The RWTH HPC-Cluster User's Guide

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What's New

These topics are added or changed significantly[1] compared to the prior release (8.3.2) of this primer:

- The Linux release changed from Scientific Linux (SL) 6.x to CentOS 7.x series.
  - All binaries had to be rebuild from scratch (including the 'configure' steps and all depending libraries).
  - The default MPI library Open MPI (http://www.openmpi.org) changed from 1.6.x series to 1.10.x series
  - The version of the default compiler changed to intel/16.0 (instead of 14.0 versions)
  - Many other modules are updated in their versions, old versions were removed.
- The BCS nodes consisting out of four 4-socket nodes coupled via a proprietary networking technology from Bull are decoupled and are available as individual 4-socket computers in the SMP complex.[2] Thus the chapter
  - *2.3.7 Big SMP (BCS) Systems*

  has been removed.
- As some older nodes reached the EOL (end-of-live) timeline, they are removed from the table 2.3 on page 14
- The HPC-Cluster has now Intel Xeon CPUs only, which are quite similar to each other. Thus these chapters:
  - *2.3.1 The Xeon X5570 "Gainestown" ("Nehalem EP") Processor*
  - *2.3.2 The Xeon X7550 "Beckton" ("Nehalem EX") Processor*
  - *2.3.3 The Xeon X5675 "Westmere EP" Processor*
  - *2.3.4 The Xeon E5-2650 "Sandy Bridge" Processor*

  are removed and superseded by table 2.4 on page 14.
- In chapter 8.1.1 on page 79 outdated and less important information removed, including
  - *Table 8.27: Hardware counter available for profiling with collect on Intel Harpertown, Tigerton and Dunnington CPUs*
  - *Chapter 8.1.4 The Performance Tools Collector Library API.*
- HPC tools evolve very quick. Any detailed information added to this document was often outdated ex works. Thus the chapters
  - *8.3 Vampir*
  - *8.4 Scalasca*

  are removed and replaced by short description of the VI-HPS tools and UNITE modules, cf. chapter 8.3 on page 84.

[1] The last changes are marked with a change bar on the border of the page

[2] Four nodes with the currently largest amount of memory available are exempt:

- 2x nodes with 2TB RAM each
- 2x nodes with 1TB RAM each.

For description of these nodes, refer to older versions of this document

- Instead of the X-Win32 software we now offer FastX, thus the chapter

  – *4.1.2.1 X-Win32*

  is removed and new chapter 4.1.2.1 on page 26 describe the FastX software.

- The **FLAGS_MKL_SCALAPACK_LINKER** environment variable introduced in order to simplify linking of ScaLAPACK using Intel MKL library, cf. chapter 9.3 on page 89.

- We introduced the general Project Based Management of the whole HPC-Cluster starting September 1st 2014 as extension of concepts used in the JARA-HPC Partition established since spring 2012. Thus the chapter

  – *4.5 JARA-HPC Partition*

  has been superseded by chapter 4.5 on page 44, which unfortunately is still TBD.

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Table of Contents

1 Introduction

The IT Center[3] of the RWTH Aachen University (IT Center der Rheinisch-Westfälischen Technischen Hochschule (RWTH) Aachen) has been operating a UNIX cluster since 1994 and supporting Linux since 2004. Today most of the cluster nodes run Linux.

The cluster is operated to serve the computational needs of researchers from the RWTH Aachen University and other universities in North-Rhine-Westphalia. This means that every employee of one of these universities may use the cluster for research purposes. Furthermore, students of the RWTH Aachen University can get an account in order to become acquainted with parallel computers and learn how to program them.[4]

This primer serves as a practical introduction to the HPC-Cluster. It describes the hardware architecture as well as selected aspects of the operating system and the programming environment and also provides references for further information. It gives you a quick start in using the HPC-Cluster at the RWTH Aachen University including systems hosted for institutes which are integrated into the cluster.

If you are new to the HPC-Cluster we provide a 'Beginner's Introduction' in appendix B on page 104, which may be useful to do the first steps.

1.1 The HPC-Cluster

The architecture of the cluster is heterogeneous: The system as a whole contains a variety of hardware platforms and operating systems. Our goal is to give users access to specific features of different parts of the cluster while offering an environment which is as homogeneous as possible. The cluster keeps changing, since parts of it get replaced by newer and faster machines, possibly increasing the heterogeneity. Therefore, this document is updated regularly to keep up with the changes.

The HPC-Cluster consists of Intel Xeon-based 12- to 128-way SMP nodes. The nodes are running Linux. An overview of the nodes is given in table 2.3 on page 14. Note that this table does not contain nodes integrated into HPC-Cluster via Integrative Hosting.

Accordingly, we offer different front ends into which you can log in for interactive access. Besides the front ends for general use, there are front ends with special features: graphical login (FastX servers), or for performing big data transfers.

See table 1.1 on page 8.

Front end name	OS
cluster.rz.RWTH-Aachen.DE **cluster-linux**.rz.RWTH-Aachen.DE	Linux
cluster-x.rz.RWTH-Aachen.DE **cluster-x2**.rz.RWTH-Aachen.DE	Linux, for graphical login (FastX software)
cluster-copy.rz.RWTH-Aachen.DE **cluster-copy2**.rz.RWTH-Aachen.DE	Linux, for data transfers

Table 1.1: Front end nodes

To improve the cluster's operating stability, the front end nodes are rebooted weekly, typically on Monday early in the morning. All the other machines are running in non-interactive mode and can be used by means of batch jobs (see chapter 4.4 on page 34).

[3] Note that three letter acronym "ITC" is not welcome.

[4] see appendix B on page 104 for a quick introduction to the Linux cluster

1.2 Development Software Overview

A variety of different development tools as well as other ISV[5] software is available. However, this primer focuses on describing the available software development tools. Recommended tools are highlighted in **bold blue**.

An overview of the available compilers is given below. All compilers support serial programming as well as shared-memory parallelization (autoparallelization and OpenMP):

- **Intel (F95/C/C++)**
- Oracle Solaris Studio (F95/C/C++)
- GNU (F95/C/C++)
- PGI (F95/C/C++)

For Message Passing (MPI) one of the following implementations can be used:

- **Open MPI**
- Intel MPI

Table 1.2 on page 9 gives an overview of the available debugging and analyzing / tuning tools.

	Tool	Ser	ShMem	MPI
Debugging	**TotalView**	**X**	**X**	**X**
	Allinea DDT	**X**	**X**	**X**
	Oracle Thread Analyzer		**X**	
	Intel Inspector		**X**	
	GNU gdb	X		
	PGI pgdbg	X		
Analysis / Tuning	**Oracle Performance Analyzer**	**X**	**X**	**X**
	GNU gprof	X		
	Intel VTune Amplifier	**X**	**X**	
	Intel Trace Analyzer and Collector			**X**
	Vampir			**X**
	Scalasca			X

Table 1.2: Development Software Overview. Ser = Serial Programming; ShMem = Shared memory parallelization: OpenMP or Autoparallelization; MPI=Message Passing

[5] Independent Software Vendor. See a list of installed products: https://doc.itc.rwth-aachen.de/display/CC/Installed+software

1.3 Examples

To demonstrate the various topics explained in this user's guide, we offer a collection of example programs and scripts.

The *example scripts* demonstrate the use of many tools and commands. Command lines, for which an example script is available, have the following notation in this document:
`$ $PSRC/pex/100|| echo ''Hello World''`
You can either run the script **$PSRC/pex/100** to execute the example. The script includes all necessary initializations. Or you can do the initialization yourself and then run the command after the "pipes", in this case **echo "Hello World"**. However, most of the scripts are offered for Linux only.

The *example programs*, demonstrating e.g. the usage of parallelization paradigms like OpenMP or MPI, are available on a shared cluster file system. The environment variable **$PSRC** points to its base directory.

The code of the examples is usually available in the programming languages C++, C and FORTRAN (F). The directory name contains the programming language, the parallelization paradigm, and the name of the code, e.g. the directory **$PSRC/C++-omp-pi** contains the Pi example written in C++ and parallelized with OpenMP. Available paradigms are:

- **ser** : Serial version, no parallelization. See chapter 5 on page 45
- **aut** : Automatic parallelization done by the compiler for shared memory systems. See chapter 6.1 on page 62
- **omp** : Shared memory parallelization with OpenMP directives. See ch. 6.1 on page 62
- **mpi** : Parallelization using the message passing interface (MPI). See ch. 6.2 on page 69
- **hyb** : Hybrid parallelization, combining MPI and OpenMP. See ch. 6.3 on page 72

The example directories contain Makefiles for the "gmake" tool available on Linux.Furthermore, there are some more specific examples in project subdirectories like *vihps*.

You have to copy the examples to a writeable directory before using them. You can copy an example to your home directory by changing into the example directory with e.g.
`$ cd $PSRC/F-omp-pi`
and running
`$ gmake cp`
After the files have been copied to your home directory, a new shell is started and instructions on how to build the example are given.
`$ gmake`
will invoke the compiler to build the example program and then run it.

Additionally, we offer a detailed beginners introduction for the Linux cluster as an appendix (see chapter B on page 104). It contains a step-by-step description about how to build and run a first program and should be a good starting point in helping you to understand many topics explained in this document. It may also be interesting for advanced Linux users who are new to our HPC-Cluster to get a quick start.

1.4 Further Information

Please check our web pages:
http://www.itc.rwth-aachen.de/hpc/
The latest version of this document is located here:
http://www.itc.rwth-aachen.de/hpc/primer/

News, like new software or maintenance announcements about the HPC-Cluster, is provided through the **rzcluster** mailing list. Interested users are invited to join this mailing list at
http://mailman.rwth-aachen.de/mailman/listinfo/rzcluster
The mailing list archive is accessible at
http://mailman.rwth-aachen.de/pipermail/rzcluster

Semi-annual, workshops on actual themes of HPC take place in Aachen:
http://www.itc.rwth-aachen.de/ppces/
http://www.itc.rwth-aachen.de/aixcelerate/

Please feel free to send feedback, questions or problem reports to

servicedesk@itc.rwth-aachen.de

Have fun using the HPC-Cluster!

2 Hardware

This chapter describes the hardware architecture of the various machines which are available as part of the RWTH Aachen University's HPC-Cluster.

2.1 Terms and Definitions

Since the concept of a processor has become increasingly unclear and confusing, it is necessary to clarify and specify some terms.[6] Previously, a processor socket was used to hold one processor chip[7] and appeared to the operating system as one logical processor. Today a processor socket can hold more than one processor chip. Each chip usually has multiple cores. Each core may support multiple threads simultaneously in hardware. It is not clear which of those should be called a processor, and everybody has another opinion on that. Therefore we try to avoid the term processor for hardware and will use the following more specific terms.

A *processor socket* is the foundation on the main board where a *processor package*[8], as delivered by the manufacturer, is installed. An 8-socket system, for example, contains up to 8 processor packages. All the logic inside of a processor package shares the connection to main memory (RAM).
A *processor chip* is one piece of silicon, containing one or more processor cores. Although typically only one chip is placed on a socket (processor package), it is possible that there is more than one chip in a processor package (multi-chip package). A *processor core* is a standalone processing unit, like the ones formerly known as "processor" or "CPU". One of today's cores contains basically the same logic circuits as a CPU previously did. Because an n-core chip consists, coarsely speaking, of n replicated "traditional processors", such a chip is theoretically, memory bandwidth limitations set aside, n times faster than a single-core processor, at least when running a well-scaling parallel program. Several cores inside of one chip may share caches or other resources.

A slightly different approach to offer better performance is *hardware threads* (Intel: *Hyper Threading*). Here, only parts of the circuits are replicated and other parts, usually the computational pipelines, are shared between threads. These threads run different instruction streams in pseudo-parallel mode. The performance gained by this approach depends much on hardware and software. Processor cores not supporting hardware threads can be viewed as having only one thread.

From the operating system's point of view every hardware thread is a *logical processor*. For instance, a computer with 8 sockets, having installed dual-core processors with 2 hardware threads per core, would appear as a 32 processor ("*32-way*") system.[9] As it would be tedious to write "logical processor" or "logical CPU" every time when referring to what the operating system sees as a processor, we will abbreviate that.

Anyway, from the operating system's or software's point of view it does not make a difference whether a multicore or multisocket system is installed.

2.1.1 Non-Uniform Memory Architecture (NUMA)

For performance considerations the architecture of the computer is crucial especially regarding memory connections. All of today's modern multiprocessors have a non-uniform memory access (*NUMA*) architecture: parts of the main memory are directly attached to the processors.

Today, all common *NUMA* computers are actually *cache-coherent NUMA* (or *ccNUMA*) ones: There is special-purpose hardware (or operating system software) to maintain the cache coherence. Thus, the terms *NUMA* and *ccNUMA* are very often used as replacement for each

[6] Unfortunately different vendors use the same terms with various meanings.
[7] A chip is one piece of silicon, often called "die".
[8] Intel calls this a processor
[9] The term "n-way" is used in different ways. For us, n is the number of logical processors which the operating system sees.

other. The future development in computer architectures can lead to a rise of non-cache-coherent NUMA systems. As far as we only have ccNUMA computers, we use ccNUMA and NUMA terms interchangeably.

Each processor can thus directly access those memory banks that are attached to it (*local memory*), while accesses to memory banks attached to the other processors (*remote memory*) will be routed over the system interconnect. Therefore, accesses to local memory are faster than those to remote memory and the difference in speed may be significant. When a process allocates some memory and writes data into it, the default policy is to put the data in memory which is local to the processor first accessing it (*first touch*), as long as there is still such local memory available.

