed by default, no need to load module
 - **aprun** to run jobs on an interactive node
- **qsub** to submit a job to a dedicated node
- More information at...

www.pdc.kth.se/resources/computers/lindgren/how-to/run



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Lindgren compilers and libraries

- Always use the wrappers
 - cc (C code), CC (C++), ftn (FORTRAN)
- PrgEnv module
 - PrgEnv-pgi (PGI), PrgEnv-Intel (Intel), PrgEnv-gnu (GNU)
 - By default PGI is loaded
 - Swap it by using command...

```
module swap PrgEnv-pgi PrgEnv-other
```

 Wrappers automatically link with math libraries if their modules are loaded

```
module load xt-libsci fftw
```

• Other libraries are lapack, blas scalapack, blacs,...



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Prior to starting a job

Get a forwardable kerberos ticket



ROYAL INSTITUTE OF TECHNOLOGY kinit -f -l 7d *username*@NADA.KTH.SE

Forward your ticket via ssh

ssh username@clustername.pdc.kth.se

Copy your code to your lustre directory

/cfs/klemming/nobackup/u/username

compilation on Lindgren



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Compile

```
ftn hello serial.f90 -o hello serial f90
```

```
cc hello_mpi.c -o hello_mpi_c
```

Compile OpenMP jobs

cc hello omp.c -mp -o hello omp c

cc hello omp.f90 -mp -o hello omp f90

Run on Lindgren

Serial jobs



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MPI jobs

aprun -n 16 ./hello mpi c

```
    OpenMP jobs
```

export OMP NUM THREADS=16

```
aprun -n 1 -d 16 ./hello_omp_f90
```

Run on Zorn

• On Zorn, setup your CUDA environment



ROYAL INSTITUTE OF TECHNOLOGY module load cuda/5.5

Compile

nvcc -o incarray incarray.cu

- Submit the job to the queue system
 - First create a PBS job script
 - Run the script

```
qsub ./batch.pbs
```

Format of PBS job script

Save this to batch.pbs



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```
#PBS -N hello_cuda_job
# 5 minute wall-clock time will be given
#PBS -1 walltime=5:00
#PBS -1 nodes=1
module load cuda/5.0
# Change to the work directory
echo $PBS_O_WORKDIR
cd $PBS_O_WORKDIR
# Run the program
./incrarr
```

PDC support

• A lot of question can be answered via our web

www.pdc.kth.se/support

The best way to contact us is via e-mail

www.pdc.kth.se/about/contact/support-requests

- The support request will be tracked
- Write descriptive subject line
- For follow ups always include support number
 - [SNIC support #NNNNN]
- Do not make new support cases by replying to old tickets



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