University of Iceland High Performance Computing

An introduction v2

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Changelog IHPC v2018

- All of Gardar removed
- 46 new nodes added
- Support staff down to 1
- New support mail queue

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In operation

- Garpur #1
  - Since 2015
  - 24/32 cores per node
  - 44 nodes + 3 GPU nodes
  - 128/256GB memory per node
  - 2x Tesla M2090 in each GPU node
- Garpur #2
  - Added late 2017
  - 32 cores per node
  - 192GB DDR4
  - interconnect: 50Gb/s Omnipath
- Jötunn
  - Since 2016
  - 24 cores per node
  - 4 nodes
  - 128GB memory per node

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In operation

Name	Garpur	Garpur #2	Jötunn	Total
Year	2015	2017	2016	
Nodes	44	46	4	94
TFLOPS	37	98	4	139
kW	17.1	16.6	2	35.7

- 136 Garpur users
  - 47 unique users connected since june 1st
- 73 Jötunn users

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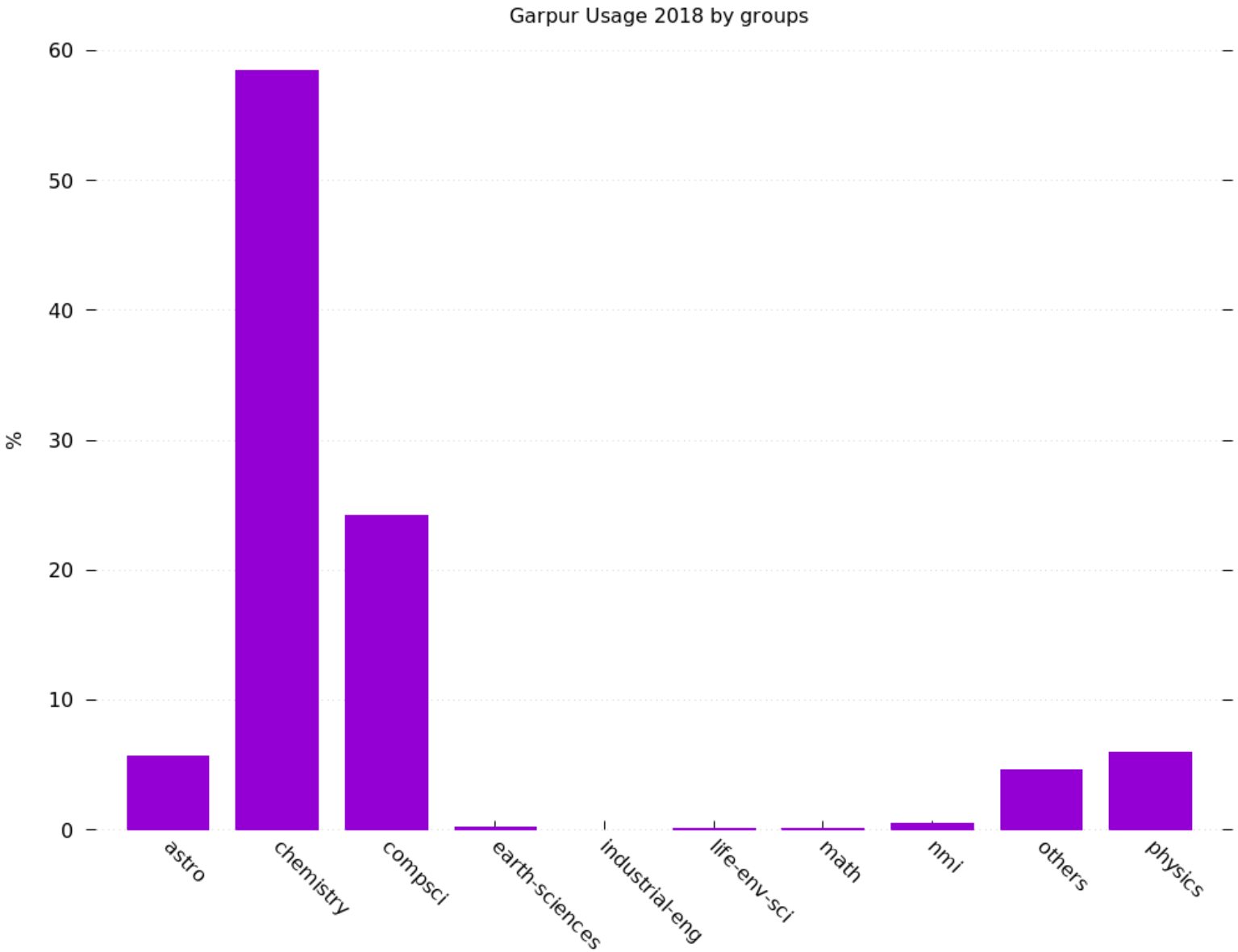
Cluster usage by groups



