

HPC @ ITV

General info

HPC Team

G.Scialabba, T.Grenga, L. Berger, D. Goeb

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Institute for Combustion Technology  
RWTH Aachen University



# HPC Group duties

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- Managing ITV user group
- Managing libraries and software
- Communication with IT Center
- Coordinate technical problem (NO fixing issues)
- Monitor cluster usage
- Maintaining job/login scripts
- Collect ITV requirements

For general information regarding the RWTH Cluster usage, please refer to the ITC documentation:

<https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/>

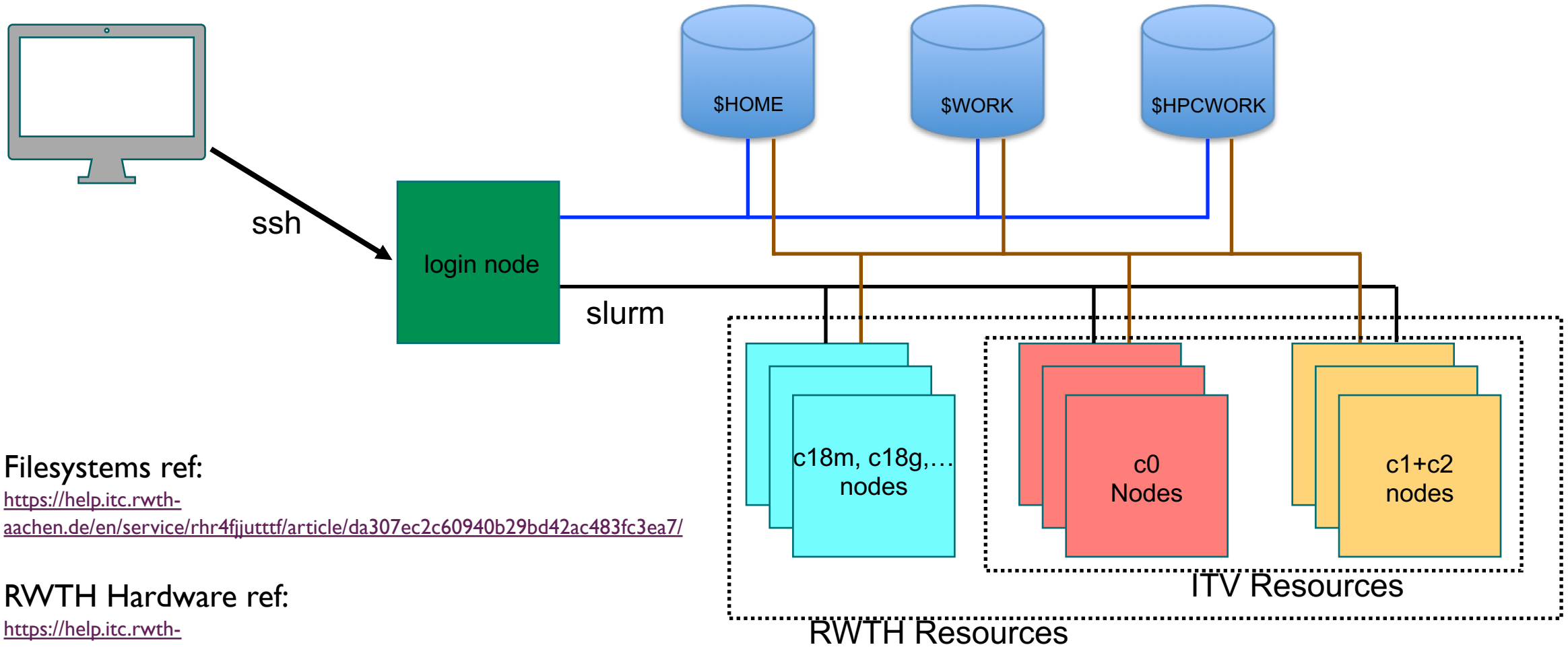


# Outline

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- **Cluster structure**
  - Hardware info
  - Usage rules (backend job submission)
  - Storage rules
  - Adding new members
- **HPC Proposal**
  - Small/Medium
  - Large scale
- **Codes**
  - Libraries
  - GitLab

# Hardware - Overview



## Filesystems ref:

<https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/article/da307ec2c60940b29bd42ac483fc3ea7/>

## RWTH Hardware ref:

<https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/article/fbd107191cf14c4b8307f44f545cf68a/>



# Login Nodes

## SSH Login ref:

<https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/article/10c8f0d9b0064013aa439f0b504cc806/>

## Dialog system ref:

<https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/article/0a23d513f31b4cf1849986aaed475789/>