To obtain the whole computing performance, the application's data placement and memory access pattern are crucial. Unfavorable access patterns may degrade the performance of an application considerably. On NUMA computers, arrangements regarding data placement must be done both by programming (accessing the memory the "right" way; see chapter 6.1.2 on page 64) and by launching the application (*Binding*,[10] see chapter 3.1.1 on page 24).

2.2 Configuration of HPC-Cluster

Table 2.3 on page 14 lists the nodes of the HPC-Cluster. The list contains only machines which are dedicated to general usage. In the course of the proceeding implementation of our Integrative Hosting concept (chapter 2.2.1 on page 13) there are a number of hosted machines that also might be used for batch production jobs. These machines are not listed in the table.

The IT Center's part of the HPC-Cluster has an accumulated peak performance of about 325 TFlops. The in 2011 new installed part of the cluster reached rank 32 in the June 2011 Top500 list: http://www.top500.org/list/2011/06/100.

2.2.1 Integrative Hosting

The IT Center offers institutes of the RWTH Aachen University to integrate their computers into the HPC-Cluster, where they will be maintained as part of the cluster. The computers will be installed in the IT Center's computer room where cooling and power is provided. Some institutes choose to share compute resources with others, thus being able to use more machines when the demand is high and giving unused compute cycles to others. Further Information can be found at http://www.itc.rwth-aachen.de/go/id/esvg/ and https://doc.itc.rwth-aachen.de/display/IH/Home

The hosted systems have an additional peak performance of about 150 TFlops (VII/2016).

2.3 The Intel Xeon based Machines

The Intel Xeon "Nehalem" and "Westmere" based Machines provide the main compute capacity in the cluster. "Nehalem" and "Westmere" are generic names, so different (but related) processors types are available. These processors support a wide variety of x86-instruction-extensions up to SSE4.2, nominal clock speed vary from 1.86 GHz to 3.6 GHz, most types can run more than one thread per core (hyperthreading).

"Sandy Bridge" is the codename for a microarchitecture developed by Intel to replace the Nehalem family of cores. The "Sandy Bridge" CPUs has the *Advanced Vector Extensions (AVX)*[11] vectors units with 256-bit instruction set.

On all desribed Intel Xeon CPUs each core can run **two** hardware threads (hyperthreading), however this feature must be activated in BIOS. Hyperthreading is in general **enabled** in HPC-Cluster except for the occasional cases.

[10] Processor/Thread Binding means explicitly enforcing processes or threads to run on certain processor cores, thus preventing the OS scheduler from moving them around.

[11] http://software.intel.com/en-us/intel-isa-extensions, http://en.wikipedia.org/wiki/Advanced_Vector_Extensions

Model	Processor type/ /LSF model name	Sockets/Cores /Threads (total)	Memory Flops/node	Hostname
Bull MPI-S (1097 nodes)	Intel Xeon X5675 "Westmere_EP"	2 / 12 / 24 3.06 GHz	24 GB 146.88 GFlops	linuxbmc0253..1350
Bull MPI-L (244 nodes)	Intel Xeon X5675 "Westmere_EP"	2 / 12 / 24 3.06 GHz	96 GB 146.88 GFlops	linuxbmc0001..0252
Bull SMP-L **s6030** (16 nodes) **s6010** (52 nodes)	Intel Xeon X7550 "Beckton"	4 / 32 / 64 2.0 GHz	256 GB 256 GFlops	linuxbsc001..014 cluster-x,cluster-x2 linuxbsc257..323
Bull SMP-S (266 nodes)	Intel Xeon X7550 "Beckton"	4x4 / 128 / 128 2.00 GHz	64 GB 1024 GFlops	linuxbsc017..252 linuxbsc325..358
Bull SMP-L (BCS) (2 nodes)	Intel Xeon X7550 "Beckton"	4x4 / 128 / 128 2.00 GHz	1 TB 1024 GFlops	linuxbcsc68,69
Bull SMP-XL (BCS) (2 nodes)	Intel Xeon X7550 "Beckton"	4x4 / 128 / 128 2.00 GHz	2 TB 1024 GFlops	linuxbcsc64,65
Bull SMP-D (BCS) (2 nodes)	Intel Xeon X7550	2x4 / 64 / 64 2.00 GHz	256 GB 512 GFlops	cluster cluster-linux

Table 2.3: Node overview (hosted systems are not included). Most up to date list of hardware: https://doc.itc.rwth-aachen.de/display/CC/Hardware+of+the+RWTH+Compute+Cluster

Each Xeon core has a L1 and a L2 cache and all cores of a package (socket) share one common L3 cache. The Level 1 cache consist of 32 KB data cache + 32 KB instruction cache (8-way associative, on chip). Level 2 cache has 256 KB for data and instructions (8-way associative, on chip). Level 3 cache for data and instructions is shared between all cores (16-way associative, on chip) and has different size depending on CPU model.

The Xeon CPUs can dynamically adjust processor voltage and core frequency (Intel Turbo Boost[12] and EIST[13] technologies), however in HPC-Cluster the clock speed of CPUs is fixed in order to stabilize the performance.

Model number	Code-named	Core process	#Cores/ #Threads	Clock Speed	Cache, L1/L2/L3	Instruction Set (top)
X7550	Beckton (Nehalem EX)	45nm	8/16	2.00GHz	32KB+32KB/ 256KB/18MB	SSE4.2
X5675	Westmere EP	32nm	6/12	3.07GHz	32KB+32KB/ 256KB/12MB	SSE4.2
E5-2650	Sandy Bridge-EP	32nm	8/16	2.00GHz	32KB+32KB/ 256KB/20MB	AVX

Table 2.4: Intel Xeon CPUs overview

2.3.1 Memory

Each processor package (Intel just calls it processor) has its own memory controller and is connected to a local part of the main memory. The processors can access the remote memory via Intel's new interconnect called "Quick Path Interconnect" and build a ccNUMA architecture.

[12] *Intel Turbo Boost*, http://www.intel.com/content/www/us/en/architecture-and-technology/turbo-boost/turbo-boost-technology.html

[13] *EIST (Enhanced Intel SpeedStep)*, http://www.intel.com/content/www/us/en/support/processors/000007073.html

On ccNUMA computers, processor binding and memory placement are important to reach the whole available performance (see chapter 2.1.1 on page 12 for details).

The machines are equipped with different amount DDR3 RAM, please refer to table 2.3 on page 14 for details. The total memory bandwidth depends on hardware type, amount of sockets (packages), amount of memory and is different from node type to node type. For example, the Westmere EP nodes reach about 37 GB/s.

2.3.2 Network

The nodes are connected via quad data rate (QDR) InfiniBand and also via Gigabit Ethernet. This QDR InfiniBand achieves an MPI bandwidth of more than 3 GB/s and has a latency of only 3 μs.

2.4 Special Systems: GPU-Cluster

The GPU-cluster comprises 30 nodes each with two GPUs, and one head node with one GPU. In detail, there are 57 NVIDIA Quadro 6000 (Fermi) and 4 NVIDIA K20x (Kepler) GPUs. Furthermore, each node is a two socket Intel Xeon "Westmere" EP (X5650) or "Sandy Bridge" EP (E5-2650) server which contains a total of 12 or 16 cores running at 2.7 or 2.0 GHz and 24GB or 64GB DDR3 memory. All nodes are conntected by QDR InfiniBand. The head node and 24 of the double-GPU nodes are used on weekdays (at daytime) for interactive visualizations by the Virtual Reality Group[14] of the IT Center. During the nighttime and on weekends, they are available for GPU compute batch jobs. The remaining nodes enable, on the one hand, GPU batch computing all-day and, on the other hand, interactive access to GPU hardware to prepare the GPU compute batch jobs and to test and debug GPU applications.

The software environment on the GPU-cluster is now as similar as possible to the one on the RWTH HPC-Cluster. GPU-related software (like NVIDIA's CUDA Toolkit, PGI's Accelerator Model or a CUDA debugger) is additionally provided.

2.4.1 Access to the GPU cluster

2.4.1.1 Access

Every regular cluster user can also directly access the GPU Cluster.

2.4.1.2 Friendly Usage

All GPUs are in the **exclusive process** compute mode, which means that whenever a GPU program is run it gets the whole GPU and does not have to compete with other programs for resources (e.g. GPU memory). Furthermore, it enables several threads in a single process to use both GPUs that are available on each node (cf. e.g. *cudaSetDevice*) instead of being restricted to one thread per device. Therefore you should use them reasonably. Please run long computations in batch mode only and close any debuggers after usage. We also appreciate compute jobs that allow other users to run their jobs once in a while. Thank you!

2.4.1.3 Interactive Mode

You can access the GPU nodes interactively via SSH. If needed, you can also first log into one of our (graphical) front ends and then use SSH to log into one of the interactive GPU nodes.

GPU login nodes are listed in the chapter 2.4.4 on page 18.

Be aware that we have special time windows for certain GPU nodes. The time frames for interactives access are also listed in the chapter 2.4.4 on page 18.

[14] http://www.itc.rwth-aachen.de/vr

2.4.1.4 GPU + MPI

If you would like to test your GPU + MPI program interactively, you can do so on the dialog nodes using our mpiexec wrapper $MPIEXEC (see chapter 6.2.1 on page 69). To get your MPI program run on the GPU machines, you have to explicitly specify their hostnames, otherwise your program will get started on the regular MPI backend which does not have any GPUs. You can do so by providing the following option:

```
-H host1,host2,host3
```

However, you should not use this option with regular MPI machines! You can also provide how many processes shall be run on a host by host basis (see the example below or call `$MPIEXEC -help`). Furthermore, it could be useful to simply specify the same number of processes to be run on all hosts (e.g. if each of your processes uses one GPU). For our interactive mpiexec wrapper use the **-m *ppn*** option where *ppn* is the desired number of processes per node.

Example with 2 processes on each host:

```
$ $MPIEXEC -np 4 -m 2 -H linuxgpud1,linuxgpud2 foobar.exe
```

Example with 1 process on the first host, 3 processes on the second:

```
$ $MPIEXEC -np 4 -H linuxgpud1:1,linuxgpud2:3 foobar.exe
```

2.4.2 GPU Programming Models

2.4.2.1 CUDA

NVIDIA provides the **CUDA C SDK** for programming their GPUs. PGI added a **CUDA Fortran** version, also for NVIDIA GPUs. On the GPU cluster, we recommend that the most-recent CUDA Toolkit Version (`module load cuda`) is used. For compatibility we also provide older versions of the toolkit (`module avail cuda`). Usage information can be found online.[15]

2.4.2.2 OpenCL

OpenCL is an open standard for programming GPUs, CPUs (NVIDIA, AMD, Intel,...) and other device using a C-like API. Usage information can be found online.[16]

2.4.2.3 OpenACC

OpenACC is an industry standard for directive-based programming of accelerators. PGI, Cray and Caps support OpenACC in their commercial compilers. The PGI compiler installed on the cluster can be used to develop OpenACC codes. Usage information can be found online.[17]

2.4.2.4 NVIDIA GPU Computing SDK

NVIDIA provides numerous examples in CUDA C (and OpenCL C). See online[18] on how to get and use them.

2.4.3 GPU Batch Mode

Information about the general usage of LSF can be found in chapter 4.4.1 on page 34.

You can use the **bsub** command to submit jobs:

```
$ bsub [options] command [arguments]
```

We advise you to use a batch script in which the #**BSUB** magic cookie can be used to specify job requirements:

```
$ bsub < gpuDeviceQueryLsf.sh
```

[15] https://doc.itc.rwth-aachen.de/display/CC/CUDA
[16] https://doc.itc.rwth-aachen.de/display/CC/OpenCL
[17] https://doc.itc.rwth-aachen.de/display/CC/OpenACC
[18] https://doc.itc.rwth-aachen.de/display/CC/NVIDIA+GPU+Computing+SDK

You can submit batch jobs for the GPU cluster at any time. However, dependent on the batch mode availability, scheduling and occupancy, it might take a while until your compute job finishes (see chapter 2.4.4 on page 18).

In the following, we differentiate between short test runs on the one hand and real program runs on the other hand.

2.4.3.1 Short test runs (daytime)

Short test runs can be done on a couple of machines which are in batch mode also during daytime. If you would like to test your batch script, add the following:

```
#BSUB -a gpu
```

If you would also like to use MPI, you can combine the requests for using GPU and MPI (please see below for more details on the usage of MPI):

```
#BSUB -a "gpu openmpi"
```

2.4.3.2 Long runs (nighttime, weekend)

Production jobs (i.e. longer runs or performance tests) have to be scheduled on the GPU cluster (nighttime and weekends). Therefore, you have to select the appropriate queue:

```
#BSUB -q gpu
```

You can either put the **-q gpu** option in your batch script file or give it to the bsub command. You will get all requested machines exclusively. BTW: If you accidentally combine **-a gpu** AND **-q gpu**, the **-q gpu** option takes precedence and your job will run during the night on the GPU cluster.

2.4.3.3 Selecting a certain GPU type (Fermi/Kepler)

Since October 2013 there are nodes with two different kinds of GPUs in the cluster. If you do not specify a certain kind, you will get an arbitrary GPU node. That is advantageous if you are not dependent on a certain GPU type because you will get any node that is available (so possibly less waiting time for the job).

