Introduction to PDC's environment

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PDC

KTH, Sweden

PDC Center for High Performance Computing

What to learn?

- How to login

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What to learn?

- How to login
- Where to store things

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What to learn?

- How to login
- Where to store things
- How to run a program

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- Never let anyone else use your PDC account. No, not even me!

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Finding Information

- `man`, `-help`, `-h`, `apropos` ...

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Modules

- Modules handles `PATH`, `MANPATH` . . .

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Common PDC modules are: `i-compilers`, `mpi`, `afsws`, `heimdal` and `easy`.

Modules

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- `module list`

Common PDC modules are: `i-compilers`, `mpi`, `afsws`, `heimdal` and `easy`. Use the Summer School module summer/10.

Kerberos

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Kerberos

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- **Kerberos server**, trusted by users and services.
- A **Kerberos principal** (*username@NADA.KTH.SE*) is a user's or service's username for a certain **Kerberos realm** (*NADA.KTH.SE*).

Getting your Kerberos ticket

- `kinit` — proves your identity

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Getting your Kerberos ticket

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

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  `klist -Tf`

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```
kinit -f -l 7d 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     afs/pdc.kth.se@NADA.KTH.SE
```

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Important!

REMEMBER! You are NOT allowed to write your password on any computer that you are remotely connected to!!!. If you expose your password you endanger not only your own work, you are putting all other cluster users at risk.

- Once you have your **local Kerberos ticket** you never need to type your password again!

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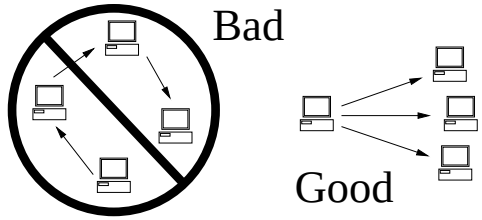

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Login using Kerberos tickets

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- Make sure you have **forwardable** Kerberos tickets
- **Forward** your forwardable tickets for remote login and secure X-windows redirect:

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- **Forward** your forwardable tickets for remote login and secure X-windows redirect:
- `ssh -Y -l username summer-10.pdc.kth.se`

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Login using Kerberos tickets

- Make sure you have **forwardable** Kerberos tickets
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- `ssh -Y -l username summer-10.pdc.kth.se`
- The `ssh` command has to use **GSSAPI key exchange**.

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Login using Kerberos tickets

- Make sure you have **forwardable** Kerberos tickets
- **Forward** your forwardable tickets for remote login and secure X-windows redirect:
- `ssh -Y -l username summer-10.pdc.kth.se`
- The `ssh` command has to use **GSSAPI key exchange**.
- Test your ssh using
  ```
  ssh -vv -Y -o GSSAPIKeyExchange=yes -o \
  GSSAPIAuthentication=yes -l elimo summer-10.pdc.kth.se
  ```

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Storage in AFS

- **AFS** is a global, distributed file system.

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- AFS data is stored on a number of **AFS server machines**
- **Client machines** request file data from servers when necessary and cache them locally.

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Your home directory

- Your **home directory** is located in **AFS**.

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- When you login you arrive in your AFS home directory, $\sim$.

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Your home directory

- Your **home directory** is located in **AFS**.
- When you login you arrive in your AFS home directory, ~.
- The path to your PDC AFS home directory is `/afs/pdc.kth.se/home/u/user` where `username` is your username and u is the first letter in your username.

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Your home directory

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- The storage space in $\sim$ is 500 MB (mega byte). Type `fs lq` to verify!

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- Some pre-existing **files and folders to keep**:
  .bashrc .forward Public Private . . .

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- **Oldfiles** contain $\sim$, as it was yesterday, i.e. a **backup**.

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AFS tokens

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- `klist -Tf` lists your **AFS tokens** and **Kerberos tickets**

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- `module add afsws`

AFS and directories

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pts member username
pts creategroup groupname
pts adduser username groupname
pts examine groupname
pts help adduser
```

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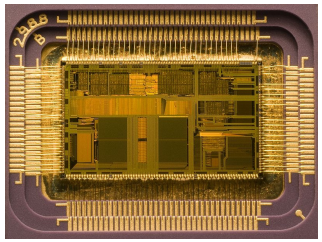
What's a computer cluster?