Login nodes

Remote session

Hostname	Hardware Node Type	CPU Code-name	CPU Model	Clock Speed [GHz]	#Sockets per Node	#Cores per Socket	#Cores per Node	Memory per Node [GB]	SSD/HDD size [GB]	Beginning of operation	Remarks
login.hpc.itc.rwth-aachen.de	NEC HP-C128Rg-2	Broadwell EP	E5-2695v4	2.1	2	18	36	256	2000	November 2016	Main dialog system for CLAI2016, Hyperthreading ON (2x)
login2.hpc.itc.rwth-aachen.de	NEC HP-C128Rg-2	Broadwell EP	E5-2695v4	2.1	2	18	36	256	2000	November 2016	Hyperthreading ON (2x)
login18-1.hpc.itc.rwth-aachen.de	intel-R2208WFTZS	Skylake	Platinum 8160	2.1	2	24	48	384	1920	November 2018	Main dialog system for CLAI2018
login18-2.hpc.itc.rwth-aachen.de	intel-R2208WFTZS	Skylake	Platinum 8160	2.1	2	24	48	384	1920	November 2018	
login18-3.hpc.itc.rwth-aachen.de	intel-R2208WFTZS	Skylake	Platinum 8160	2.1	2	24	48	384	1920	November 2018	
login18-4.hpc.itc.rwth-aachen.de	intel-R2208WFTZS	Skylake	Platinum 8160	2.1	2	24	48	384	1920	November 2018	
login18-x-1.hpc.itc.rwth-aachen.de	supermicro-1029GP-TR	Skylake	Platinum 8160	2.1	2	24	48	384	1920	November 2018	Dedicated to remote desktop sessions
login18-x-2.hpc.itc.rwth-aachen.de	supermicro-1029GP-TR	Skylake	Platinum 8160	2.1	2	24	48	384	1920	November 2018	Dedicated to remote desktop sessions
login-g.hpc.itc.rwth-aachen.de	NEC-GPS12G3Rg-1 2 x Tesla P100	Broadwell EP	E5-2650v4	2.2	2	24	24	128	120	November 2016	GPU Cluster

## “Broadwell” node list

→ 89 nodes

2 Intel E5-2650 v4 processors “Broadwell”  
(2.2 GHz, 12 cores each)

24 cores per node,  
128 GB main memory per node  
( ~5 GB main memory per core)

→ Total 2136 cores

Nodes 1-4 for **debug only** (‘c0’)

Nodes 5-89 for production (‘c1+c2’)

## Rules

1. Runtime must be less than 24h on c1 and c2 (*Inih005-Inih089*)
2. Runtime \* max(<Number of cores>, 24\* <exclusive nodes>) must be equal or less than 48 on **c0** during working hours
3. If you run multiple serial jobs, e.g. FlameMaster simulations, make sure that you fill up a node before touching a new node.
4. If you need to run jobs longer than 24h or require any other exception, please notify the HPC group via e-mail ([hpc@itv.rwth-aachen.de](mailto:hpc@itv.rwth-aachen.de)).

**To run exclusively on the production nodes, specify the node list “Broadwell”**

# ITV Cluster Slurm Scripts

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```
-rw-rw---- 1 kr843742 itv 3.0K Apr 28 14:49 SlurmScript_FM_serial
-rw-rw---- 1 kr843742 itv 3.0K Jun 15 23:52 SlurmScript_FM
-rw-rw-r-- 1 kr843742 itv 2.7K Jun 22 14:56 SlurmScript_CIAO_Intel2018
-rw-rw-r-- 1 kr843742 itv 2.7K Apr 28 14:49 SlurmScript_CIAO_Intel2016
-rw-rw-r-- 1 kr843742 itv 468 Jul 26 09:54 Readme
-rw-rw-r-- 1 kr843742 itv 1.2K Jun 3 2019 INTEL2016_libraries
drwxrwsr-x 2 kr843742 itv 147 Apr 26 22:53 archive
[gandalf@login18-4 SLURM_submission_scripts]$ pwd
/home/itv/SLURM_submission_scripts
```

Some template scripts are located in

**/home/itv/SLURM\_submission\_scripts**

- Single node/core jobs submission script (e.g. FlameMaster)
- Multiple core jobs submission script (e.g. CIAO)

SLURM ITC Ref:

<https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/article/6e4d3ad2573d4e41a5fab9b65dbd320a/>



# ITV Cluster Slurm Script Example 1/4