If you need a certain GPU type, you have to request it in you batch script with either

```
#BSUB -R fermi
```

or

```
#BSUB -R kepler
```

Please note that in batch mode all (correct working) GPU machines are available, including one node with only *one* GPU attached (linuxgpum1). If you would like to exclude this particular node from your hostlist (e.g. due to the fact that you want to use 2 processes per node and each process uses one GPU), please specify additionally the following (so that you will only get machines that have *two* GPUs):

```
#BSUB -m bull-gpu-om
```

A combination of a certain GPU type with a certain number of GPUs, i.e. Fermi nodes with two GPUs per node, could be requested as well:

```
#BSUB -R fermi
#BSUB -m bull-gpu-om
```

2.4.3.4 Example Scripts

In order to save some trees the example scripts are not included in this document. The example scripts are available on the HPC-Cluster in the $PSRC/pis/LSF/ directory and online at https://doc.itc.rwth-aachen.de/display/CC/GPU+batch+mode.

- Simple GPU Example - Run **deviceQuery** (from NVIDIA SDK) on one device: **$PSRC/pis/LSF/gpuDeviceQueryLsf.sh** or Docuweb[19]

[19] https://doc.itc.rwth-aachen.de/display/CC/GPU+batch+mode#GPUbatchmode-GPUSimple

- MPI GPU Example - Run **deviceQuery** (not a real MPI application!) on 4 nodes (use one device on each: **$PSRC/pis/LSF/gpuMPIExampleLsf.sh** or Docuweb[20]

Since we do not have requestable GPU slots in LSF at the moment, you have to explicitly specify how many processes you would like to have per node (see **ptile** in the script file). This is usually one or two, depending on how you would like to use the GPUs and how many GPUs you would like to use per node. Examples:

- 1 process per node (*ppn*):
  - If you would like to use only one GPU per node;
  - If your process uses both GPUs at the same time, e.g. via cudaSetDevice.
- 2 processes per node (*ppn*):
  - If each process communicates to a single GPU.
- More than 2 processes per node:
  - If you also have processes that do computation on the CPU only. Be aware that our GPUs are set to "exclusive process" mode, which is the reason why no more than one process could use each GPU.

2.4.4 Limitations Within the GPU Cluster

2.4.4.1 Operation modes

The 24 render nodes (+ head node) are used on weekdays (during daytime) for interactive visualizations by the Virtual Reality Group (VR) of IT Centerand are NOT available for GPGPU computations during that period. However, during the night and during the weekends they can be used for GPU compute batch jobs. Furthermore, few nodes run in batch mode the whole day long (see below) for the purpose of executing short batch jobs (e.g. for testing). Several dialogue nodes enable interactive access to the GPU hardware. There the GPU compute batch jobs can be prepared and GPU applications can be tested and debugged. A couple of dialogue nodes (see below) stay in interactive mode the whole day. The others are switched to batch mode during the evening.

Between switch from interactive visualization to batch computation mode each system is rebooted.

- **Interactive Mode**
  dialogue nodes

#nodes	node names	GPU type	operating time
1	linuxgpud1	Fermi	whole day [24/7]
2	linuxgpud[2-3]	Fermi	working days: 7:40 am - 8 pm
1	linuxnvc01	Kepler	whole day [24/7]

- **Batch Mode**
  all nodes (excluding linuxgpud1, linuxnvc01)

#nodes	node names	GPU type	operating time
1	linuxgpud4	Fermi	whole day (short test runs only!)
27	linuxgpud[2-3] linuxgpus[01-24] linuxgpum1	Fermi	working days: 8 pm - 7:30 am weekends: whole day
1	linuxnvc02	Kepler	whole day (short test runs only!)

[20] https://doc.itc.rwth-aachen.de/display/CC/GPU+batch+mode#GPUbatchmode-GPUMPI

2.4.4.2 Exclusive Mode

As the GPUs are set to "exclusive" mode, you will get an error message if you try to run your program on a GPU device that is already in use by another user. If possible, simply choose another device number for execution of your program. For CUDA applications do not explicitly set the device number in your program (e.g. with a call to cudaSetDevice) if not strictly necessary. Then your program will automatically use any available GPU device (if there is one). However, if you set a specific device number, you will have to wait until that device becomes available (and try it again).

Keep in mind that debugging sessions always run on device *0* (default) and therefore you might exhibit the same problem there.

If you would like to run on a certain GPU (e.g. debugging a non-default device), you may mask certain GPUs by setting a environment variable:

```
$ export CUDA_VISIBLE_DEVICES=<GPU ID>
```

2.4.4.3 X Configuration

We have different **X** configurations on different GPU nodes. This may impact your programs in certain situations. To find out about the current setup use **nvidia-smi** and look for *"Disp. On"* or *"Disp. Off"*.

Current settings:

- Login nodes: An X session runs on the display of GPU *1*.
  On GPU *0* is the display mode disabled.
- Batch nodes: Display mode is disabled on both GPUs

2.5 Special Systems: Intel Xeon Phi Cluster

Note: For latest info take a look at this wiki:
https://doc.itc.rwth-aachen.de/display/CC/Intel+Xeon+Phi+cluster

The Intel Xeon Phi Cluster comprises 9 nodes each with two Intel Xeon Phi coprocessors (MIC). One of these nodes is used as front end and the other 8 nodes run in batch mode. More specifically, each node consists of two 60-core MICs running at 1.05 GHz with 8 GB of memory each and two 8-core Intel Xeon E5-2650 (codename **Sandy Bridge**) CPUs running at 2.0 GHz with 32 GB of main memory.

2.5.1 Access to the Intel Xeon Phi cluster

2.5.1.1 Access

To get access to this system your account has to be authorized first. If you are interested in using the machine, please write to servicedesk@itc.rwth-aachen.de with your user ID and let us know that you would like to use the Intel Xeon Phi cluster.

2.5.1.2 Interactive Mode

The front end system can be used interactively. It should only be used for programming, debugging, preparation and post-processing of batch jobs. It is not allowed to run production jobs on it.

Login from Linux is possible via Secure Shell (ssh). For example:

```
$ ssh cluster-phi.rz.rwth-aachen.de
```

From the front end you can then login to the coprocessors:

```
$ ssh cluster-phi-mic0
```

or

```
$ ssh cluster-phi-mic1
```

Please note that the host system **cluster-phi** is only accessible from our normal dialog systems, therefore you should first log into one of them and then use SSH to log into **cluster-phi**. The coprocessors are only accessible from their host system.

Like every other front end system in the HPC-Cluster, **cluster-phi** is rebooted every Monday at 6 am.

Registered users can access their $HOME and $WORK directories at the coprocessors under /home/<userid> and /work/<userid>.

Due to the fact that programs using the Intel Language Extension for Offload (LEO) are started under a special user ID (**micuser**), file IO within an offloaded region is not allowed.

2.5.2 Programming Models

Three different programming models can be used. Most programs can run *natively* on the coprocessor. Also, parallel regions of the code can be offloaded using the *Intel Language Extension for Offload (LEO)*. Finally, *Intel MPI* can be used to send messages between processes running on the hosts and on the coprocessors.

2.5.2.1 Native Execution

Cross-compiled programs using OpenMP, Intel Threading Building Blocks (TBB) or Intel Cilk Plus can run natively on the coprocessor.

To prepare an application for native execution, the Intel compiler on the host must be instructed to cross-compile the application for the coprocessor (e.g. by adding the **-mmic** switch to your makefile). Once the program executable is properly built, you can log into the coprocessor and start the program in the normal way, e.g.:

```
$  ssh cluster-phi-mic1
$  cd /path/to/dir
$  ./a.out
```

The LD_LIBRARY_PATH and the PATH environment variables will be set automatically.

2.5.2.2 Language Extension for Offload (LEO)

The Intel Language Extension for Offload offers a set of pragmas and keywords that can be used to tag code regions for execution on the coprocessor. Programmers have additional control over data transfer by clauses that can be added to the offload pragmas. One advantage of the LEO model compared to other offload programming models is that the code inside the offloaded region may contain arbitrary code and is not restricted to certain types of constructs. The code may contain any number of function calls and it can also use any parallel programming model supported (e.g. OpenMP, Fortran's do concurrent, POSIX Threads, Intel TBB, Intel Cilk Plus).

2.5.2.3 MPI

An MPI program with host-only ranks may employ LEO in order to utilize the performance of the coprocessors. An MPI program may also run in native mode with ranks on both the processors and the coprocessors. That way MPI can be used for reduction of the parallel layers.

To compile an MPI program on the host, the MPI module must be switched:

```
$ module switch openmpi intelmpi/5.0mic
```

The module defines the following variables:

I_MPI_MIC=enable
I_MPI_MIC_POSTFIX=.mic

After that two different versions of the executable must be build. One with the **-mmic** switch and an added **.mic** suffix to the name of the executable file and one without:

```
$ $MPICC micproc.c -o micproc
$ $MPICC micproc.c -o micproc.mic -mmic
```

In order to start MPI applications over multiple MICs, the interactive $MPIEXEC wrapper can be used. The wrapper is only allowed to start processes on MICs when you are logged in on a MIC-enabled host, e.g. cluster-phi.rz.rwth-aachen.de.

The mpiexec wrapper can be used as usual with dynamic load balancing. In order to distinguish between processes on the host and processes on the MICs, there are 2 different command line parameters, shown in the following examples.

Start 2 processes on the host:

```
$ $MPIEXEC -nph 2 micproc
```

Start 2 processes on the coprocessors:

```
$ $MPIEXEC -npm 2 micproc.mic
```

The parameters can also be used simultaneously like:

```
$ $MPIEXEC -nh 2 -nm 30 micproc
```

Also there is the option to start MPI application on coprocessors and hosts without the load balancing. The value for each host defines the number of processes on this host, NOT the compute slots.

16 processes on the host and 10 processes spanning both coprocessors:

```
$ $MPIEXEC -H cluster-phi:16,cluster-phi-mic0:10,cluster-phi-mic1:10 <exec>
```

2.5.2.4 Batch Mode

Information about the general usage of LSF can be found in chapter 4.4.1 on page 34. You can use the **bsub** command to submit jobs:

```
$ bsub [options] command [arguments]
```

We advise you to use a batch script in which the #**BSUB** magic cookie can be used to specify job requirements:

```
$ bsub < jobscript.sh
```

Please note that the coprocessor(s) will be rebooted for every batch job, therefore it could take some time before your application starts and you can see any output from **bpeek**. For general information on job submission please refer to chapter 4.4.1 on page 34.

To submit a job for the Intel Xeon Phi's you have to put

```
#BSUB -a phi
```

in your submission script. Furthermore, you have to specify a special job description parameter that determines the job type (offload (LEO), native or MPI job):

- For Language Extension for Offload (LEO), put
  `#BSUB -Jd "leo=a;b"`
  where:
  - **a** is the number of MICs
  - **b** is the number of threads on the MICs
- For native job use
  `#BSUB -Jd "native"`
- For MPI specify
  `#BSUB -Jd "hosts=a;b;mics=c;d""`
  where:
  - **a** is the number of hosts
  - **b** is a comma separated list of MPI processes on the hosts
  - **c** is the number of MICs
  - **d** is a comma separated list of MPI processes on the MICs

2.5.2.5 Example Scripts

In order to save some trees the example scripts are not included in this document. The example scripts are available on the HPC-Cluster in the $PSRC/pis/LSF/ directory and online at https://doc.itc.rwth-aachen.de/display/CC/Batch+mode.

- LEO (Offload) Job - **$PSRC/pis/LSF/phi_leo.sh** or Docuweb[21]
- MPI Job - **$PSRC/pis/LSF/phi_mpi.sh** or Docuweb[22]
- Native Job - **$PSRC/pis/LSF/phi_native.sh** or Docuweb[23]

2.5.2.6 Special MPI Job Configurations

If you would like to run all your processes on the MICs only please follow the next example. It shows how to use two MICs with 20 processes on each of them:

```
...
### The number of compute slots must be >= the number of hosts
#BSUB -n 1
...
### Now specify the type of Phi job:
###  "hosts" -> MPI-Job

###  "hosts=a;b;mics=c;d"
###    a: number of hosts
###    b: comma separated list of MPI processes on the ordered hosts
###       !!! you can even specify a "0" for each host !!!
###    c: number of MICs
###    d: comma separated list of MPI processes on the ordered MICs
#BSUB -Jd "hosts=1;0;mics=2;20,20"
...
```

You have to reserve the hosts and each host needs at least one process, otherwise the job will not start.

2.5.2.7 Limitations

At the moment the following limitations are in place:

- We do not guarantee availability of Intel Xeon Phi cluster.
- There is no module system at the coprocessors.
- Only one compiler version (always the default Intel compiler) and one MPI version (intelmpi/*mic) are supported.
- Intel MPI: LSF does not terminate the job after your MPI application has finished. Please use a small run time limit (#BSUB -W) in order to prevent resources from being blocked for extended periods of time. The job will terminate after reaching that limit.
- Offloading is not supported in MPI jobs.
- Our **mpi_bind** script (see chapter 4.4.1 on page 42) does not work for jobs on the Intel Xeon Phi. Please refer to the Intel MPI manual for details on how to enable process binding/pinning.

[21] https://doc.itc.rwth-aachen.de/display/CC/Batch+mode#Batchmode-LEO(Offload)Job
[22] https://doc.itc.rwth-aachen.de/display/CC/Batch+mode#Batchmode-MPIJob
[23] https://doc.itc.rwth-aachen.de/display/CC/Batch+mode#Batchmode-NativeJob

2.5.2.8 Further Information

Introduction to the Intel Xeon Phi in the RWTH Compute Cluster Environment, 2013-08-07: Slides,[24] Exercises.[25]

[24] https://sharepoint.ecampus.rwth-aachen.de/units/rz/HPC/public/Shared Documents/2013-08-07_mic_tutorial.pdf

[25] https://sharepoint.ecampus.rwth-aachen.de/units/rz/HPC/public/Shared Documents/2013-08-07_ex_phi.tar.gz

3 Operating Systems

Today we are running one single operating systems on the machines of the HPC-Cluster at the RWTH Aachen University: Linux (see chapter 3.1 on page 24).

