OpenFoam training

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Introduction to PDC

Centre for high performance computing

Arash Alizad Banaei/PDC

What is PDC?

- A supercomputing centre founded in 1990
  - SNIC centre(SNIC > Swedish National Infrastructure for Computing)
  - Under administration of School of Electrical Engineering and Computer Science (EECS) at KTH
- Providing high performance computing (HPC) services for academic and business/industrial research.
  - Services include HPC systems for performing computations and simulations (as well as pre- and post-processing of data), short- and long-term data storage, and assistance from application and systems experts

History of PDC

Year	Rank	Procs.	peak TFlops	vendor	name
2017	69	67456	2438.1	Cray	Beskow
2014	32	53632	1973.7	Cray	Beskow
2011	31	36384	365.63	Cray	Lindgren
2010	76	11016	92.534	Cray	Lindgren
2010	89	9800	86.024	Dell	Ekman
2005	65	886	5.6704	Dell	Lenngren
2003	196	180	0.6480	HP	Lucidor
1998	60	146	0.0934	IBM	Strindberg
1996	64	96	0.0172	IBM	Strindberg
1991	341	256	0.0025	Thinking Machines	Bellman

HPC Systems

- Beskow:
  - Cray XC40 system
  - Intel Haswell and Broadwell processors
  - Designed for running large parallel jobs
- Tegner
  - Pre and post processing system for Beskow
  - Intel CPUs + NVIDIA Tesla GPUs
  - 24 cores per node
  - Has large memory nodes: 0.5-1-2 TB
  - Will be used for OpenFOAM training

- Dardel
  - New system of PDC arrived a few months ago!
  - Dual AMD EPYC™ 2.25 GHz 64 core processor
  - AMD Instinct™ MI200 GPUs

Dardel Compute nodes

Number of nodes	RAM (GB)	Name
488	256	Thin
20	512	Large
8	1024	Huge
2	2048	Giant
36	256	Business

Getting started with Tegner
How to login

- Apply for a PDC account!
    - https://pdc-web.eecs.kth.se/accounts/
    - Receive your password by SMS
- Follow steps in:
  https://www.pdc.kth.se/support/documents/login/login.html#step-by-step-login-tutorial

- Contact PDC support in case of login issues:

support@pdc.kth.se

Getting started with Tegner
How to login: two step login using Kerberos ticket

1. Enter your password and get a ticket (you only have to do it once)

Kerberos Authentication Server

TICKET

2. Login with your ticket safe and hassle-free

PDC

Kinit –f <username>@NADA.KTH.SE
ssh –X <username>@tegner.pdc.kth.se

OpenFOAM on Tegner

- Once logged in, you will be on your home directory:
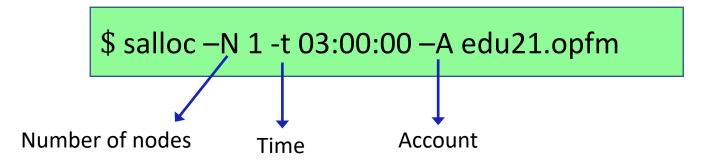/afs/pdc.kth.se/home/<letter>/<username>

```
[arash2@tegner-login-1 ~]$ pwd
/afs/pdc.kth.se/home/a/arash2
[arash2@tegner-login-1 ~]$ 
```

All the operations will be performed on your home directory

- All the software on Tegner are available through modules
- You need to load a module to your environment to access it

How to run OpenFOAM on Tegner

- You are already on the 'login node' and do not have access to the compute resources. You need to request a compute node:

- Request a compute node using 'salloc' command

$ salloc –N 1 -t 03:00:00 –A edu21.opfm

Number of nodes   Time   Account

15 nodes are reserved for this course. Each compute node has 24 cores

- You should see Something like this once you're granted a compute node:

```
salloc: Pending job allocation 63554
salloc: job 63554 queued and waiting for resources
salloc: job 63554 has been allocated resources
salloc: Granted job allocation 63554
```

How to run OpenFOAM on Tegner

- Try to login to the compute node

```
$ echo $SLURM_NODELIST
```

- Name of compute node will be printed

```
$ ssh –X <username>@<compute node>.pdc.kth.se
```

- Example

```
$ ssh –X arash2@t02n01.pdc.kth.se
```

OpenFOAM on Tegner

- Run 'module avail openfoam' to see which versions are available:

```
[[arash2@t02n01 ~]$ module avail openfoam

--------------------------------------------------------------- /pdc/modules/system/base ---
openfoam/1612+ openfoam/1712   openfoam/1812   openfoam/2.3.1 openfoam/5.0   openfoam/7
openfoam/1706  openfoam/1806   openfoam/1912   openfoam/4.1    openfoam/6
[arash2@t02n01 ~]$
```

- Run 'module load openfoam/1912'

- Run 'module list' to see the loaded modules and make sure OpenFOAM is loaded:

```
[[arash2@t02n01 ~]$ module list
Currently Loaded Modulefiles:
  1) gcc/7.2.0                 2) openmpi/3.0-gcc-7.2   3) openfoam/1912
[arash2@t02n01 ~]$
```

OpenFOAM on Tegner
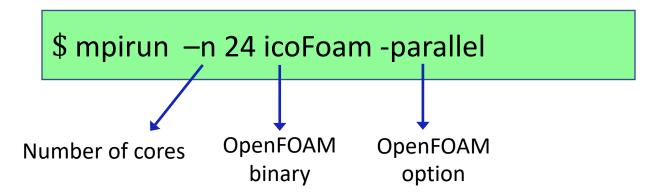
- Now you have access to OpenFOAM on Dardel!

- You need to run a script to set some environment variables and paths for OpenFOAM:

```
. $FOAM_BASHRC
```

- Copy OpenFOAM tutorials to your home directory:

Now You're ready for the analysis! You have Necessary files on your home directory

```
$ cp -r $WM_PROJECT_DIR/tutorials .
```

How to run OpenFOAM on Tegner

- To run your job you use srun command:

$ mpirun −n 24 icoFoam -parallel

Number of cores

OpenFOAM
binary

OpenFOAM
option

How to run OpenFOAM on Tegner

- Jobs can also be submitted through a batch script from the login node:

```
#!/bin/bash
#SBATCH -J mytest
#SBATCH -t 1:00:00
#SBATCH -A edu21.opfm
#SBATCH --nodes=1
module load openfoam/1912
. $FOAM_BASHRC
mpirun -n  24 icoFoam -parallel > my_output_file 2>&1
```

- Submit with 'sbatch' command'

```
$sbatch <name of the script>
```

How to run OpenFOAM on Tegner

- Use 'squeue' command to see your job status

$squeue -u <username>

- The output will look like this:

```
        JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
      1059071      main   my_job   arash2  R       0:08      1 t02n01
```

- Use 'scancel' command to cancel your job

$scancel <job-ID>

Good luck with the computations!