```
1 #!/bin/bash
2
3 ## Double ## is a comment , #SBATCH is a command      ## indicates a comment, #SBATCH is a SLURM command
4
5 ## Job name and files
6 #SBATCH --job-name=flame_test_sbatch      ← Name of the job that will appear in itv_jobs
7
8 ## OUTPUT AND ERROR
9 #SBATCH -o job.%j.out      ← Set job output and error files name
10 #SBATCH -e job.%j.err
11
12 ## Initial working directory
13 ##SBATCH -D /hpcwork/ab123456/Your_folder/      ← Set working directory (" -D . " for current directory)
14
15 ## specify your mail address (send feedback when job is done)
16 #SBATCH --mail-type=begin      # send email when process begins...
17 #SBATCH --mail-type=end      # ...and when it ends...
18 #SBATCH --mail-type=fail      # ...or when it fails.      Mail notification settings
19 #SBATCH --mail-user=luca.toni@itv.rwth-aachen.de      # send notifications to this email REPLACE WITH YOUR EMAIL
20
21 ## Setup of execution environment
22 #SBATCH --export=NONE
```

# ITV Cluster Slurm Script Example 2/4

```
22 #SBATCH --export=NONE
23
24 ## account and partition selection
25 #SBATCH --account='itv'
26 #SBATCH --partition='itv'
27
28 ## Select list of nodes (use itv_jobs / itv_status / itv_status_long for more info)
29 ## 'broadwell' = previously CITV6-7 ('c2') + Honda nodes
30 # Use the 'broadwell' option to run in the 'c1+c2' nodes only
31 # Remove the option to include also the 'c0' debug nodes (Limited runtime for these nodes!)
32 #SBATCH -C 'broadwell' ## Specify the cluster
33 ##SBATCH -w 'lnih09' ## Specify one particular single node
34
35 ## Request the number of nodes
36 #SBATCH --nodes=2 # number of nodes
37
38 ##### Check 'itv_status_long' for more information about cores
39 ## Set tasks per node = Number of tasks per node (for MPI applications = numero of MPI processes (cores) per node)
40 ## Default values for different nodes:
41 ## 'broadwell' = 24
42 #SBATCH --tasks-per-node=24
43
44
```

Account and partition selection necessary to run in the itv cluster

Selection of node list (Comment out to include also the debug nodes)

Specific node selection (optional)

Number of required nodes

Task per node (Number of MPI processes)

# ITV Cluster Slurm Script Example 3/4

```
45 ## Set cores per task (OMP_NUM_THREADS)
46 #SBATCH --cpus-per-task=1
47
48 #SBATCH --threads-per-core=1
49
50 ## memory per cpu (IMPORTANT: specify a suitable value for your job)
51 ##SBATCH --mem-per-cpu=3000 # INSERT VALUE IN MB
52
53 ## do not share nodes
54 ##SBATCH --exclusive
55
56 ## OPTIONAL
57 ## set max. file size to 500Gbyte per file
58 ##SBATCH -F 500000000
59
60 ## execution time in [hours]:[minutes]:[seconds]
61 ## recommended: less than 24:00:00
62 #SBATCH --time=00:30:00
63
64 #####
65 #####
66 ##### END OF SLURM INSTRUCTION #####
67 ##!!! DO NOT PLACE SHELL VARIABLES ABOVE!!!###
```

CPU options (sets OMP\_NUM\_THREADS) and hyperthreading

Core memory option (1 GB / core if not specified, max 5GB for Broadwell)

Reserve the whole node even if not all the cores are used. Unless it is necessary, do not use this option for a more efficient use of the cluster resources.

Job execution time.  
Cluster rule < 24h

# ITV Cluster Slurm Script Example 4/4

```
71
72 ## Optional lines to remove all modules loaded and load the one desired
73 ## Not need to use them if you use the default modules
74 ## In the case the code has been compiled with the intel2016, change the following line accordingly
75
76 module purge; module load DEVELOP DEPRECATED
77 module load intel
78 module load intelmpi/2018.3.222
79
80
81 export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/itv/compile_centos7/lib/sundials/2.7.0_intel19.0_intelmpi_2018_mkl/Install_DIR/lib/
82
83
84 ## #executable name (e.g. arts_cf)
85 exe='arts'
86
87 ### executable arguments
88 args='input'
89
90
91 date
92
93 $MPIEXEC $FLAGS_MPI_BATCH ./$exe $args
94
95 date
96 █
```

Module loading

Additional library export

Executable selection

Input selection

Execution line



# SLURM Script node settings comparison

Single node job settings (e.g. OpenMP FlameMaster):

1 node \* 12 core per node = 12 cores

Multi node job settings example (e.g. CIAO):

2 nodes \* 24 tasks (cores per node) = 48 cores