3.1 Linux

Linux is a UNIX-like operating system. We are running the 64-bit version of Scientific Linux (SL), with support for 32-bit binaries, on our systems. Scientific Linux is a binary-compatible clone of RedHat Enterprise Linux (RHEL).

The Scientific Linux release is displayed by the command:

```
$ cat /etc/issue
```

The Linux kernel version can be printed with the command

```
$ uname -r
```

3.1.1 Processor Binding

Note: The usage of user-defined binding may destroy the performance of other jobs running on the same machine. Thus, the usage of user-defined binding is only allowed in batch mode, if cluster nodes are reserved exclusively. Feel free to contact us if you need help with binding issues.

During the runtime of a program, it could happen (and it is most likely) that the scheduler of the operating system decides to move a process or thread from one CPU to another in order to try to improve the load balance among all CPUs of a single node. The higher the system load is, the higher is the probability of processes or threads moving around. In an optimal case this should not happen because, according to our batch job scheduling strategy, the batch job scheduler takes care not to overload the nodes. Nevertheless, operating systems sometimes do not schedule processors in an optimal manner for HPC applications. This may decrease performance considerably because cache contents may be lost and pages may reside on a remote memory location where they have been first touched. This is particularly disadvantageous on NUMA systems because it is very likely that after several movement many of the data accesses will be remote, thus incurring higher latency. *Processor Binding* means that a user explicitly enforces processes or threads to run on certain processor cores, thus preventing the OS scheduler from moving them around.

On Linux you can restrict the set of processors on which the operating system scheduler may run a certain process (in other words, the process is *bound* to those processors). This property is called the *CPU affinity* of a process. The command **taskset** allows you to specify the CPU affinity of a process prior to its launch and also to change the CPU affinity of a running process.

You can get the list of available processors on a system by entering

```
$ cat /proc/cpuinfo
```

The following examples show the usage of **taskset**. We use the more convenient option **-c** to set the affinity with a CPU list (e.g. 0,5,7,9-11) instead of the old-style bitmasks.

```
$ $PSRC/pex/321|| taskset -c 0,3 a.out
```

You can also retrieve the CPU affinity of an existing task:

```
$ taskset -c -p pid
```

Or set it for a running program:

```
$ taskset -c -p list pid
```

Note that the Linux scheduler also supports natural CPU affinity: the scheduler attempts to keep processes on the same CPU as long as this seems beneficial for system performance.

Therefore, enforcing a specific CPU affinity is useful only in certain situations.

If using the Intel compilers with OpenMP programs, processor binding of the threads can also be done with the KMP_AFFINITY environment variable (see chapter 6.1.3 on page 64). Similar environment variables for the Oracle compiler are described in section 6.1.4 on page 65 and for the GCC compiler in section 6.1.5 on page 67.

The MPI vendors also offer binding functionality in their MPI implementations; please refer to the documentation.

Furthermore we offer the R_Lib library. It contains portable functions to bind processes and threads (see 9.8 on page 92 for detailed information).

3.2 Addressing Modes

Programs can be compiled and linked either in 32-bit mode or in 64-bit mode. This affects memory addressing, the usage of 32- or 64-bit pointers, but has no influence on the capacity or precision of floating point numbers (4- or 8-byte real numbers). Programs requiring more than 4 GB of memory have to use the 64-bit addressing mode. You have to specify the addressing mode at compile and link[26] time. On Linux the default mode is 64-bit.

Note: *long int* data and pointers in C/C++ programs are stored with 8 bytes when using 64-bit addressing mode, thus being able to hold larger numbers. The example program shown below in listing 1 on page 25 prints out "4" twice in the 32-bit mode:

```
$ $CC $FLAGS_ARCH32 $PSRC/pis/addressingModes.c; ./a.out
```

and "8" twice in the 64-bit mode:

```
$ $CC $FLAGS_ARCH64 $PSRC/pis/addressingModes.c; ./a.out
```

Listing 1: Show length of pointers and long integer variables

```
1  #include <stdio.h>
2  int main (int argc, char **argv)
3  {
4      int* p;
5      long int li;
6      printf ("%lu %lu\n",
7              (unsigned long int)sizeof(p),
8              (unsigned long int)sizeof(li));
9      return 0;
10 }
```

[26] Note the environment variables $FLAGS_ARCH64 and $FLAGS_ARCH32 which are set for compilers by the module system (see chapter 5.2 on page 45).

4 The RWTH Environment

4.1 Login to Linux

4.1.1 Command line Login

The secure shell **ssh** is used to log into the Linux systems. Usually **ssh** is installed by default on Linux and Unix systems. Therefore you can log into the cluster from a *local*[27] Unix or Linux machine using the command

```
$ ssh -l username cluster.rz.rwth-aachen.de
```

For data transfers use the **scp** command.

A list of front end nodes you can log into is given in table 1.1 on page 8.

To log into the Linux cluster from a *Windows* machine, you need to have an SSH client installed. Such a client is provided for example by the cygwin (http://www.cygwin.com) environment, which is free to use. Other software is available under different licenses, for example PuTTY (http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html) or SSH Client for Windows (ftp://ftp.cert.dfn.de/pub/tools/net/ssh).

The SSH Client for Windows provides a graphical file manager for copying files to and from the cluster as well (see chapter 4.2.1 on page 29); another tool providing such functionality is WinSCP (http://winscp.net/eng/docs/start).

If you log in over a weak network connection you are welcome to use the **screen** program, which is a full-screen CLI window manager. Even if the connection breaks down, your session will be still alive and you will be able to reconnect to it after you logged in again.[28]

4.1.2 Graphical Login

If you need graphical user interface (GUI), you can use the **X Window System**.[29] The forwarding of GUI windows using the X Window System is possible when logged in in any Linux front end(see table 1.1 on page 8).

When logging from Linux or Unix you usually do not need to install additional packages. Depending on your local configuration it may be necessary to use the **-X**[30] flag of the **ssh** command to enable the forwarding of graphical programs.

On Windows, to enable the forwarding of graphical programs a **X server** on your local computer must run, e.g. the **cygwin** http://www.cygwin.com/ contains one. Another X server for Windows is **Xming**: http://sourceforge.net/projects/xming/

However, the *X Window System* can be quite slow over weak network connection, and in case of a temporary network failure your program will die and the session is lost. In order to prevent this we offer special front ends capable to run the **FastX** software (see table 1.1 on page 8). These sofware packages allow you to run remote X11 sessions even across low-bandwidth network connections, as well as reconnecting to running sessions.

4.1.2.1 FastX

We provide the software FastX from *StarNet Communications* http://www.starnet.com/ for running remote desktop sessions. You have the choice to use either a desktop client software or to start a session from inside a browser window (which does not achieve the performance of the desktop client though).

[27] To login from *outside* of the RWTH network you will need VPN: https://doc.itc.rwth-aachen.de/display/VPN

[28] The **screen** command is known to lose the value of the $LD_LIBRARY_PATH environment variable just after it started. In order to fix it we changed the global initialization file */etc/screenrc*. Be aware of this if you are using your own **screen** initialization file *$HOME/.screenrc*.

[29] http://en.wikipedia.org/wiki/X_Window_System

[30] If your X11 application is not running properly try to use the (less secure) **-Y** option instead of **-X**.

Native desktop clients are available for

- Windows https://cluster-x.rz.rwth-aachen.de:3443/downloads/setup.exe
- Windows (non-root) https://cluster-x.rz.rwth-aachen.de:3443/downloads/setup_nonroot.exe
- Linux (32Bit) https://cluster-x.rz.rwth-aachen.de:3443/downloads/fastx-32.tar.gz
- Linux (64Bit) https://cluster-x.rz.rwth-aachen.de:3443/downloads/fastx-64.tar.gz
- MacOS https://cluster-x.rz.rwth-aachen.de:3443/downloads/FastX.dmg

The vendor documentation[31] describes in detail how to configure and use the desktop client. You may use one of the dedicated servers (see table 1.1 on page 8) to connect your FastX session.

Choose *ssh* as the connection method.

Browser based client: To use the browser based client follow one of the following links:

- http://cluster-x.rz.rwth-aachen.de:3000/
- http://cluster-x2.rz.rwth-aachen.de:3000/

You will then get redirected to a SSL-secured connection on port 3443 where you can login with your usual HPC account.

More information can be found in the vendor documentation.[32]

Further notes: Currently, solely the desktop environments MATE and XFCE can be started. KDE as well as GNOME tend to consume many hardware resources and are therefore not available for selection.

Note that the above links and FastX work only from inside the RWTH network. From an external network you can use a VPN connection to get an RWTH network address.

4.1.3 Kerberos

Kerberos[33] is a computer network authentication protocol. It is not extensively used in HPC-Cluster but became more and more important.

A Kerberos *ticket* is needed to get acess to any services using Kerberos. It will be granted automatically if you are logged in using ssh, unless you are using a self-made ssh user key. This ticket has limited lifetime (typically 24h).

Note: You can obtain a valid ticket by calling the command **kinit**. This utility will ask for your cluster password and will create a ticket valid for another 24 hours.

Note: With the **klist** utility you can check your Kerberos ticket.

4.1.4 cgroups

Control Groups (cgroups)[34] provide a mechanism which can be used for partitioning resources between tasks for resource tracking purposes on Linux.

We have now activated the cgroups memory subsystem on a range of HPC-Clusterfront ends. This means that there are now limits on how much physical memory and swap space a single user can expend. Current usage and limits are shown by the command

```
$ memquota
```

The cgroups CPU subsystem is also active on the front ends and ensure the availability of minimal CPU time for all users.

[31] http://www.starnet.com/xwin32kb/fastx-desktop-client/
[32] http://www.starnet.com/xwin32kb/fastx-browser-client/
[33] Kerberos RFC: http://tools.ietf.org/html/rfc4120,
Kerberos on Wikipedia: http://en.wikipedia.org/wiki/Kerberos_(protocol)
[34] http://www.kernel.org/doc/Documentation/cgroups/cgroups.txt

4.2 The RWTH User File Management

Every user owns directories on shared file systems (**home**, **work** and **hpcwork** directories), a scratch directory (**tmp**) and is also welcome to use the **archive** service.

Permanent, long-term data has to be stored in the **home** directory **$HOME=/home/*username***

Note: Please do not use the home directory for significant amounts of short-lived data because repeated writing and removing creates load on the back-up system. Please use **work** or **tmp** file systems for short-living files.

The $HOME data will be backed up in regular intervals. We offer *snapshots* of the home directory so that older versions of accidentally erased or modified files can be accessed, without requesting a restore from the backup. The snapshots are located in each directory in the **.snapshot/.snapshot/*name*** subdirectory, where the *name* depends on the snapshot interval rule and is *hourly*, *nightly* or *weekly* followed by a number. Zero is the most recent snapshot, higher numbers are older ones. Alternativly, you can access the snapshot of your home directory with the environment variable $HOME_SNAPSHOT.

The date of a snapshot is saved in the access time of these directories and can be shown for example with the command

```
$ ls -ltru
```

The **work** file system is accessible as **$WORK=/work/*username*** and is intended for medium-term data like intermediate compute results, and especially for sharing the data with the Windows part of the cluster.

As far as you do not depend on sharing the data between Linux and Windows, you should use the **hpcwork** instead of the work direktory.

Note: There is no backup of the $WORK file system!

Do not store any non-reproducible or non-recomputable data, like source code or input data, on the **work** file system!

Note: As long as there is some free volume, we will offer the *snapshots* on the **work** file system in the same way as they are provided on the **home** filesystem. Silent removement of the snapshots in the **work** file system stays reserved.

The **hpcwork** file system is accessible as **$HPCWORK=/hpcwork/*username*** from the Linux part of the HPC-Cluster and is currently *not* available from the Windows part. This high-performance Lustre file system (see chapter 4.2.2 on page 29) is intended for very large data consisting of not so many big (and huge) files. You are welcome to use this file system instead of the $WORK file system.

There is no backup of the $HPCWORK file system!

Note: The **hpcwork** filesystem is also available from the old (legacy, non-Bull) part of the HPC-Cluster but with limited speed only, so do not run computations with huge amount of input/output on the old machines.

Note: The constellation of the $WORK and the $HPCWORK (Lustre) file systems may be subject to change. Stay tuned!

Note: Every user has limited space (quota) on file systems. Use the **quota** command to

figure out how much of your space is already used and how much is still available. Due to the amount of HPC-Cluster users the quota in the **home** directory is rather small in order to reduce the total storage requirement. If you need more space or files, please contact us.

Note: In addition to the space, also the number of files is limited.

Note: The Lustre quotas on **hpcwork** are *group* quotas (this may have impact to very old HPC-Clusteraccounts). The number of available files is rather small by contrast with the **home** and **work** filesystems.

Furthermore, the **tmp** directory is available for session-related temporary (scratch) data. Use the **$TMP** environment variable on the Linux command line. The directory will be automatically created before and deleted after a terminal session or batch job. Each terminal session and each computer has its own tmp directory, so data sharing is not possible this way! Usually, the tmp file system is mapped onto a local hard disk which provides fast storage. Especially the number of file operations may be many times higher than on network-mounted work and home file systems. However, the size of the tmp file system is rather small and depends on the hardware platform.

