This publication shall facilitate the beginning of work with HP XC3000 (HC3) at Steinbuch Centre for Computing (SCC) of KIT. HP XC3000 is a distributed memory parallel computer with 356 compute nodes. All nodes are equipped with 8 cores, local disks and network adapters; 312 compute nodes have 24 GB main memory, 32 nodes have 48 GB main memory and 12 nodes have 144 GB main memory. The operating system is the same as on the login nodes. The parallel file system Lustre is used for globally visible user data like the home- and a work- directory.

If you run into troubles when working on HC3 please contact the hc-hotline (see chapter 9) or responsible staff members of SCC.

Figure 1: Configuration of HP XC3000 (HC3)
1 Configuration

HP XC3000 (HC3) is a distributed memory parallel computer with 340 so-called thin compute nodes and 12 so-called fat compute nodes. The thin nodes are equipped with 8 cores, 24 or 48 GB main memory, local disks and network adapters, whereas the fat nodes are equipped with 8 cores, 144 GB main memory, bigger local disks and network adapters.

The parallel file system Lustre is used for globally visible user data like the home- and a work-directory. The environment variable $HOME points to the home-directory and $WORK points to the work-directory. The home-directories of IC2 and HC3 are the same.

2 Login

HC3 has 2 dedicated login nodes. Both login nodes are equipped with 8 cores, 48 GB main memory, local disks and network adapters. The operating system Linux (SLES 11) runs on the login nodes (and all other nodes), so that working on a single node of HC3 is comparable with working on a workstation.

2.1 Login on a Login Node

The selection of the login node is done automatically. If you are connecting another time to a login node, the sessions might run on the other (login) node of HC3. Only the secure shell ssh is allowed to login. Other commands like telnet or rlogin are not allowed for security reasons.

A connection to HC3 can be established by the command

```
ssh kit-account@hc3.scc.kit.edu
```

Be aware that the password can not be changed directly on IC2! Please change it on the web site:

https://intra.kit.edu (Link: Meine Daten)

If you are using OpenSSH (usually installed on Linux based systems) and you want to use a GUI-based application on HC3 like e.g. the debugger DDT, you should use the command

```
ssh -X kit-account@hc3.scc.kit.edu
```

with the option -X.

3 Copying Data onto HC3

You will see the home-directory of hc3 and IC2 if you have an account on one of them. There is additional file space that can be accessed by using the environment variable $WORK.

To achieve a high security level the files must be transferred by the secure copy command scp or the command rsync that again uses the command scp.

The command rsync is used similar to the command scp. In the following recommendation the specified directory and all subdirectories of the computer you are logged in are copied recursively to the user typed instead of kit-account on HC3 into the directory Copy_of_dir.

```
rsync -av local_computer_directory/ kit-account@ic2.scc.kit.edu:Copy_of_dir
```
To guarantee consistent data neither batch jobs on your workstation nor batch jobs on HC3 should run while the data are copied.

Further informations on the command rsync are available by manual pages (man rsync).

4 Choosing your User Environment

HC3 supports the use of Modules software to make it easier to configure and modify the user environment. Modules software enables dynamic modification of your environment by the use of modulefiles. A modulefile contains information to configure the shell for an application.

We provide modules for all supported compilers, debuggers, tools and libraries. Modulefiles that are available on HC3 can be viewed by the command module available. To view the modulefiles that are currently loaded in your environment, issue the command module list. By default the following modulefiles are available:

- dot adding the current directory to your environment variable PATH,
- intel loading the Intel C/C++ and Fortran compiler in a stable version and
- openmpi loading OpenMPI in the latest stable version.

You can load a modulefile in to your environment to enable easy access to software that you want to use by executing the command module add <modulefile>. To unload a modulefile that is currently loaded the command module rm <modulefile> must be executed.

If e.g. you want to use the GNU compiler instead of the Intel compiler (this is the default compiler), you just have to type module add gcc. The command module rm intel can be omitted because unloading of an arbitrary loaded compiler will be done automatically within our Module environment when loading another compiler.

5 Compiler and Parallelization Environment

On HC3 different compilers are available for the programming languages Fortran90/95, C, C++ and Java. The most important parallelization environments are the Message Passing Interface MPI for jobs running on many nodes and OpenMP for jobs running within one node.

The default compiler is the Intel compiler called by ifort for Fortran programs, icc for C programs and icpc for C++ programs. The GNU compiler suite can also be chosen for both Fortran and C/C++; exchanging of the compiler can simply be done by the command module add gcc.

For the compilation of message passing applications with MPI there are special compiler scripts like mpif77 for Fortran77 programs, mpif90 for Fortran95 programs, mpicc for C programs and mpicc for C++ programs.

Further information on compilers and the parallelization environment can be found in HP XC3000 User Guide.
6 Batch System JMS

A few nodes are provided for interactive operations. All other nodes can only be accessed by
the batch system JMS using SLURM. Batch jobs are submitted by the command job_submit.
A required parameter is the name of the executable for jobs running on a single core or rather
"mpirun name_of_executable" for jobs running on more than one core or a shellscript;
required options are the required resources like number of cores, CPU-time and main memory.
Information on job_submit can be displayed by the command job_submit -H and actual
limitations of the job queues by the command job_info.

7 User Guide

All manuals on HP XC3000 are available online in PDF-format. The substantial local adjust-
ments on usage of HC3 are outlined in HP XC3000 User Guide.

8 Important Addresses for Online Informations

- HP XC3000 Website at Steinbuch Centre for Computing
  http://www.scc.kit.edu/dienste/hc3.php

- HP XC3000 User Guide

- Homepage of HPC and Clustercomputing
  http://www.scc.kit.edu/dienste/hpc.php

- Homepage of Steinbuch Centre for Computing (SCC)
  http://www.scc.kit.edu/

- Maintenance and Repair Information
  http://www.scc.kit.edu/dienste/stoerungen.php

9 Contact

- HC3 Hotline
  hc-hotline@lists.uni-karlsruhe.de
  Phone: +49 721 608-48011