```
29 ## Select list of nodes (use itv_jobs / itv_status / itv_status_long for more info)
30 ## 'broadwell' = previously CITV6-7 ('c2') + Honda nodes
31 # Use the 'broadwell' option to run in the 'c1+c2' nodes only
32 # Remove the option to include also the 'c0' debug nodes (Limited runtime for these nodes!)
33 #SBATCH -C 'broadwell' ## Specify the cluster
34 ##SBATCH -w 'lnih09' ## Specify one particular single node
35
36 ## Request the number of nodes
37 #SBATCH --nodes=1 # number of nodes
38
39 ##### Check 'itv_status_long' for more information about cores
40 ## Set tasks per node = Number of tasks per node (for MPI applications = number of MPI processes (cores) per node)
41 ## Default values for different nodes:
42 ## 'broadwell' = 24
43 #SBATCH --tasks-per-node=1
44
45
46 ## Set cores per task (OMP_NUM_THREADS)
47 #SBATCH --cpus-per-task=12
48
49 #SBATCH --threads-per-core=1
50
51 ## memory per cpu (IMPORTANT: specify a suitable value for your job)
52 #SBATCH --mem-per-cpu=3000 # INSERT VALUE IN MB
```

```
28 ## Select list of nodes (use itv_jobs / itv_status / itv_status_long for more info)
29 ## 'broadwell' = previously CITV6-7 ('c2') + Honda nodes
30 # Use the 'broadwell' option to run in the 'c1+c2' nodes only
31 # Remove the option to include also the 'c0' debug nodes (Limited runtime for these nodes!)
32 #SBATCH -C 'broadwell' ## Specify the cluster
33 ##SBATCH -w 'lnih09' ## Specify one particular single node
34
35 ## Request the number of nodes
36 #SBATCH --nodes=2 # number of nodes
37
38 ##### Check 'itv_status_long' for more information about cores
39 ## Set tasks per node = Number of tasks per node (for MPI applications = number of MPI processes (cores) per node)
40 ## Default values for different nodes:
41 ## 'broadwell' = 24
42 #SBATCH --tasks-per-node=24
43
44
45 ## Set cores per task (OMP_NUM_THREADS)
46 #SBATCH --cpus-per-task=1
47
48 #SBATCH --threads-per-core=1
49
50 ## memory per cpu (IMPORTANT: specify a suitable value for your job)
51 ##SBATCH --mem-per-cpu=3000 # INSERT VALUE IN MB
```

# SLURM Script execution

```
## #executable name (e.g. arts_cf)
exe='/Your/FlameMaster/Path/FlameMan'

### executable arguments
args='-i FlameMaster.input'

date
##### EXECUTION LINE #####

$exe $args

##### END OF EXECUTION PART #####
```

## FlameMaster execution

```
## Request the number of nodes
#SBATCH --nodes=1          # number of nodes

## Set tasks per node
#SBATCH --tasks-per-node=2

## Set cpus per task (multiple tasks for hyperthreading)
#SBATCH --cpus-per-task=1
##SBATCH --threads-per-core=1

srun -c 1 $exe $args
srun -c 1 $exe $args2
##### END OF EXECUTION PART #####
```

```
71
72 ## Optional lines to remove all modules loaded and load the one desired
73 ## Not need to use them if you use the default modules
74 ## In the case the code has been compiled with the intel2016, change the following line accordingly
75
76 module purge; module load DEVELOP DEPRECATED
77 module load intel
78 module load intelmpi/2018.3.222
79
80
81 export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/itv/compile_centos7/lib/sundials/2.7.0_intel19.0_intelmpi_2018_mkl/Install_DIR/lib/
82
83
84 ## #executable name (e.g. arts_cf)
85 exe='arts'
86
87 ### executable arguments
88 args='input'
89
90
91 date
92
93 $MPIEXEC $FLAGS_MPI_BATCH ./$exe $args
94
95 date
96 █
```

## CIAO execution

Two parallel single core processes in a single job script (srun needed)

# Hardware – Interactive job

---

## Procedure to follow

- `srun --pty -A itv -p ih -C broadwell -n 1 --mem-per-cpu=120000`  
`--tasks-per-node=1 -t 01:00:00 $SHELL`
- `queue -u <TIM-ID>`
- `ssh -Y <TIM-ID>@<nodename>` (from a new terminal)
- Load modules (if necessary)
- Launch software (e.g.: Matlab)

# HW – ITV Cluster monitoring

## Useful bash scripts for ITV cluster monitoring:

- `itv_jobs`, `itv_jobs_long`

Gives info on the cluster job queue (with user names).

- `itv_status`

Gives info on the status of the nodes

- `itv_status_long`

Gives detailed info on the status of the nodes  
(number of free cores if partially empty)

To use them add this line to your `.zshrc` / `.bashrc` → `source /home/itv/tools`