Some computers[35] have a network-mounted **tmp** file system because they do not have sufficient local disk space.

We also offer an **archive** service to store large long-term data, e.g. simulation result files, for future use. A description how to use the archive service can be found at this page:
https://doc.itc.rwth-aachen.de/display/ARC

4.2.1 Transferring Files to the Cluster

To transfer files[36] to the *Linux* cluster the secure copy command **scp** on Unix or Linux, or the *Secure File Transfer Client* on Windows, can be used. Usually the latter is located in *"Start"* → *"Programs"* → *"SSH Secure Shell"* → *"Secure File Transfer Client"*, if installed. To connect to a system, use the menu *"File"* → *"Quick Connect"*. Enter the host name and user name and select *Connect*. You will get a split window: The left half represents the local computer and the right half the remote system. Files can be exchanged by drag-and-drop. As an alternative to *Secure File Transfer Client*, the *PS-FTP* program can be used, refer to http://www.psftp.de/

4.2.2 Lustre Parallel File System

4.2.2.1 Basics

Lustre is a file system designed for high throughput when working with few large files.

Note: When working with many small files (e.g. source code) the Lustre file system may be many times slower than the ordinary network file systems used for **$HOME**. To the user it is presented as an ordinary file system, mounted on every node of the cluster as **$HPCWORK**.

Note: There is no backup of the Lustre file system!

Programs can perform I/O on the Lustre file system without modification. Nevertheless, if your programs are I/O-intensive, you should consider optimizing them for parallel I/O.

For details on this technology refer to:

- `http://www.whamcloud.com/`

[35] Currently, only the Sun Blade X6275 computers (see table 2.3 on page 14) have a network-mounted **tmp** directory (on a Lustre file system). See 4.2.2 on page 29)

[36] Although the data transfer is possible over any HPC-Clusterfront end, we recommend the usage of the dedicated **cluster-copy**.rz.RWTH-Aachen.DE node.

4.2.2.2 Mental Model

A Lustre setup consists of one metadata server (MDS) and several object storage servers (OSS). The actual contents of a file are stored in chunks on one or more OSSs, while the MDS keeps track of file attributes (name, size, modification time, permissions, ...) as well as which chunks of the file are stored on which OSS.

Lustre achieves its throughput performance by striping the contents of a file across several OSSs, so I/O performance is not that of a single disk or RAID (hundreds of MB/s), but that of all OSSs combined (up to ∼5 GB/s, sequential).

An example: You want to write a 300 MiB file, with a stripe size of 16 MiB (19 chunks), across 7 OSSs. Lustre would pick a list of 7 out of all available OSSs. Then your program would send chunks directly to each OSS like this:

OSS:	1	2	3	4	5	6	7
Chunks:	1	2	3	4	5	6	7
	8	9	10	11	12	13	14
	15	16	17	18	19		

So when your program writes this file, it can use the bandwidth of all requested OSSs, the write operation finishes sooner, and your program has more time left for computing.

4.2.2.3 Optimization

If your MPI application requires large amounts of disk I/O, you should consider optimizing it for parallel file systems. You can of course use the known POSIX APIs (**fopen**, **fwrite**, **fseek**, ...), but MPI as of version 2.0 offers high-level I/O APIs that allow you to describe whole data structures (matrices, records, ...) and I/O operations across several processes. An MPI implementation may choose to use this high-level information to reorder and combine I/O requests across processes to increase performance. The biggest benefit of MPI's parallel I/O APIs is their convenience for the programmer.

Recommended reading:

- "Using MPI-2". Gropp, Lusk, and Thakus. MIT Press.
  Explains in understandable terms the APIs, how they should be used and why.
- "MPI: A Message-Passing Interface Standard", Version 2.0 and later. Message Passing Interface Forum.
  The reference document. Also contains rationales and advice for the user.

4.2.2.4 Tweaks

The **lfs** utility controls the operation of Lustre. You will be interested in **lfs setstripe** since this command can be used to change the stripe size and stripe count. A directory's parameters are used as defaults whenever you create a new file in it. When used on a file name, an empty file is created with the given parameters. You can safely change these parameters; your data will remain intact.

Please do use sensible values though. Stripe sizes should be multiples of 1 MiB, due to characteristics of the underlying storage system. Values larger than 64 MiB have shown almost no throughput benefit in our tests.

4.2.2.5 Caveats

The availability of our Lustre setup is specified as 95 %, which amounts to 1-2 days of expected downtime per month.

Lustre's weak point is its MDS (metadata server); all file operations also touch the MDS, for updates to a file's metadata. Large numbers of concurrent file operations (e.g. a parallel **make** of the Linux kernel) have reliably resulted in slow down of our Lustre setup.

4.3 Defaults of the RWTH User Environment

The default login shell is the **Z** (**zsh**) shell. Its prompt is symbolized by the dollar sign. With the special "." dot command a shell script is executed as part of the current process ("sourced"). Thus changes made to the variables from within this script affect the current shell, which is the main purpose of initialization scripts.

```
$ .  $PSRC/pex/440
```

For most shells (e.g., bourne shell) you can also use the *source* command:

```
$ source $PSRC/pex/440
```

Environment variables are set with

```
$ export VARIABLE=value
```

This corresponds to the C shell command (the C shell prompt is indicated with a "%" symbol)

```
% setenv VARIABLE value
```

If you prefer to use a different shell, keep in mind to source initialization scripts before you change to your preferred shell or inside of it, otherwise they will run after the shell exits.

```
$ .  init_script
$ exec tcsh
```

If you prefer using a different shell (e.g. bash) as default, please append the following lines at THE END of the *.zshrc* file in your home directory:

```
if [[ -o login ]]; then
        bash; exit
fi
```

4.3.1 Z Shell (zsh) Configuration Files

This section describes how to configure the zsh to your needs.

The user configuration files for the zsh are ~/**.zshenv** and ~/**.zshrc**, which are sourced (in this order) during login. The file ~/**.zshenv** is sourced on *every* execution of a zsh. If you want to initialize something e.g. in scripts that use the zsh to execute, put it in ~/.zshenv. Please be aware that this file is sourced during login, too.

Note: Never use a command which calls a zsh in the ~/.zshenv, as this will cause an endless recursion and you will not be able to login anymore.

Note: Do not write to standard output in ~/.zshenv or you will run into problems using **scp**.

In login mode the file ~/**.zshrc** is also sourced, therefore ~/.zshrc is suited for interactive zsh configuration like setting aliases or setting the look of the prompt. If you want more information, like the actual path in your prompt, export a format string in the environment variable **PS1**. Example:

```
$ export PS1='%n@%m:%~$'
```

This will look like this:

user@cluster:~/directory$

You can find an example **.zshrc** in $PSRC/psr/zshrc.

You can find further information about zsh configuration here:
https://doc.itc.rwth-aachen.de/pages/viewpage.action?pageId=2721075

4.3.2 The Module Package

The **Module package** provides the dynamic modification of the user's environment. Initialization scripts can be loaded and unloaded to alter or set shell environment variables such as $PATH, to choose for example a specific compiler version or use software packages. The need to load modules will be described in the according software sections in this document.

The advantage of the module system is that environment changes can easily be undone by unloading a module. Furthermore dependencies and conflicts between software packages can be easily controlled. Color-coded warning and error messages will be printed if conflicts are detected.

The **module** command is available for the **zsh**, **ksh** and **tcsh** shells. **csh** users should switch to tcsh because it is backward compatible to csh.
Note: **bash** users have to add the line
. /usr/local_host/etc/bashrc
into ~/**.bashrc** to make the module function available.

The most important options are explained in the following. To get help about the module command you can either read the manual page (man module), or type

```
$ module help
```

to get the list of available options. To print a list of available initialization scripts, use

```
$ module avail
```

This list can depend on the platform you are logged in to. The modules are sorted in categories, e.g. CHEMISTRY and DEVELOP. The output may look like the following example, but will usually be much longer.

```
------- /usr/local_rwth/modules/modulefiles/linux/linux64/DEVELOP -------
intel/11.1                          intel/14.0(default)
intel/12.1                          openmpi/1.6.5(default)
intel/13.1                          openmpi/1.6.5mt
```

An available module can be loaded with

```
$ module load modulename
```

This will set all necessary environment variables for the use of the respective software. For example, you can either enter the full name like **intel/11.1** or just **intel**, in which case the default **intel/14.0** will be loaded.

A module that has been loaded before but is no longer needed can be removed by

```
$ module unload modulename
```

If you want to use another version of a software (e.g., another compiler), we *strongly recommend*[37] switching between modules:

```
$ module switch oldmodule newmodule
```

This will unload all modules from bottom up to the *oldmodule*, unload the *oldmodule*, load the *newmodule* and then reload all previously unloaded modules. Due to this procedure the order of the loaded modules is not changed and dependencies will be rechecked. Furthermore some modules adjust their environment variables to match previous loaded modules.

You will get a list of loaded modules with

```
$ module list
```

A short description about the software initialized by a module can be obtained by

```
$ module whatis modulename
```

and a detailed description by

```
$ module help modulename
```

The list of available categories inside of the GLOBAL category can be obtained by

```
$ module avail
```

To find out in which category a module *modulename* is located try

```
$ module apropos modulename
```

If your environment seems to be insane, e.g. the environment variable $LD_LIBRARY_PATH

[37] The loading of another version by unloading and then loading may lead to a broken environment.

is not set properly, try out
```
$ module reload
```

You can add a directory with your own module files with
```
$ module use path
```

By default, only the DEVELOP software category module is loaded, to keep the available modules clearly arranged. For example, if you want to use a chemistry software you need to load the CHEMISTRY category module. After doing that, the list of available modules is longer and you can now load the software modules from that category.

On Linux the Intel compilers and Open MPI implementation are loaded by default.

Note: If you loaded module files in order to compile a program and subsequently logged out and in again, you probably have to load the same module files before running that program. Otherwise, some necessary libraries may not be found at program startup time. The same situation arises when you build your program and then submit it as a batch job: You may need to put the appropriate module commands in the batch script.

Note: We *strongly discourage* the users from loading any modules defaultly in your environment e.g. by adding any **module** commands in the **.zshenv** file. The modification of the standard environment may lead to unpredictable, strong-to-discover behaviour. Instead you can define a module loading script (containig all the needed switches) and source it once at the beginning of any interactive session or batch job.

4.3.3 Self-administration of UNIX groups

Each user account, e.g. *xy123456*, has its own primary UNIX group which accidentally bears the same name *xy123456*. In order to allow each user to manage his group by himself, we provide a tool called **member**. Besides of changing the members of a UNIX group, member can also be used to add further managers for a UNIX group - users that are also allowed to change the list of members of a group. The following authorization rules hold:

- You must be the owner or a manager of a group in order to be allowed to change its members. The owner of group *xy123456* is always the user with the same name *xy123456*.
- You must be the owner of the group in order to be allowed to change its managers.

Some typical use cases are shown below. All commands shown are executed by user *xy123456*, i.e. the owner of group *xy123456*. To print the manual page of member use the following command:
```
$ member -man
```

Add other users to your UNIX group

To add a user *ab65431* to your group *xy123456* use the following command:
```
$ member add ab654321
```

The **member** tool relies on Kerberos to authenticate against our LDAP server. Unless you have already a valid Kerberos ticket (see chapter 4.1.3 on page 27), member will ask for your password in order to get a ticket. Subsequently, you can use member without the need to enter your password again until your Kerberos ticket expires.

Note: It will take some minutes until the change actually becomes active on the system. You can print the members of the group *xy123456* with the command:
```
$ getent group xy123456
```

Note: The user *ab654321* has to log in again in order to become a member of the group *xy123456*. He can print the groups he is a member of using the command
```
$ groups
```

Note: In a remote desktop environment, i.e. FastX, it is usually not sufficient to start a new terminal instance to reflect membership changes of groups. You will have to restart the whole desktop session.

Project accounts and groups
If you have a project account, e.g. *jara9876*, you can add yourself to the list of managers by
```
$ member add -auth jara9876 -g jara9876 -m xy123456
```
Afterwards, you are allowed to add yourself to the group itself:
```
$ member add -g jara9876 xy123456
```
A Unix project group *jara9876* will usually have a corresponding LSF project group *p_jara9876*. Unfortunately, LSF needs to be reconfigured to reflect membership changes. This is done only once every night, so it takes up to 24 hours, until a project account can be used within LSF. You can check if you are already a member of a LSF group by
```
$ bugroup p_jara9876
```

List your groups
Use the following command to list all groups you are manager for:
```
$ member list -m -g '*' | grep $USER | awk -F : '{ print $1 }'
```

4.4 The RWTH Batch Job Administration

A batch system controls the distribution of *tasks* (also called *batch jobs*) to the available machines and the allocation of other resources which are needed for program execution. It ensures that the machines are not overloaded as this would negatively impact system performance. If the requested resources cannot be allocated at the time the user *submits* the job to the system, the batch job is queued and will be executed as soon as resources become available. Please use the batch system for jobs running longer than 15 minutes or requiring many resources in order to reduce load on the front end machines.

4.4.1 The Workload Management System LSF

Batch jobs on our Linux systems are handled by the workload management system IBM Platform LSF. [38]

Note: All information in this chapter may be subject to change, since we are collecting further experiences with LSF in production mode. For latest info take a look at this wiki:
https://doc.itc.rwth-aachen.de/display/CC/Using+the+batch+system

Job Submission For job submission you can use the **bsub** command:
```
$ bsub [options] command [arguments]
```
We advise to use a batch script within which you can use the magic cookie *#BSUB* to specify the job requirements:
```
$ bsub < jobscript.sh
```
Attention: Please note the left < arrow. If you do not use it the job will be submitted, but all resource requests will be ignored, because the *#BSUB* is not interpreted by the workload management. Example scripts can be found in chapter 4.4.1 on page 42.