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Cluster Software

Garpur

- OpenHPC
- OS: Centos 7
- GCC & Intel compilers
- OpenMPI, IntelMPI, MPICH
- Python, R, Matlab
- VASP, GROMACS, PISM

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Application Process

Are you

- studying/working at an Icelandic University/Academic Institution?
- Doing a project supported by RANNIS?

→ then send an email to support-hpc@hi.is

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What do I get with an account?

- SSH login
- Disk space
  - Home partition: 100GB +
  - Work partition: Unlimited[1]
  - Jotunn disk space is more limited
- Unlimited CPU hours[1]
- Support from us[1]

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[1]Within resonable limits

Communication

- Account requests
  - support-hpc@hi.is
- Software requests
  - ihpc@hi.is
  - Request site is public
- News
  - ihpc@listar.hi.is
- Chat
  - ihpcgroup.slack.com

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Cluster workflow

You should have recieved your login credentials by email.

1. Connect with ssh
   - ssh mani@jotunn.rhi.hi.is
2. Check cluster status
   - sinfo
   - squeue
3. Load modules *or* compile program on login node
   - module avail
   - module load ...
4. Create job file
5. Submit job to queue
   - sbatch myjob.sh
6. Check results
   - Use slurm directives to send email when job completes

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Modules

Software on the cluster is provided in modules.

```
Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

[mani@garpur-main ~]$ module avail

------------------------------------------------------- /opt/ohpc/pub/moduledeps/gnu-openmpi -------------------------------------------
   boost/1.61.0    netcdf/4.4.1        netcdf-fortran/4.4.4    phdf5/1.8.17       scalasca/2.3.1    sionlib/1.7.0
   fftw/3.3.4      netcdf-cxx/4.2.1    petsc/3.7.0             scalapack/2.0.2    scorep/3.0

------------------------------------------------------------ /opt/ohpc/pub/moduledeps/gnu ---------------------------------------------
   R_base/3.3.1    gsl/2.2.1    hdf5/1.8.17    mpich/3.2    openblas/0.2.19    openmpi/1.10.4 (L)    pdtoolkit/3.22

---------------------------------------------------------- /opt/ohpc/pub/modulefiles ----------------------------------------------
   gnu/5.4.0 (L)    ohpc    papi/5.4.3    prun/1.1

------------------------------------------------------------ /opt/share/modulefiles -------------------------------------------------
   ADF/2017_r61726        gpaw/1.2.0               matlab/R2016a              proj4/4.9.2               tensorflow/1.1-cpu
   ADF/2017.109    (D)    gromacs/5.1.4-w-plumed   ncl/6.4.0                  pypy3/6.0                 udunits/2.2.24
   ase/3.13               gurobi/7.0.2             nco/4.6.1                  python/intel-3.6          vasp/5.4.1-impi
   cdo/1.8.2              intel/compiler/2017.2    openmpi/intel/2.1.0        python/2.7.13             vasp/5.4.1-tbdyn-impi
   cp2k/5.1               intel/impi/2017.4        openmpi/intel/2.1.1 (D)    python/3.6.1       (D)    vasp/5.4.1
   gcc/4.9.4              intel/mkl/2017.2         pism/0.7                   siesta/gcc/4.1.b3         vasp/5.4.4-impi       (D)
   go/1.10.2              julia/0.6                pism/1.0            (D)    siesta/intel/4.0.1

  Where:
   L:  Module is loaded
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
```

Anything missing?