```
[gandalf@login18-4 ~]$ itv_jobs_long
-----
--- ITV Cluster ---
-----
--- CLUSTER CONFIGURATION ---
Partition 1 = DEBUG/POST PROCESING NODES 'c0' (4 nodes with 24 cores each = 96 slots, 128 GByte per node)
Partition 2 = PRODUCTION NODES 'broadwell' (85 nodes with 24 cores each = 2040 slots, 128 GByte per node)
--- NOTES ---
- Each job can use nodes of either 'broadwell' or CITV5 ('ivybridge').
- Runtime must be less than 24h on 'broadwell' ('c1' and 'c2').
- <Runtime> * max(<Number of cores>,24*<touched nodes>) must be equal or less than 48 on 'c0' during working hours.
- To run in the c0 nodes, the keyword 'broadwell' in #SBATCH -C must be removed.
- For regular jobs, keep the 'broadwell' option. Jobs running in 'c0' which don't follow the rules above will be cancelled.
--- FREE CORES READY ON 'c0' ---
FREE: 48
TOTAL: 96
--- FREE CORES READY ON BROADWELL ('c2' + former 'honda' nodes) ---
FREE: 743
TOTAL: 2040
--- Running jobs on ITV ---
JOBID  NAME      USER      TIME      TIME_LIMIT  TIME_LEFT  CPUS      NODELIST(REASON)
22442081 Water3    xi685912   3:17:41   23:00:00    19:42:19   1        lnih089
22443823 zsh       jh238254   17:30     1-00:00:00  23:42:30   12       lnih035
22439276 sc_phi_sweep ck777362   1:41:06    3:00:00     1:18:54   12       lnih049
22439275 sc_phi_sweep ck777362   1:46:35    3:00:00     1:13:25   12       lnih061
22439274 sc_phi_sweep ck777362   1:51:25    3:00:00     1:08:35   12       lnih067
22439273 sc_phi_sweep ck777362   1:53:45    3:00:00     1:06:15   12       lnih010
22439272 sc_phi_sweep ck777362   1:56:36    3:00:00     1:03:24   12       lnih017
```



# HW – SBATCH Queue Monitoring

---

- Check your job queue:

```
squeue -u <yourTIM-ID>
```

- Check itv job queue (as in itv\_jobs)

```
squeue -A itv
```

- Check itv cluster node info (long list, as in itv\_status\_long)

```
sinfo -p ih -A itv -N
```

For additional command options see:

<https://slurm.schedmd.com/sbatch.html>

<https://slurm.schedmd.com/sinfo.html>

<https://slurm.schedmd.com/squeue.html>

<https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/article/3d20a87835db4569ad9094d91874e2b4/>

- Storage space of 1,5 PetaByte (Lustre 16 filesystem) available for ITV group members.
- Storage location → **/itv/hpcwork/**
- Its usage should make the share of simulation data more efficient, avoiding unnecessary copies among individual cluster accounts.
- Simulation with medium/large outputs should be run directly from this partition of the cluster.

# HW – ITV Storage rules 1/2

---

## General guidelines:

- The shared space is intended to be used mainly for large simulation data
- Files should be organized by user or project
- In order to avoid accidental removal of the data, the owner should change the permission on this data to **READ-ONLY** (HPCWORK doesn't have a backup).
- When the owner of some data is going to leave ITV, it is his responsibility either to remove the data (if no longer needed in the institute) or to change their permission accordingly.

Change permissions of your directories with `chmod` (group) or `setfacl` (single user)

EXAMPLE: Give read, write and execute permission on a specific directory to a specific user:

```
setfacl -Rm u:TIM_ID:rwX,d:u:TIM_ID:rwX DIRECTORY
```

Check permissions with `getfacl`

# HW – ITV Storage rules 2/2

---

## General guidelines:

- Total file limit of 10m → **File number per user limit set to 150-200k** (please keep it as low as possible!)
- Compress large number of small files that are not accessed frequently in a .tar file
- **Keep the output file number of your codes to a reasonable level**
- Remove unnecessary or obsolete "transfer", "copy", "tmp"

To check the number of files in your directory → `find DIR_NAME -type f | wc -l`

For any doubt or request on the storage space please contact us at:

[hpc@itv.rwth-aachen.de](mailto:hpc@itv.rwth-aachen.de)

# Access to the ITV Group

Access to the ITV nodes and storage is only for the ITV linux group member

To get access (also for student, HiWis, etc...)

- Get an RWTH cluster account ([ITC ref](#))
- Send an email to [hpc@itv.rwth-aachen.de](mailto:hpc@itv.rwth-aachen.de) specifying the TIM-ID and attaching the Datenschutzrechtliche Einwilligung form filled

(The form can be found in sciebo  
[itv\\_public/orga/Datenschutzrechtliche  
Einwilligung\\_en.pdf](#))

## Datenschutzrechtliche Einwilligung

Name: \_\_\_\_\_

TIM-ID: \_\_\_\_\_

Ich willige ein, dass meine personenbezogenen Daten (Name, E-Mail-Adresse, TIM-ID) durch die HPC-Gruppe des Instituts für Technische Verbrennung gespeichert und genutzt werden. Die Datenverarbeitung erfolgt ausschließlich zur Administration des internen Rechenclusters, das am IT-Center der RWTH Aachen University integrativ gehostet wird. Hierdurch können meine TIM-ID und Name durch andere Nutzer des internen Rechenclusters miteinander in Verbindung gebracht werden.

Die Einwilligung erfolgt auf freiwilliger Basis und ich kann sie jederzeit mit Wirkung für die Zukunft widerrufen. Ab Zugang der Widerrufserklärung dürfen meine Daten nicht weiterverarbeitet werden. Sie sind unverzüglich zu löschen. Durch den Widerruf meiner Einwilligung wird die Rechtmäßigkeit der bis dahin erfolgten Verarbeitung nicht berührt. Meine Widerrufserklärung kann ich per E-Mail an [hpc@itv.rwth-aachen.de](mailto:hpc@itv.rwth-aachen.de) richten.

\_\_\_\_\_  
Ort, Datum  
Place and Date

\_\_\_\_\_  
Unterschrift  
Signature

## Non-binding English translation:

*I agree that my personal data (name, email address, TIM-ID) are stored and used by the HPC group of the Institute for Combustion Technology. The collected data will be exclusively used for administration of the internal computing cluster, integratively hosted at the IT Center of RWTH Aachen University. As a result of this, my TIM-ID and name can be connected by other users of the internal computing cluster.*