Job Output (stdout, stderr) The job output (stdout) is written into a file during the runtime of a job. The job error output (stderr) is merged into this file, if no extra option for a stderr file is given.

If the user does not set a name for the output file(s), the LSF system will set it during submission to **output_%J_%I.txt** (located in the working directory of the job), where **%J**

[38] http://www-03.ibm.com/systems/services/platformcomputing/lsf.html

and **%I** are the batch job and the array IDs. Please do not specify the same output file for stdout and stderr files, but just omit the definition of stderr file if you want the output merged with stdout.

The output file(s) are available only after the job is finished. Nevertheless using the command **bpeek** the output of a running job can be displayed as well.

Parameter	Function
`-J <name>`	Job name
`-o <path>`	Standard out (and error if no option `-e <path>` used)
`-e <path>`	Standard error

Table 4.5: Job output options

Mail Dispatching Mail dispatching needs to be explicitly requested via the options shown in the table 4.6 on page 35:

Parameter	Function
`-B`	Send mail when when job is dispatched (starts running)
`-N`	Send mail when job is done
`-u <mailaddress>`	Recepient of mails

Table 4.6: Mail dispatching options

If no mail address is given, the Email is redirected to the mail account defined for the user in the RWTH identity management system system (IdM)[39]. The Email size is restricted to a size of 1024kB.

Job Limits / Resources If your job needs more resources or higher job limits than the preconfigured defaults you need to specify these. Please note that your application will be killed, if it consumes more resources than specified.

Parameter	Function	Default
`-W <runlimit>`	Set the runtime limit in format `[hour:]minute` After the expiration of this time the job will be killed. *Note*: No seconds can be specified	00:15
`-M <memlimit>`	Set the per-process memory limit in MB	512
`-S <stacklimit>`	Set a per-process stack size limit in MB Try to increase this limit, if your application crashed (e.g. OpenMP and Fortran can consume a lot of stack)	10
`-x`	Request node(s) exclusive - please do not use without good reasons (especially do not use for serial jobs)	OFF

Table 4.7: Job resources options

To get an idea how much memory your application needs you can use **memusage**, see chapter 5.10 on page 59. Note that there is less memory per slot available than the naive calculation "memory size / number of slots" may suggest. A part of memory (0.5-2.0 GB) is not accessible at all due to addressing restriction. The operating system also need some memory (up to another gigabytes). In order to use all slots of a machine you should order less memory per process than the naive calculation returns (of course only if your job can run with this memory limit at all).

[39] Selfservice: https://www.rwth-aachen.de/selfservice

Special Resources If you want to submit a job to a specific machine type or a predefined host group you can use the option `-m <hostgroup>`.

The values for `<hostgroup>` can be the host groups you get with the **bhosts** command. A range of recommended host groups[40] are denoted in the table 4.8 on page 36.

Host Group	Architecture	Slots	Memory	Max. Mem.[42]
mpi-s	Westmere EP	12	24 GB	1850 MB
mpi-l	Westmere EP	12	96 GB	7850 MB

Table 4.8: Recommended host groups

More information about the hardware can be found in the chapter 2.2 on page 13.

Compute Units To ensure MPI jobs run on nodes directly connected through a high speed network, so called Compute Units are used. The selection of such a compute unit is done automatically for you, when an MPI job is submitted.

We have defined several compute unit types, see table 4.9 on page 36.

Compute Unit	example name	meaning
`chassis`	C<number>	up to eighteen of the mpi-s and mpi-l machines are combined into one chassis
`rack`	R<number>	up to five chassis are combined into one rack
`mtype`	mpi-s | mpi-l	for different machine types like mpi-s, mpi-l ...

Table 4.9: Compute Units

Using Compute Units you can e.g. tell LSF, that you want all processes of your job to run on *one* chassis. This would be done by selecting

```
#BSUB -R "cu[type=chassis:maxcus=1]"
```

Which means *"I want to run on a chassis* (type=chassis) *and I want to run on max one chassis* (maxcus=1)."

You normally do not want to mix SMP-Nodes and MPI-Nodes in one job, so, if you do not use the *#BSUB -m* option, we set for you:

```
#BSUB -R "cu[type=mtype:maxcus=1]"
```

If you want to know, which machines are in one compute unit, you can use the **bhosts -X <compute unit name>** command.

CPU models If you want to run on a specific CPU-Architecture, you can also ask for a specific model the following way:

```
#BSUB -R "select[model==<modelname>]"
```

As model name you can choose one shown in the second column (LSF model name) of the node overview in table 2.3 on page 14.

HPCWORK (Lustre) availability The HPCWORK file system is based on the Lustre high performance technology. This file system offers huge bandwidth but it is not famous for their stability. The availability goal is 95%, which means some 2 weeks per year of planned downtime in virtually error free environment. Due to fact that Lustre works over InfiniBand (IB), it also is troubled any times when IB is impacted.

[40] *Note*: The hostg roups are subject to change, check the actual stage before submitting.

[42] Max. Mem. means the recommended maximum memory per process, if you want to use all slots of a machine. It is not possible to use more memory per slot, because the operating system and the LSF needs approximately 3% of the total amount of memory.

If your batch job uses the HPCWORK file system you should set this parameter:
`#BSUB -R "select[hpcwork]"`
This will ensure that the job will run on machines with up'n'running Lustre file system.

On some machines (mainly the hardware from pre-Bull installation and some machines from Integrative Hosting) the HPCWORK is connected via ethernet instead of InfiniBand, providing no advantage in terms of speed in comparison to the HOME and WORK file system. If your batch job do a lot of input/output in HPCWORK you should set this parameter:
`#BSUB -R "select[hpcwork_fast]"`
This will ensure that the job will run on machines with a fast connection to the Lustre file system.

Parallel Jobs If you want to run a job in parallel you need to request more compute slots. To submit a parallel job with the specified number of processes use the option `-n <min_proc>[,max_proc]`.

Shared Memory Parallelization Nowadays, shared memory parallelized jobs are usually OpenMP jobs. Nevertheless you can use other shared memory parallelisation paradigms like pthreads in a very similar way.

In order to start a shared memory parallelized job, use
`#BSUB -a openmp`
in your script in addition with the `-n` parameter for the number of threads.

Note: This option will set `-R "span[hosts=1]"` which ensures that you get the requested compute slots on the same host. Furthermore it will set the **OMP_NUM_THREADS** environment variable for OpenMP jobs to the number of threads you specified with `-n`, see example in listing **??** on page **??**.

MPI Parallelization In order to start a MPI program you have to tell LSF how many processes you need and eventually how they should be distributed over the hosts. Additionally you have to specify which MPI you want to use with the option
`#BSUB -a open|intelmpi`
in your job file. Do not forget to switch the module, if you do not use the default MPI (see **??** on page **??**).

To call the **a.out** MPI binary use in your submit script the line
`$MPIEXEC $FLAGS_MPI_BATCH a.out`
The batch system set these environment variables accordingly to your request and used MPI. You can call the MPI program multiple times per batch job, however it is not recommended.

Note: Usage of only *one* MPI library implementation per batch job is supported, so you have to submit discrete jobs for e.g. Open MPI and Intel MPI programs.

Note: Usage of deviant (less than specified) number of processes is currently not supported. Submit a separate batch job for each number of MPI processes you want your program to run with.

Example MPI Jobs can be found in listings **??** on page **??** and **??** on page **??**.

Open MPI The Open MPI is loaded by default. It is tightly integrated within LSF which means that Open MPI and LSF communicate directly. Thus the $FLAGS_MPI_BATCH variable is intentionally left empty. To specify the Open MPI use:
`#BSUB -a openmpi`

Intel MPI In order to get access to Intel MPI you need to specify it and to switch the MPI module:

```
#BSUB -a intelmpi
module switch openmpi intelmpi
```

Hybrid Parallelization Hybrid jobs are those with more than one thread per MPI process.

The Platform LSF built-in mechanism for starting such jobs supports only one single MPI process per *node*, which is mostly insufficient because the sweet-spot often is to start an MPI process per *socket*. A feature request for support of general hybrid jobs is open.

Nevertheless you can start hybrid jobs by the following procedure:

- Request a certain node type, see table 4.8 on page 36
- Request the nodes for exclusive use with `-x`
- Set the number of MPI processes as usually with `-n ...`
- Define the grouping of the MPI processes over the nodes with `-R "span[ptile=...]"`
- Manually set the OMP_NUM_THREADS environment variable to the desired number of threads per process with
  `$ export OMP_NUM_THREADS=...`

Note: For correct function of such jobs, the LSF affinity capabilities (see page 40) must be **disabled**. If the LSF's built-in binding is active, all threads will be pinned to the single slot reserved for the MPI process which is probably not what you want.

Note: For hybrid jobs, the MPI library must provide threading support. See chapter 6.3 on page 72 for details.

Note: The described procedure to start of hybrid jobs is general and can be used for all available node types. For Big SMP (BCS) systems, there is also an alternative way to start the hybrid jobs (see page 41).

Non-MPI Jobs Over Multiple Nodes It is possible to run jobs using more than one node which do *not* use MPI for communication, e.g. some client-server application. In this case, the user has to start (and terminate!) the partial processes on nodes advised by LSF manually. The distribution of slots over machines can be found in environment variables set by LSF, see table 4.15 on page 44. An example script can be found in listing **??** on page **??**. Note that calls for SSH are wrapped in the LSF batch.

Array Jobs Array jobs are the solution for running jobs, which only differ in terms of the input (e.g. running different input files in the same program in the context of parameter study / sensitivity analysis). Essentially the same job will be run repeatedly only differing by an environment variable. The LSF option for array jobs is `-J`. The following example would print out *Job 1 ... Job 10*:

```
$ bsub -J "myArray[1-10]" echo "Job \$LSB_JOBINDEX"
```

The variable $LSB_JOBINDEX contains the index value which can be used to choose input files from a numbered set or as input value directly. See example in listing **??** on page **??**.

Another way would be to have parameter sets stored one per row in a file. The index can be used to select a corresponding row, every time one run of the job is started, e.g. so:

```
INPUTLINE=‘awk "NR==$LSB_JOBINDEX" input.txt‘
echo $INPUTLINE
a.out -input $INPUTLINE
```

Note: Multiple jobs of the same array job can start and run at the same time, the number of concurrently running array jobs can be restricted. Of the the following array job with 100 elements only 10 would run concurrently:

```
$ bsub -J "myArray[1-100]%10" echo "Job \$LSB_JOBINDEX"
```

Environment variables available in array jobs are denoted in the table 4.10 on page 39.

Environment Variable	Description
LSB_JOBINDEX_STEP	Step at which single elements of the job array are defined
LSB_JOBINDEX	Contains the job array index
LSB_JOBINDEX_END	Contains the maximum value of the job array index

Table 4.10: Environment variables in Array Jobs

More details on array jobs can be found in WiKi.[43]

Chain Jobs It is highly recommended to divide long running computations (several days) into smaller parts. It minimizes the risk of loosing computations and reduces the pending time. Such partial computations form a *chain* of batch jobs, in which every successor waits until its predecessor is finished. There are multiple ways to define chain jobs:

- A chain job can be created by submitting an array job with up to 1000 elements and limiting the number of concurrently running subjobs to 1. Example with 4 subjobs:
  `#BSUB -J "ChainJob[1-4]%1`

  Note: The order of the subtasks is not guaranteed.
  The above example could result in 1 - 3 - 4 - 2.

If the execution order is crucial (e.g. in case of different computation stages), you have to define the order explicitly.

- Submit the follow-up job(s) from within a batch job (after the computation). Submitting after the computation ensure the genuine sequence, but will prolong pending times.
- Make the follow-up's start dependent on predecessor's jobs ending using the *job dependencies*[44] feature with the bsub option `-w <condition>`. Besides being very flexible job dependencies are complex and every single dependency has to be defined explicitly.
  Example (the job *second* will not start until the job *first* is is done):

```
$ bsub -J "first" echo "I am FIRST!"
$ bsub -J "second" -w 'done(first)' echo "I have to wait..."
```

When submitting a lot of chain jobs, scripted production is a good idea in order to minimize typos. An example for can be found on the pages[45] of TU Dresden.

Project Options Project Options (e.g. helpful for resource management) are given in the table 4.11 on page 39.

Parameter	Function
`-P <projectname>`	Assign the job to the specified project
`-G <usergroup>`	Associate the job with the specified group for fairshare scheduling

Table 4.11: Project options

[43] http://lsf-manual.itc.rwth-aachen.de/9.1.2/lsf_admin/index.htm?job_array_create.html~main
[44] http://lsf-manual.itc.rwth-aachen.de/9.1.2/lsf_admin/job_dependency.html
[45] https://doc.zih.tu-dresden.de/hpc-wiki/bin/view/Compendium/PlatformLSF?skin=plainjane.nat%2cnat#Chain_Jobs

Integrative Hosting Users taking part in the Integrative Hosting, who are member of a project group, can submit jobs using the bsub option `-P <project group>`. The submission process will check the membership and will conduct additional settings for the job. Further information concerning the Integrative Hosting can be found in chaper 2.2.1 on page 13.