CPU/core

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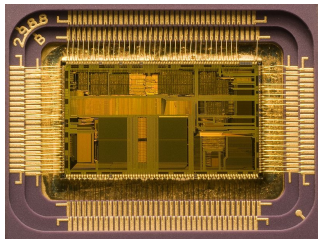

CPU/core

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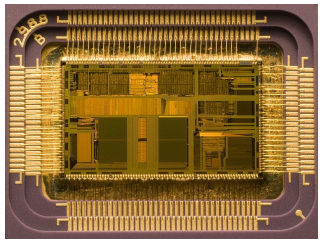

CPU/core

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Rack

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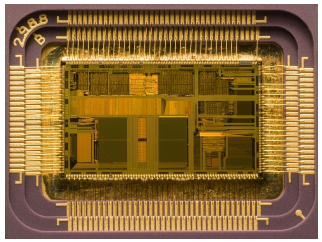

CPU/core

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Where to run your programs

- Login nodes — don’t run jobs here!

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Where to run your programs

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- Interactive nodes — for test runs, shared among users

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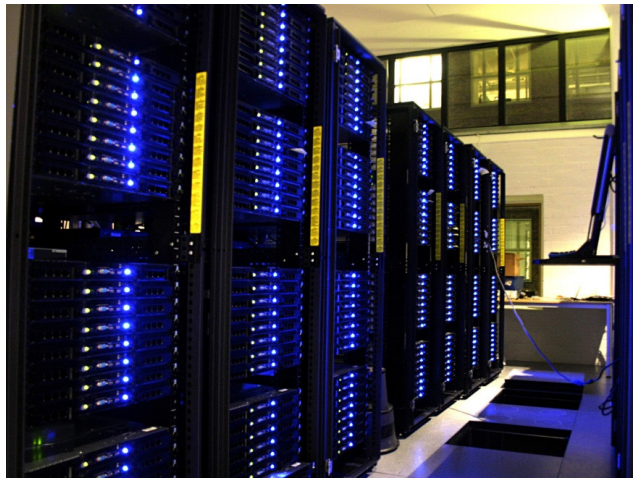
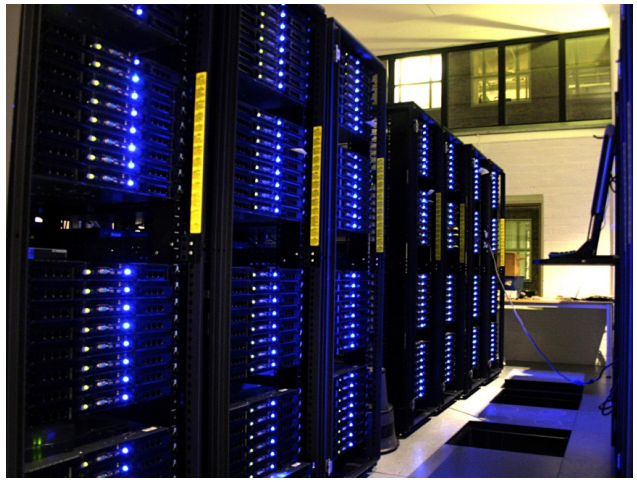


Where to run your programs

- Login nodes — don’t run jobs here!
- Interactive nodes — for test runs, shared among users
- Dedicated nodes (batch nodes) — for running final programs



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Run a serial program on an interactive node

- Login on the login node **summer-10.pdc.kth.se**

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- Login on the login node **summer-10.pdc.kth.se**
- Find which nodes are interactive ones:

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- Run the program:
  ```
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  ```

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  esubmit -n1 -t5 ./example1
  ```
- Watch the progress of your job:
  ```
  spq -u $USER
  ```

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Run a serial program on a dedicated node

- Login on the login node **summer-10.pdc.kth.se**
- Setup your environment:
  `module add summer/10`
- Compile your program:
  ```
  ifort -FR -o example1 -O2 example1.f
  ```
- Run the program on a dedicated node:
  `esubmit -n1 -t5 ./example1`
- Watch the progress of your job:
  ```
  spq -u $USER
  ```
- You will **receive two e-mails** — one when your job starts and later another containing the output of your program.

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When does my job start?

- Many users continuously submit jobs to the cluster

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- Every user belongs to at least one **time allocation** on a cluster. You belong to the time allocation (CAC) **summer-2010**
- A CAC states **how many node hours per month you have on a specific cluster**.