*This consent is given on a voluntary basis and I can revoke it at any time with effect for the future. My data may not be further used after my revocation of this agreement has been received. They must be deleted immediately. The revocation of my consent does not affect the legality of usage that has taken place up to that point. I can send my declaration of revocation by e-mail to [hpc@itv.rwth-aachen.de](mailto:hpc@itv.rwth-aachen.de).*

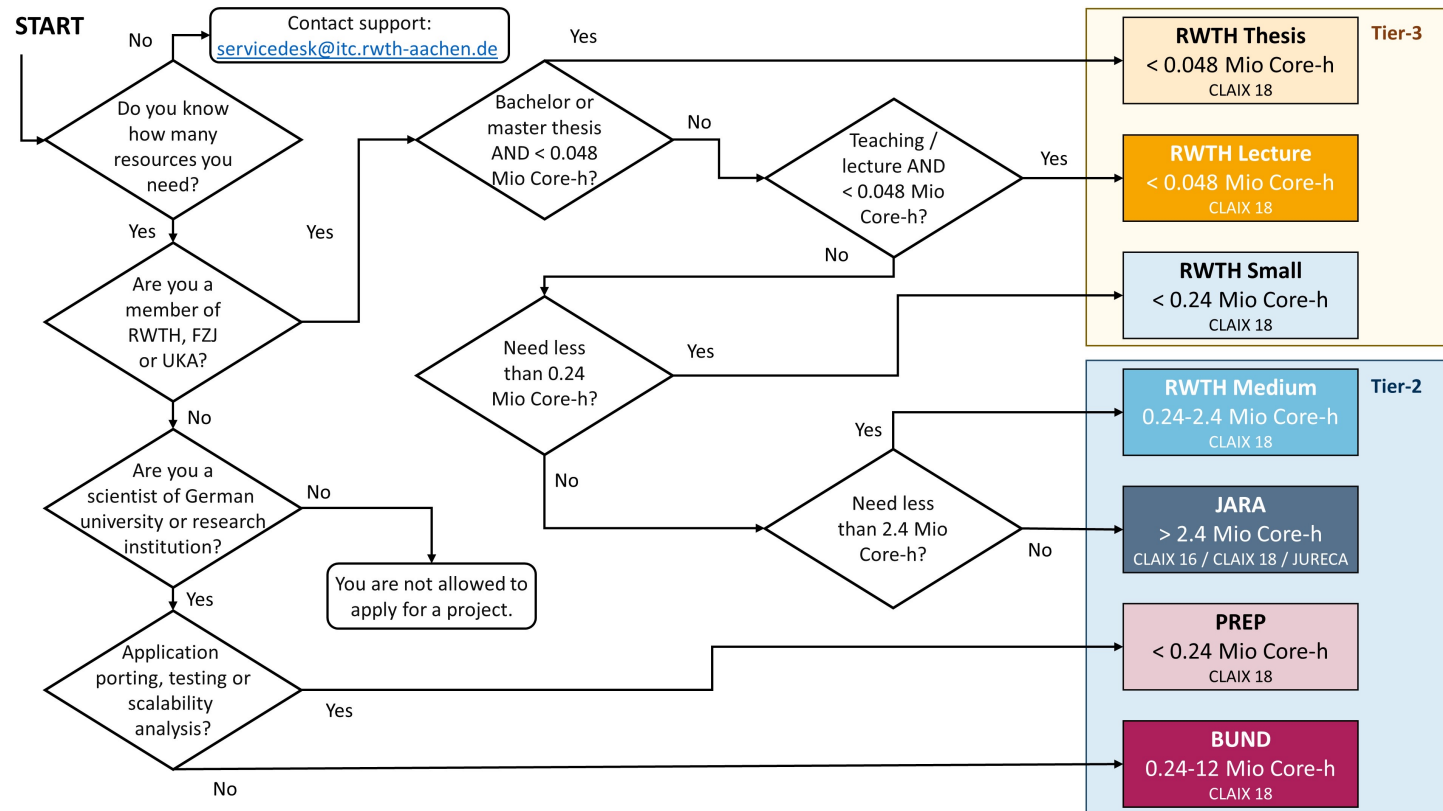
# Outline

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- Codes
  - Libraries
  - GitLab

# HPC Resources and Applications – Small and Medium

- For very small computational requirements (e.g. FlameMaster simulations, small CIAO tests) there's no need for HPC applications → Use the ITV cluster
- For small (i.e. Thesis) to medium application (up to 2.4 million Core-h), please consider the RWTH-JARA applications ([Ref.](#)):



- Small applications (up to 240k Core-h) only require a small abstract of 1-2 pages.
- Fast approval
- RWTH Small proposal examples on Sciebo (ITVPublic/proposals)
- Contact us at [hpc@itv.rwth-aachen.de](mailto:hpc@itv.rwth-aachen.de) before submission

# HPC Resources and Applications – Large Scale

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For medium to large scale applications (i.e. DNS/LES simulations) with larger computational requirements (above 2.4m Core-h) it is necessary to apply to external HPC Centres:

- Leibniz Supercomputing Center (LRZ, SuperMUC)
- High-Performance Computing Center Stuttgart (HLRS)
- Jülich Supercomputing Center (JSC, JARA)

**Only HLRS and LRZ are suitable for large (>20m Core-h) CPU only applications**

How to apply:

- HLRS → Rolling calls up to 100m, twice a year for larger requirements (Gauss Call, PRACE)
- LRZ (SuperMUC) → Rolling calls up to 45m, twice a year for larger requirements (Gauss Call, PRACE)
- JSC → Only twice a year, for anything above 2.4m (Gauss Call, PRACE)



# HPC Resources and Applications – Large Scale

- Submission of a proposal with detailed requirements and research motivation is required (10-15 pages)
- Previous proposals from ITV can be found on Sciebo (ITVPublic/proposals)

## Useful links:

→ HLRS : <https://www.hlrs.de/solutions-services/academic-users/hlrs-systems-access/>



→ LRZ: <https://doku.lrz.de/display/PUBLIC/Application+for+a+project+on+SuperMUC-NG>



→ JSC/JARA: <https://www.jara.org/en/research/center-for-simulation-and-data-sciences/jara-partition/applying-for-computing-time>



→ Gauss Centre for Supercomputing (GCS): <https://www.gauss-centre.eu/results/large-scale-projects/>



→ PRACE: <https://prace-ri.eu/hpc-access/project-access/project-access-how-to-apply/>



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  - Libraries
  - GitLab

# Codes – Libraries in home/itv