Advanced Reservation An advanced reservation reserves job slots for a specified period of time. By default the user can not do this by his own. In case such an advanced reservation was made for you, use the reservation ticket with `-U <reservation_ID>` submit option.

The command

```
$ brsvs
```

displays all advanced reservations.

Overloading Systems Oversubscription of the slot definition (e.g. usage of hyperthreading) is currently not supported by LSF. However, for shared memory and hybrid jobs, the number of threads can be adjusted by setting the OMP_NUM_THREADS environment variable manually. Do not forget to request the nodes for exclusive usage to prevent disturbance by other jobs possibly running on the same node if you wish to experiment with overloading.

Binding and pinning The Platform LSF built-in capabilities for hardware affinity are currently not used in our environment. Feel free to bind/pin the processes and threads using e.g. the **taskset** command or compiler-specific options. However, if you want to use some affinity options in your batch job, request the nodes for exclusive usage to prevent disturbance by other jobs possibly running on the same node. For an easy vendor independed MPI binding you can use our **mpi_bind** script, see chapter 4.4.1 on page 42.

Big SMP (BCS) systems

The SMP systems consists actually from *four* separate boars, connected together using the proprietary Bull Coherent Switch (BCS) technology, see chapter **??** on page **??**.

Because of the fact that theses systems are kind of special you have to request them explicitly and you are not allowed to run serial or small OpenMP jobs there. We decided to schedule only jobs in the granularity of a board (32 Cores) as the smallest unit. This means that you only should submit jobs with the size of 32, 64, 96 or 128 Threads. For MPI jobs the nodes will be reserved always exclusive, so that you should have a multiple of 128 MPI processes (e.g. 128, 256, 384, ...) to avoid a waste of resources.

Please note that the binding of MPI processes and threads is very important for the performance. For an easy vendor independed MPI binding you can use our **mpi_bind** script, see chapter 4.4.1 on page 42.

In order to submit a job to the BCS queue you have to specify

```
#BSUB -a bcs
```

in your batch script in addition with the `-n` parameter for the number of threads or processes.

- For shared memory (OpenMP) jobs you have to specify

  ```
  #BSUB -a "bcs openmp"
  ```

  To minimize the influence of several jobs on the same node your job will be bound to the needed number of boards (32 cores). The binding script will tell you on which boards your job will run. E.g.

```
...
Binding BCS job...
0,2
...
```

means that your job will run on board `0` and `2`, so that you can use up to 64 threads.

- For MPI jobs you have to specify

```
#BSUB -a "bcs openmpi"
```

or

```
#BSUB -a "bcs intelmpi"
module switch openmpi intelmpi
```

depending on the MPI you want to use.

- For hybrid job you have additionally to specify the `ptile`, which tells LSF how many processes you want to start per host. Depending on the MPI you want to use you have to specify

```
#BSUB -a "bcs openmpi openmp"
#BSUB -n 64
#BSUB -R "span[ptile=16]"
```

or

```
#BSUB -a "bcs intelmpi openmp"
#BSUB -n 64
#BSUB -R "span[ptile=16]"
module switch openmpi intelmpi
```

This will start a job with 64 MPI processes with 16 processes on each node. This means the job will use 64/16=4 BCS nodes in sum. The OMP_NUM_THREADS variable will be set to 128/16=8 automatically.

Note: This way to define hybrid jobs is available on Big SMP (BCS) systems only. On other nodes use the general procedure (see page 38).

The table 4.12 on page 41 give a brief overview of BCS nodes.

Model	Architecture	Slots	Memory	Max. Mem.[47]
SMP-S (BCS)	Beckton (Nehalem EX)	128	256 GB	1950 MB
SMP-L (BCS)	Beckton (Nehalem EX)	128	1 TB	7550 MB
SMP-XL (BCS)	Beckton (Nehalem EX)	128	2 TB	15150 MB

Table 4.12: Available BCS nodes

[47] Max. Mem. means the recommended maximum memory per process, if you want to use all slots of a machine. It is not possible to use more memory per slot, because the operating system and the LSF needs approximately 3% of the total amount of memory.

MPI Binding Script Especially for big SMP machines (like the BCS nodes) the binding of the MPI processes and the threads (e.g. hybrid codes) is very important for the performance of an application. To overcome the lack of functionality in the vendor MPIs and for convenience we provide a binding script in our environment. The script is not designed to get the optimal distribution in *every* situation, but it covers all usual case (e.g. one process per socket). The script makes the following assumptions:

- It is executed within a batch job (some LSF environment variable are needed).
- The job reserved the node(s) exclusively.
- The job does not overload the nodes.
- The OMP_NUM_THREADS variable is set correctly (e.g. for hybrid jobs).

To use this script set **mpi_bind** between the **mpiexec** command and your application **a.out**:

```
$  $MPIEXEC $FLAGS_MPI_BATCH mpi_bind a.out
```

Note, that the threads are not pinned at the moment. If you want to pin them as well you can use the vendor specific environment variables.

Vendor	Environment Variable
Intel	KMP_AFFINITY
Oracle	SUNW_MP_PROCBIND
GNU	GOMP_CPU_AFFINITY
PGI	MP_BLIST

Table 4.13: Pinning: Vendor specific environment variables

In case of the Intel Compiler this could look like this:

```
$ export KMP_AFFINITY=scatter
```

For bug questions please contact the service desk: servicedesk@itc.rwth-aachen.de

Submitting a job with GUI To submit a job with a GUI to the batch system, one needs to add this additional option:

```
#BSUB -XF
```

The **bsub** command will block the terminal and wait until the actual job is dispatched. Once dispatched, the actual command of the job script will be executed (e.g. a GUI program started). The batch job ends when this command is done (e.g. GUI program is closed).

General example of a GUI batch script with a **xterm** terminal (remember: **xterm** is a GUI program) is available on the HPC-Clusterin **$PSRC/pis/LSF/GUI_xterm.sh** file or online at https://doc.itc.rwth-aachen.de/display/CC/Submitting+a+job+with+GUI

Once **xterm** is open you can execute commands in it, especially you can also start other GUI programs.

Instead of starting a GUI program from **xterm** as above you can also directly start it from the batch script, e.g. like described for Intel VTune Amplifier in chapter 8.2.1 on page 82.

Example Scripts In order to save some trees the example scripts are not included in this document. The example scripts are available on the HPC-Cluster in the $PSRC/pis/LSF/ directory and online at https://doc.itc.rwth-aachen.de/display/CC/Example+scripts.

- Serial Job - **$PSRC/pis/LSF/serial_job.sh** or Docuweb[48]

[48] https://doc.itc.rwth-aachen.de/display/CC/Example+scripts#Examplescripts-SerialJob

- Array Job - **$PSRC/pis/LSF/array_job.sh** or Docuweb[49]
- GUI Job (xterm) - **$PSRC/pis/LSF/GUI_xterm.sh** or Docuweb[50]
- Shared-memory (OpenMP) parallelized Job - **$PSRC/pis/LSF/omp_job.sh** or Docuweb[51]
- MPI Jobs
  - Open MPI Example - **$PSRC/pis/LSF/openmpi_job.sh** or Docuweb[52]
  - Intel MPI Example - **$PSRC/pis/LSF/intelmpi_job.sh** or Docuweb[53]
  - Hybrid Example - **$PSRC/pis/LSF/hybrid_job.sh** or Docuweb[54]
- Non-MPI Job over multiple Nodes - **$PSRC/pis/LSF/non-mpi_job.sh** or Docuweb[55]

Some application specific (e.g. Gaussian) examples can be found in the Docuweb.[56]

Job Monitoring You can use the **bjobs** command to display information about jobs:

```
$ bjobs [options] [job_ID]
```

The output prints for example the state, the submission time or the job ID:

```
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
3324    tc53084 RUN   serial     linuxtc02   ib_bull     BURN_CPU_1 Jun 17 18:14
3325    tc53084 PEND  serial     linuxtc02   ib_bull     BURN_CPU_1 Jun 17 18:14
3326    tc53084 RUN   parallel   linuxtc02   12*ib_bull  *RN_CPU_12 Jun 17 18:14
3327    tc53084 PEND  parallel   linuxtc02   12*ib_bull  *RN_CPU_12 Jun 17 18:14
```

Some useful options of the **bjobs** command are denoted in the table 4.14 on page 43. Please note especially the **-p** option: you may get a hint to the reason *why* your job is not starting.

Option	Description
`-l`	Long format - displays detailed information for each job
`-w`	Wide format - displays job information without truncating fields
`-r`	Displays running jobs
`-p`	Displays pending job and the pending reasons
`-s`	Displays suspended jobs and the suspending reason

Table 4.14: Parameters of **bjobs** command

Delete a Job For an already submitted job you can use the **bkill** command to remove it from the batch queue:

```
$ bkill [job_ID]
```

To control an individual job submitted from a job array, specify the command using the job ID of the job array and the index value of the corresponding job. The job ID and index

[49] https://doc.itc.rwth-aachen.de/display/CC/Example+scripts#Examplescripts-ArrayJob
[50] https://doc.itc.rwth-aachen.de/display/CC/Submitting+a+job+with+GUI
[51] https://doc.itc.rwth-aachen.de/display/CC/Example+scripts#Examplescripts-Shared-Memory(OpenMP)ParallelJob
[52] https://doc.itc.rwth-aachen.de/display/CC/Example+scripts#Examplescripts-OpenMPIExample
[53] https://doc.itc.rwth-aachen.de/display/CC/Example+scripts#Examplescripts-IntelMPIExample
[54] https://doc.itc.rwth-aachen.de/display/CC/Example+scripts#Examplescripts-HybridExample
[55] https://doc.itc.rwth-aachen.de/display/CC/Example+scripts#Examplescripts-Non-MPIJobOverMultipleNodesExample
[56] https://doc.itc.rwth-aachen.de/display/CC/Usage+of+software

value must be enclosed in quotes:

```
$ bkill "12345678[5]"
```

If you want to kill all your jobs please use this:

```
$ bkill 0
```

LSF Environment Variables There are several environment variables you might want to use in your submission script, see table 4.15 on page 44

Note: These variables will *not* be interpreted in combination with the magic cookie *#BSUB* in the submission script.

Environment Variable	Description
LSB_JOBNAME	The name of the job
LSB_JOBID	The job ID assigned by LSF
LSB_JOBINDEX	The job array index
LSB_JOBINDEX_STEP	Step at which single elements of the job array are defined
LSB_JOBINDEX_END	Contains the maximum value of the job array index
LSB_HOSTS	The list of hosts selected by LSF to run the job
LSB_MCPU_HOSTS	The list of the hosts and the number of CPUs used
LSB_DJOB_HOSTFILE	Path to the hostfile
LSB_DJOB_NUMPROC	The number of slots allocated to the job

Table 4.15: LSF environment variables

Further Information More documentation on Platform LSF is available here: http://lsf-manual.itc.rwth-aachen.de/

Also, there is a man page for each LSF command.

4.5 Project-based management of the cluster resources

The HPC-Cluster is an expensive and valuable but limited resource. In order to secure the fairness of use and the quality of the scientific output, we established the JARA-HPC Partition since spring 2012, and introduced the general Project Based Management of the whole HPC-Cluster starting September 1st 2014.

TBD.

Missed chapters:

- Project-based management of the cluster resources https://doc.itc.rwth-aachen.de/display/CC/Projektbewirtschaftung
- JARA-HPC Partition https://doc.itc.rwth-aachen.de/display/CC/Using+the+JARA-HPC+partition
- r_batch_usage https://doc.itc.rwth-aachen.de/display/CC/Accounting+information+with+r_batch_usage

5 Programming / Serial Tuning

5.1 Introduction

The basic tool in programming is the compiler, which translates the program source to executable machine code. However, not every compiler is available for the provided operating systems.

On the **Linux** operating system the freely available GNU/GCC[57] compilers are the somewhat "natural" choice. Code generated by these compilers usually performs acceptably on the cluster nodes. Since version 4.2 the GCC compilers offer support for shared memory parallelization with OpenMP. Since version 4 of the GNU compiler suite a FORTRAN 95 compiler – *gfortran* – is available. Code generated by the old *g77* FORTRAN compiler typically does not perform well, so gfortran is recommended.

To achieve the best possible performance on our HPC-Cluster, we recommend using the Intel compilers. The Intel compiler family in version 11.1 now provides the default FORTRAN/C/C++/ compilers on our Linux machines. Although the Intel compilers in general generate very efficient code, it can be expected that AMD's processors are not the main focus of the Intel compiler team. As alternatives, the Oracle Studio compilers and PGI compilers are available on Linux, too. Depending on the code, they may offer better performance than the Intel compilers.

The Intel compiler offers interesting features and tools for OpenMP programmers (see chapter 6.1.3 on page 64 and 7.4.2 on page 78). The Oracle compiler offers comparable tools (see chapter 7.4.1 on page 77).

A word of caution: As there is an almost unlimited number of possible combinations of compilers and libraries and also the two addressing modes, 32- and 64-bit, we expect that there will be problems with incompatibilities, especially when mixing C++ compilers.

5.2 General Hints for Compiler and Linker Usage

To access non-default compilers you have to load the appropriate module file.[58] You can then access the compilers by their original name, e.g. g++, gcc, gfortran, or via the environment variables $CXX, $CC, or $FC. However, when loading more than one compiler module, you have to be aware that the environment variables point to the *last* compiler loaded.

For convenient switching between compilers, we added environment variables for the most important compiler flags. These variables can be used to write a generic makefile that compiles with any loadable compiler. The offered variables are listed below. Values for different compilers are listed in tables 5.16 on page 46 and 6.20 on page 63.