Anything outdated?

Send an email to ihcp@hi.is

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Slurm Partitions

name	Time limit	nodecount	comment
short	4 hours	82	Default, limited to 1 node
normal	15 days	36	
long	30 days	36	
omnip	15 days	46	
himem	15 days	5	256GB memory nodes
himem-bigdisk	15 days	3	256GB memory and bigger disk
gpu	15 days	3	GPU Nodes

or use *sinfo* command

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Interactive job

```
[mani@garpur ~]$ salloc -N 1 -p gpu --exclusive
salloc: Granted job allocation 203466
[mani@garpur ~]$ squeue -u mani
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            203466       gpu     bash     mani  R       0:03      1 gpu-1
[mani@garpur ~]$ ssh $SLURM_NODELIST
Last login: Tue Jun 12 19:13:53 2018 from garpur.localdomain
[mani@gpu-1 ~]$ module load python/2.7.13
[mani@gpu-1 ~]$ module li

Currently Loaded Modules:
  1) prun/1.1   2) gnu/5.4.0   3) openmpi/1.10.4   4) ohpc   5) python/2.7.13

[mani@gpu-1 ~]$ nvidia-smi
Tue Jun 12 19:15:35 2018
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 375.26                 Driver Version: 375.26                    |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Tesla M2090         Off  | 0000:21:00.0     Off |                    0 |
| N/A   N/A    P0    76W /  N/A |      0MiB /  5301MiB |      0%      Default |
+-------------------------------+----------------------+----------------------+
|   1  Tesla M2090         Off  | 0000:22:00.0     Off |                    0 |
| N/A   N/A    P0    77W /  N/A |      0MiB /  5301MiB |      0%      Default |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID  Type  Process name                               Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
[mani@gpu-1 ~]$ exit
logout
Connection to gpu-1 closed.
[mani@garpur ~]$ exit
exit
salloc: Relinquishing job allocation 203466
salloc: Job allocation 203466 has been revoked.
[mani@garpur ~]$
```

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Job Scheduler

Typical slurm job workflow:

1. Decide how many nodes you need and on which partition (himem, default, gpu)
2. Create bash script with slurm directives
   - #SBATCH -J jobname
   - #SBATCH -N 2
   - #SBATCH –ntasks-per-node=2
   - #SBATCH –mail-user mani@hi.is
   - #SBATCH –mail-type=END
   - #SBATCH –array=0-15
3. Submit to queue
   - sbatch myjob.sh

```
[mani@garpur-main src]$ sbatch imb.sh
Submitted batch job 7303
```

Further examples available on our website `http://ihpc.is`

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Rules of thumb

1. Be respectful of others. Don't submit 10 jobs requiring 1 node each at once.
2. Allocate your job to 1 core, half a node or the whole node.
3. Tidy up unused disk space
4. Keep in mind resources other than CPU cores (e. g. memory)
5. If you know how long your job will run for, allocate only the needed walltime