```
drwxrws--- 2 mb472681 itv 263 Jul 19 17:45 zsh
drwxrws--- 5 mb472681 itv 257 Jul 26 12:59 tools
drwxrws--- 32 mb472681 itv 1.5K Jun 28 19:06 tmp
drwxrwsr-x 3 kr843742 itv 19 Jun 23 2020 soo_l
drwxrwsr-x 3 kr843742 itv 245 Jul 26 13:35 SLURM_submission_scripts
drwxrws--- 3 ic400715 itv 28 Feb 8 08:50 scripts
drwxrws--- 7 re838602 itv 200 Feb 10 2020 Regression_TMP
drwxrws--- 4 re838602 itv 241 Sep 20 2019 Molpro
drwxrws--- 2 jh42442a itv 0 Jan 16 2015 Mixing
-rw-rw---- 1 ff219929 itv 59K Jan 13 2020 lpt_spray.f90
drwxrws--- 3 kr843742 itv 27 Jan 18 2021 LIBRARIES
drwxrwxr-x 6 mg261650 itv 142 Jun 10 2014 LES_psDNS_15.06.10_beta
drwxrwsr-x 2 mg261650 itv 264K Aug 18 2015 jet
drwxrws--- 6 kk032690 itv 230 Jan 21 2019 itv_thf
-rw-rw-r-- 1 mg261650 itv 197K Sep 9 2014 io_m.f90
drwxrws--- 2 md777659 itv 112 Oct 16 2019 fluent
drwxrwsr-x 3 dd734732 itv 947 Nov 4 2020 DE_vr
drwxrws--- 8 22048 itv 161 Mar 6 2017 CONVERGE_Studio
drwxrwx--- 4 mb472681 itv 42 Jan 16 2021 compile_centos7
drwxrws--- 4 re838602 itv 57 Jan 18 2021 CLAI2018
drwxrws--- 5 kk032690 itv 110 Aug 29 2019 CIAO_thfVerification
drwxrws--- 9 r1945150 itv 281 Jun 14 2018 cantera
drwxrwsr-x 2 mg261650 itv 1.7K Sep 21 2014 budget_4
-rw-rw-r-- 1 mg261650 itv 6.0K Sep 8 2015 box.xmf
-rw-rw---- 1 kr843742 itv 396 Oct 21 2020 artsModules.sh
drwxrws--- 5 az601284 itv 331 Jul 28 2020 AH_Project_2D
drwxrwxr-x 6 mg261650 itv 101 Jun 5 2014 3dt_Achim
drwxrws--- 9 jh424426 itv 487 Jan 18 2021 2015
```

Shared scripts and libraries stored in /home/itv/

- Working libraries for CIAO stored in /compile\_centos7/ → **DO NOT MODIFY!**
- Useful compiled libraries for other users can be stored in LIBRARIES
- /home/itv shared space intended only for libraries/codes and scripts → **NO STORAGE OF DATA**

# Codes – RWTH GitLab



Codes should be handled through version controlled repositories → **GitLab** provided by RWTH

- Better maintainability, keeps track of changes
- Suitable for codes, scripts, LaTeX templates
- General codes and templates should be added in the **ITV GitLab group**
  - Ask the HPC group or other colleagues to be added
  - Previously existing repositories can be added to the group's repositories
- General repositories with Post-Processing scripts and tools will be soon created

Link to the ITV Git → <https://git.rwth-aachen.de/ITV>

The screenshot shows the GitLab interface for the 'ITV' group. The left sidebar contains navigation options: Group information, Epics (0), Issues (6), Merge requests (2), Security & Compliance, Push Rules, Kubernetes, Packages & Registries, Analytics, Wiki, and Settings. The main content area shows the group name 'ITV' with a group ID of 2908 and a 'Leave group' link. Below this, a 'Recent activity' section shows 1 Merge Request opened, 0 Issues opened, and 8 Members added in the last 90 days. The 'Subgroups and projects' section is active, displaying a list of projects with their names, descriptions, star counts, and update dates.

Project Name	Description	Stars	Last Updated
egc	EGLIB is a general-purpose Fortran library designed to evaluate transport propertie...	0	6 months ago
FlameMaster	The open source code FlameMaster is a comprehensive tool for numerical modeling...	6	3 months ago
Mech	A chemical kinetic model repository.	2	3 months ago
OpenFoam	This is the repository of OpenFOAM ESI version used and extended at the ITV.	0	3 weeks ago
Surrogate Fitting Tool	Tool for determining surrogate composition based on target data. Example in the fol...	0	3 weeks ago
thermodynamik1		0	9 months ago
compare_reaction_rates_coefficients	A minimal example that generates a figure with a comparison of reaction rate coeffi...	0	3 months ago
SootMasterLeland	C++ Library for Soot Moments computation with HMOM/MOMIC closure	2	8 months ago

Thanks for your attention

HPC Group

[hpc@itv.rwth-aachen.de](mailto:hpc@itv.rwth-aachen.de)

Institute for Combustion Technology  
RWTH Aachen University