Time Allocations

- Check which time allocation, **CAC**, you belong to:
  ```
  cac members username
  cac examine summer-2010
  cac help
  ```

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Time Allocations

- Check which time allocation, **CAC**, you belong to:

```
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cac help
```

- Get current status of a time allocation:

```
spjobsummary -h
spjobsummary -c summer-2010
spjobsummary -u username -f 201008 -w
spsummary -h
spusage -h
spfree -h
```

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Time Allocations

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spjobsummary -c summer-2010
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spfree -h
```

- If your time allocation has run out of time for the month, your jobs are automatically assigned to a virtual CAC that runs only when no other jobs can run called `free.username`

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Submitting jobs with EASY

- Jobs should be submitted from the login node using `esubmit`

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- Submitting a MPI program (in a script) on four nodes for 30 minutes in the time allocation summer-2010:
  `esubmit -n 4 -t 30 -c summer-2010 ./myscript.sh`

Submitting jobs with EASY

- Jobs should be submitted from the login node using `esubmit`
- Please look at `esubmit -h -v`
- `spattach` is intended for use with `mpirun` and also **runs on the submit node**
- Submitting a MPI program (in a script) on four nodes for 30 minutes in the time allocation summer-2010:
  `esubmit -n 4 -t 30 -c summer-2010 ./myscript.sh`
- Redirecting STDOUT for your program to the file job.out:
  `esubmit -n 4 -t 30 ./myscript.sh "> job.out"`

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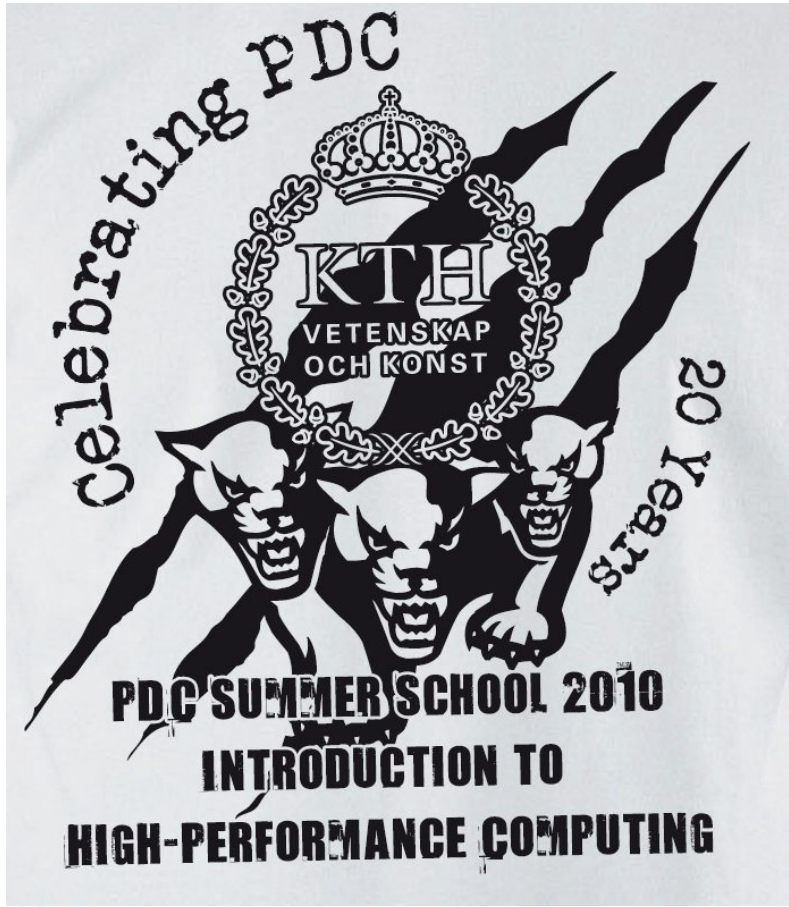
Thank you for listening!



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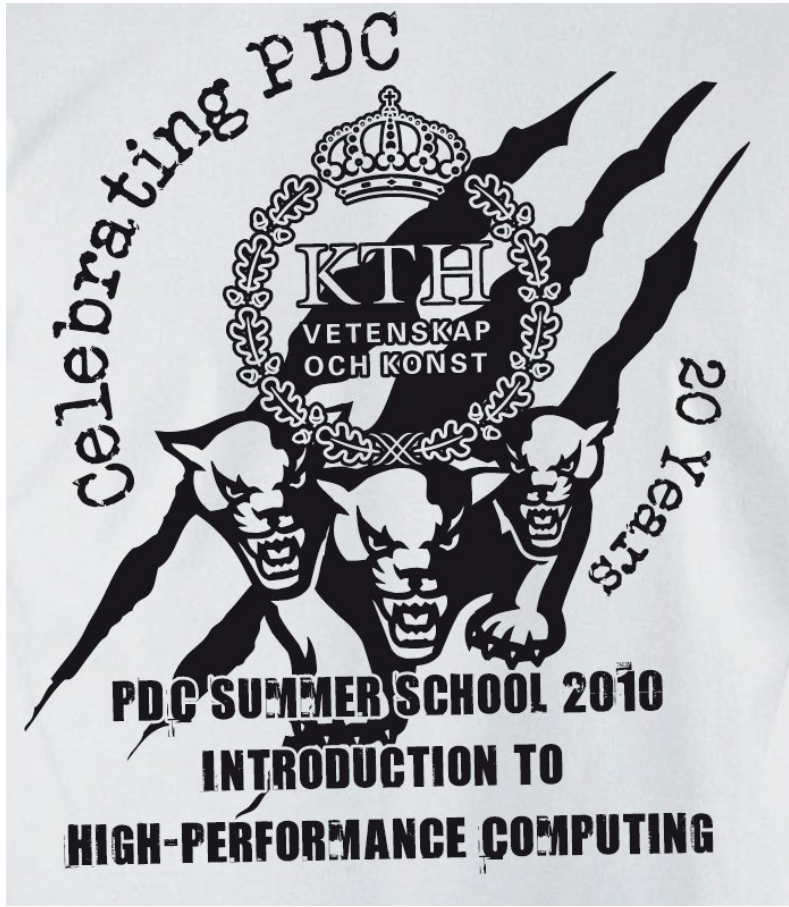

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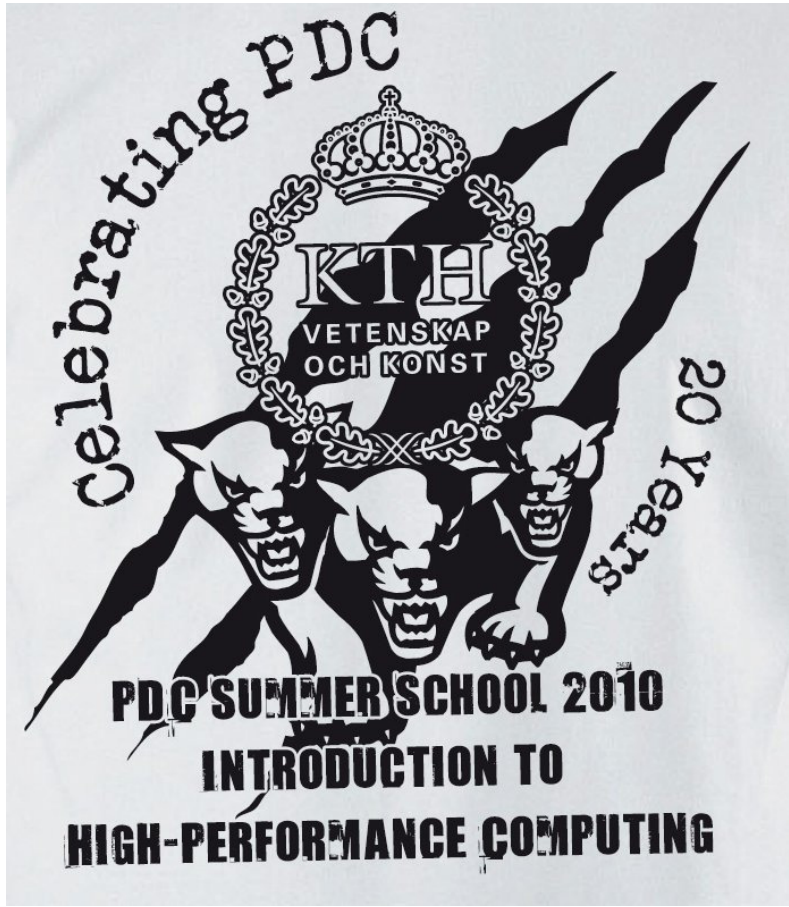

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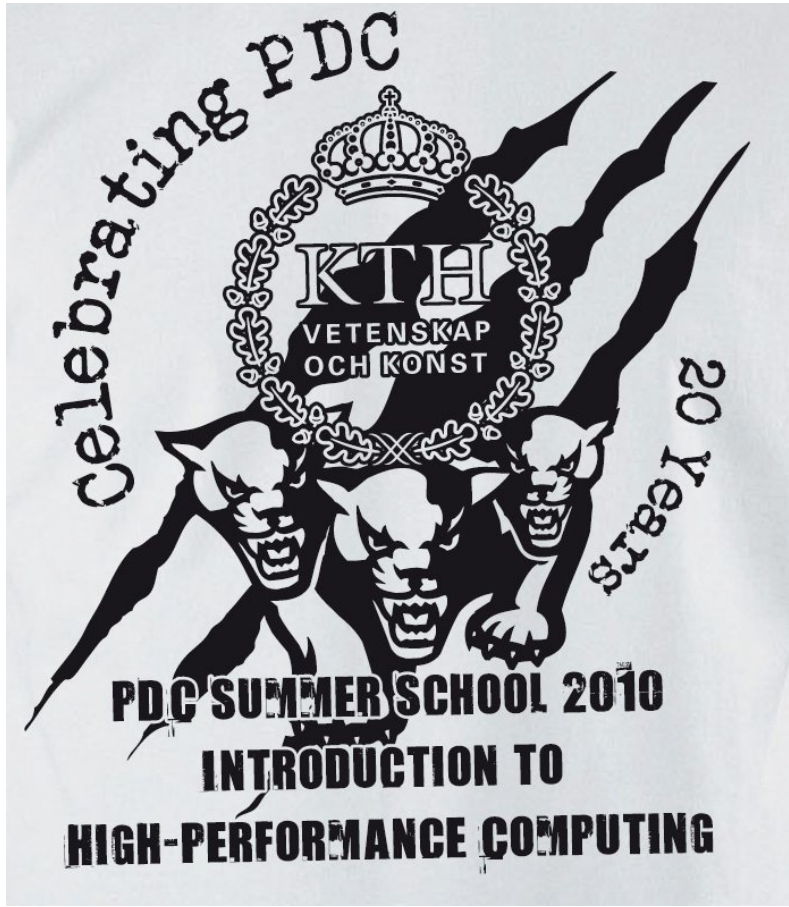

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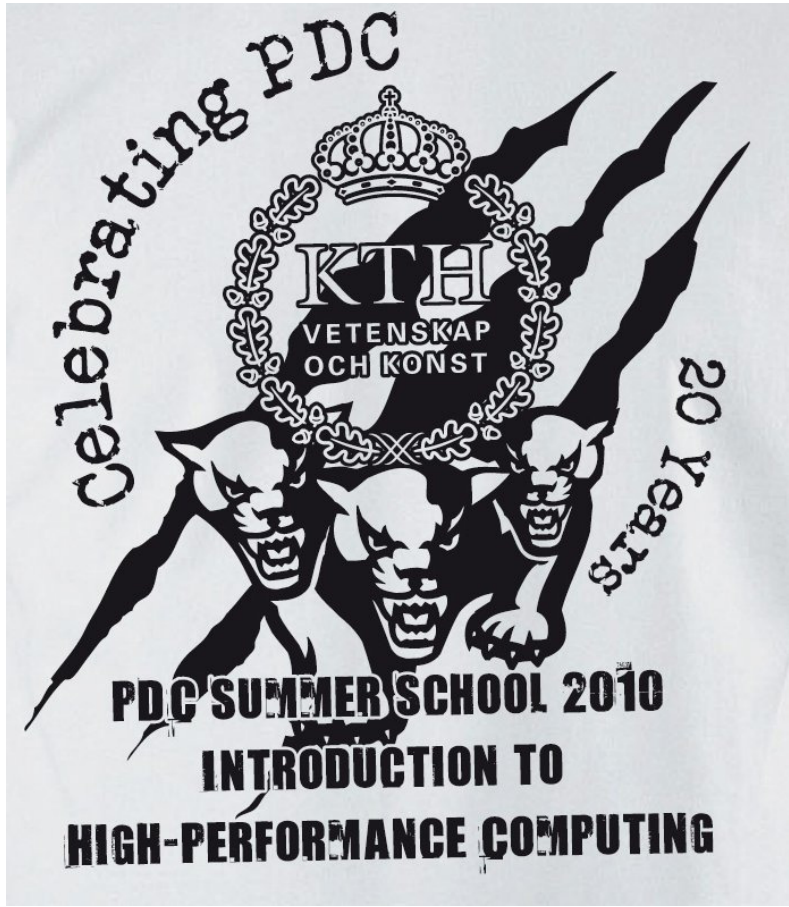

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