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System status

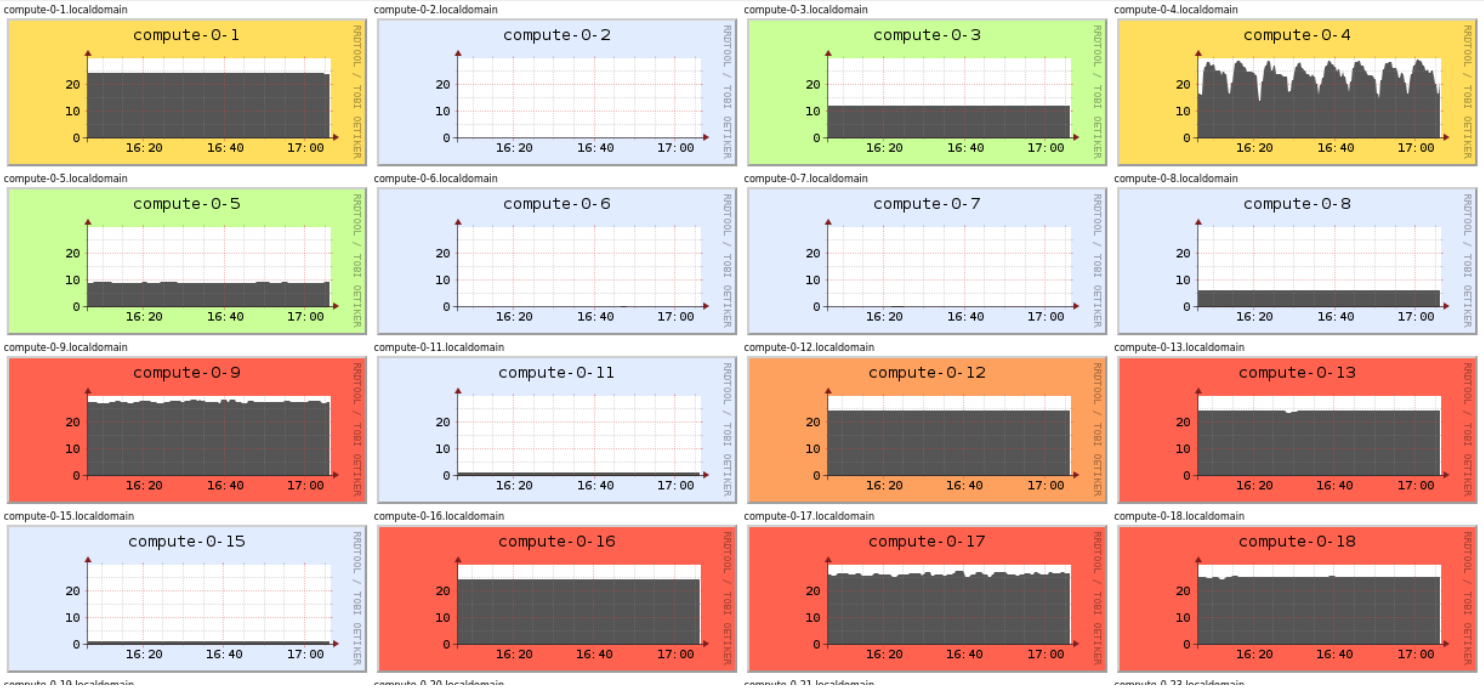
Check the status of the queue with

squeue

or

squeue -u mani

We also have a website with the system status `http://ihpc.is`



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Reporting examples

```
[mani@garpur-main ~]$ sreport user top
--------------------------------------------------------------------------------
Top 10 Users 2018-06-12T00:00:00 - 2018-06-12T23:59:59 (86400 secs)
Use reported in TRES Minutes
--------------------------------------------------------------------------------
  Cluster     Login     Proper Name         Account     Used   Energy
--------- --------- --------------- --------------- -------- --------
   garpur  jianyang       Jian Yang        jianyang   846483        0
   garpur      asod    Asmus O Dohn            asod   829440        0
   garpur elena.pa+   Elena Papaleo   elena.papaleo   593512        0
   garpur     seb21  Sebastian Bohr     jesus-group   548301        0
   garpur      jdb5      Jan Burger     jesus-group   217493        0
   garpur  etayyebi Ebrahim Tayyebi        etayyebi   152608        0
   garpur   aleksei  Aleksei Ivanov         aleksei   131781        0
   garpur     bab29 Barði Benedik+           bab29   119862        0
   garpur christia+  Christian Bean   christianbean   108730        0
   garpur      nra1 Nzar Rauf Abdu+            nra1    46080        0
[mani@garpur-main ~]$ sreport job SizesByAccount user=mani START=2018-06-01
--------------------------------------------------------------------------------
Job Sizes 2018-06-01T00:00:00 - 2018-06-12T23:59:59 (1036800 secs)
Time reported in Minutes
--------------------------------------------------------------------------------
  Cluster   Account     0-49 CPUs   50-249 CPUs  250-499 CPUs  500-999 CPUs  >= 1000 CPUs % of cluster
--------- --------- ------------- ------------- ------------- ------------- ------------- ------------
   garpur    kerfis             39             0             0             0             0      100.00%
```

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Support

Any questions?

Send them to support-hpc@hi.is

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