- $FC, $CC, $CXX – a variable containing the appropriate compiler name.
- $FLAGS_DEBUG – enables debug information.
- $FLAGS_FAST – includes the options which usually offer good performance. For many compilers this will be the **-fast** option. But beware of possible incompatibility of binaries, especially with older hardware.
- $FLAGS_FAST_NO_FPOPT – equally to FAST, but disallows any floating point optimizations which will have an impact on rounding errors.
- $FLAGS_ARCH32, $FLAGS_ARCH64 – builds 32 or 64 bit executables or libraries.
- $FLAGS_AUTOPAR – enable auto-parallelization, if supported by the compiler.
- $FLAGS_OPENMP – enables OpenMP support, if supported by the compiler.

[57] GCC, the GNU Compiler Collection: http://gcc.gnu.org/
[58] see chapter 4.3.2 on page 31.

- $FLAGS_RPATH – contains a set of directories (addicted to loaded modules) to add to the runtime library search path of the binary, with a compiler-specific command (according to the last loaded compiler) to pass these paths to the linker.[59]

In order to be able to mix different compilers all these variables (except $FLAGS_RPATH) also exist with the compiler's name in the variable name, such as $GCC_CXX or $FLAGS_GCC_FAST.
Example:

```
$ $PSRC/pex/520|| $CXX $FLAGS_FAST $FLAGS_ARCH64 $FLAGS_OPENMP $PSRC/cpop/pi.cpp
```

The makefiles of the example programs also use these variables (see chapter 1.3 on page 10 for further advice on using these examples).

Flag ↓ Compiler →	Oracle	Intel	GCC
$FLAGS_DEBUG	-g | -g0	-g	-g
$FLAGS_FAST	-fast	-axAVX,SSE4.2,SSE4.1 -O3 -ip -fp-model fast=2	-O3 -ffast-math
$FLAGS_FAST_NO_FPOPT	-fast -fsimple=0	-axAVX,SSE4.2,SSE4.1 -O3 -ip -fp-model precise	-O3
$FLAGS_ARCH32|64	-m32 | -m64	-m32 | -m64	-m32 | -m64

Table 5.16: Compiler options overview

In general we strongly recommend using the same flags for both compiling and linking. Otherwise the program may not run correctly or linking may fail.

The order of the command line options while compiling and linking does matter.

The rightmost compiler option, in the command line, takes precedence over the ones on the left, e.g. **cc ... -O3 -O2**. In this example the optimization flag O3 is overwritten by O2. Special care has to be taken if macros like **-fast** are used because they may overwrite other options unintentionally. Therefore it is advisable to enter macro options at the beginning of the command line.

If you get unresolved symbols while linking, this may be caused by a wrong order of libraries. If a library xxx uses symbols from the library yyy, the library yyy has to be right of xxx in the command line, e.g. **ld ... -lxxx -lyyy**.

The search path for header files is extended with the **-I*directory*** option and the library search path with the **-L*directory*** option.

The environment variable LD_LIBRARY_PATH specifies the search path where the program loader looks for shared libraries. Some compile time linkers (e.g., the Oracle linker) also use this variable while linking, but the GNU linker does not.

Consider the static linking of libraries. This will generate a larger executable, which is however a lot more portable. Especially on Linux the static linking of libraries may be a good idea since every distribution has slightly different library versions which may not be compatible with each other.

5.3 Tuning Hints

There are some excellent books covering tuning application topics:

- G. Hager and G. Wellein: Introduction to High Performance Computing for Scientists and Engineers. CRC Computation Science Series, 2010, ISBN: 978-1-4398-1192-4

[59] If linked with this option, the binary "knows" at runtime where its libraries are located and is thus independent of which modules are loaded at the runtime.

- J. Hennessy and D. Patterson: Computer Architecture. A Quantitative Approach. Morgan Kaufmann Publishers, Elsevier, 2011, ISBN: 978-0123838728

Contiguous memory access is crucial for reducing cache and TLB misses. This has a direct impact on the addressing of multidimensional fields or structures. FORTRAN arrays should therefore be accessed by varying the leftmost indices most quickly and C and C++ arrays with rightmost indices. When using structures, all structure components should be processed in quick succession. This can frequently be achieved with *loop interchange*.

The limited memory bandwidth of processors can be a severe bottleneck for scientific applications. With *prefetching* data can be loaded prior to the usage. This will help reducing the gap between the processor speed and the time it takes to fetch data from memory. Such a prefetch mechanism can be supported automatically by hardware and software but also by explicitly adding prefetch directives (FORTRAN) or function calls in C and C++.

The re-use of cache contents is very important in order to reduce the number of memory accesses. If possible, blocked algorithms should be used, perhaps from one of the optimized numerical libraries described in chapter 9 on page 88.

Cache behavior of programs can be improved frequently by *loop fission* (=*loop splitting*), *loop fusion* (=*loop collapsing*, *loop unrolling*, *loop blocking*, *strip mining*), and combinations of these methods. Conflicts caused by the mapping of storage addresses to the same cache addresses (*false sharing*) can be eased by the creation of buffer areas (*padding*).

The compiler optimization can be improved by integrating frequently called small subroutines into the calling subroutines (*inlining*). This will not only eliminate the cost of a function call, but also give the compiler more visibility into the nature of the operations performed, thereby increasing the chances of generating more efficient code.

Consider the following general program tuning hints:

- Turn on high optimization while compiling. The use of $FLAGS_FAST options may be a good starting point. However keep in mind that optimization may change rounding errors of floating point calculations. You may want to use the variables supplied by the compiler modules. An optimized program runs typically 3 to 10 times faster than the non-optimized one.

- Try another compiler. The ability of different compilers to generate efficient executables varies. The runtime differences are often between 10% and 30%.

- Write efficient code that can be optimized by the compiler. We offer a lot of materials (videos, presentations, talks, tutorials etc.) that are a good introduction into this topic, please refer to
  https://sharepoint.ecampus.rwth-aachen.de/units/rz/HPC/public/Lists/Presentations and Training Material/Events.aspx

- Try to perform as little input and output as possible and bundle it into larger chunks.

- Try to allocate big chunks of memory instead of many small pieces, e.g. use arrays instead of linked lists, if possible.

- Access memory continuously in order to reduce cache and TLB misses. This especially affects multi-dimensional arrays and structures. In particular, note the difference between FORTRAN and C/C++ in the arrangement of arrays! Tools like Intel VTune Amplifier (chapter 8.2.1 on page 82) or Oracle Sampling Collector and Performance Analyzer (chapter 8.1.1 on page 79 and 8.1.3 on page 81) may help to identify problems easily.

- Use a profiling tool (see chapter 8 on page 79), like the Oracle (Sun) Collector and Analyzer, Intel VTune Amplifier or gprof to find the computationally intensive or time-consuming parts of your program, because these are the parts where you want to start optimization.

- Use optimized libraries, e.g. the Intel MKL, the Oracle (Sun) Performance Library or the ACML library (see chapter 9 on page 88).

- Consider parallelization to reduce the runtime of your program.

5.4 Endianness

In contrast to e.g. the UltraSPARC architecture, the x86 AMD and Intel processors store the least significant bytes of a native data type first (**little endian**). Therefore care has to be taken if binary data has to be exchanged between machines using **big endian** – like the UltraSPARC-based machines – and the x86-based machines. Typically, FORTRAN compilers offer options or runtime parameters to write and read files in different byte ordering.

For other programming languages than FORTRAN the programmer has to take care of swapping the bytes when reading binary files. Below is a C++ example to convert from big to little endian or vice versa. This example can easily be adapted for C; however, one has to write a function for each data type since C does not know templates.
Note: This only works for basic types, like integer or double, and not for lists or arrays. In case of the latters, every element has to be swapped.

Listing 2: $PSRC/pex/542

```
template <typename T> T swapEndian( T x){
    union{ T x; unsigned char b[sizeof(T)];} dat1, dat2;

    dat1.x = x;
    for (int i = 0; i < sizeof(T); ++i)
    {
        dat2.b[i] = dat1.b[sizeof(T)-1-i];
    }
    return dat2.x;
}
```

5.5 Intel Compilers

On Linux, a version of the Intel FORTRAN/C/C++ compilers is loaded into your environment per default. They may be invoked via the environment variables $CC, $CXX, $FC or directly by the commands **icc | icpc | ifort**. The corresponding manual pages are available for further information. An overview of all the available compiler options may be obtained with the flag **-help**.

You can check the version which you are currently using with the **-v** option. Please use the `module` command to switch to a different compiler version. You can get a list of all the available versions with *module avail intel*. In general, we recommend using the latest available compiler version to benefit from performance improvements and bug fixes.

5.5.1 Frequently Used Compiler Options

Compute intensive programs should be compiled and linked (!) with the optimization options which are contained in the environment variable $FLAGS_FAST. For the Intel compiler, $FLAGS_FAST currently evaluates to

```
$ echo $FLAGS_FAST
-O3 -ip -axAVX,SSE4.2,SSE4.1 -fp-model fast=2
```

These flags have the following meaning:

- **-O3**: This option turns on aggressive, general compiler optimization techniques. Compared to the less aggressive variants **-O2** and **-O1**, this option may result in longer compilation times, but generally faster execution. It is especially recommended for code that processes large amounts of data and does a lot of floating-point calculations.

- **-ip**: Enable additional interprocedural optimizations for single-file compilation.

- **-axAVX,SSE4.2,SSE4.1**: This option turns on the automatic vectorizer[60] of the compiler and enables code generation for processors which employ the vector operations contained in the AVX2, AVX, SSE4.2, SSE4.1, SSE3, SSE2, SSE, SSSE3 and RDRND instruction set extensions. Compared to the similar option **-xCORE-AVX2**, this variant also generates machine code which does not use the vector instruction set extensions so that the executable can also be run on processors without these enhancements. This is reasonable on our HPC-Cluster, because not all of our machines support the same instruction set extensions.

- **-fp-model fast=2**: This option enables aggressive optimizations of floating-point calculations for execution speed, even those which might decrease accuracy.

Other options which might be of particular interest to you are:

- **-openmp**: Turns on OpenMP support. Please refer to Section 6.1 on page 62 for information about OpenMP parallelization.

- **-heap-arrays**: Puts automatic arrays and temporary arrays on the heap instead of the stack. Needed if the maximum stack space (2 GB) is exhausted.

- **-parallel**: Turns on auto-parallelization. Please refer to Section 6.1 on page 62 for information about auto-parallelizing serial code.

- **-vec-report**: Turns on feedback messages from the vectorizer. If you instruct the compiler to vectorize your code[61] (e.g. by using **-axAVX,SSE4.2,SSE4.1**) you can make it print out information about which loops have successfully been vectorized with this flag. Usually, exploiting vector hardware to its fullest requires some code re-structuring which may be guided by proper compiler feedback. To get the most extensive feedback from the vectorizer, please use the option **-vec-report3**. As the compiler output may become a bit overwhelming in this case, you can instruct the compiler to only tell about failed attempts to vectorize (and the reasons for the failure) by using **-vec-report5**.

- **-convert big_endian**: Read or write big-endian binary data in FORTRAN programs.

Table 5.17 on page 50 provides a concise overview of the Intel compiler options.

[60] Intel says, for the Intel Compiler, vectorization is the unrolling of a loop combined with the generation of packed SIMD instructions.

[61] If the compiler fails to vectorise a piece of code you can influence it using pragmas, e.g. *#pragma ivdep* (indicate that there is no loop carried dependence in the loop) or *#pragma vector always/aligned/unaligned* (compiler is instructed to always vectorize a loop and ignore internal heuristtics). There are more compiler pragmas available. For more information please refer to the compiler documentation. In Fortran there are compiler directives instead of pragmas used, with the very same meaning.
Note: Using pragmas may lead to broken code, e.g. if mocking no loop dependence in a loop which has a dependence!

[64] For this option the syntax -Ob*N* is still available on Linux but is deprecated.

[65] Objects compiled with -ipo are not portable, so do not use for libraries.

Linux	Description
-c	compile, but do not link
-o *filename*	specify output file name
-O0	no optimization (useful for debugging)
-O1	some speed optimization
-O2	(default) speed optimization, the generated code can be significantly larger
-O3	highest optimization, may result in longer compilation times
-fast	a simple, but less portable way to get good performance. The -fast option turns on -O3, -ipo, -static and -no-prec-div. *Note*: -no-prec-div enables optimizations that give slightly less precise results than full IEEE division.
-inline-level=N[64]	N = 0: disable inlining(default if -O0 specified) N = 1: enable inlining(default) N = 2: automatic inlining
-xC	generate code optimized for processor extensions C (see compiler manual). The code will only run on this platform.
-axC_1,C_2,..	like -x, but you can optimize for several platforms, and baseline code path is also generated
-vec-report*[X]*	emits level X diagnostic information from the vectorizer; if X is left out, level 1 is assumed
-ip	enables additional interprocedural optimizations for single-file compilation
-ipo	enables interprocedural optimization between files Functions from different files may be inlined[65]
-openmp	enables generation of parallel code based on OpenMP directives
-openmp-stubs	compiles OpenMP programs in sequential mode; the OpenMP directives are ignored and a sequential version of the OpenMP library is linked
-parallel	generates multi-threaded code for-loops that can be safely executed in parallel (auto-parallelization)
-par-report*[X]* -opt-report *[X]*	emit diagnostic information from the auto-parallelizer, or an optimization report
-g	produces symbolic debug information in object file
	set the default stack size in byte
-Xlinker *val*	passes *val* directly to the linker for processing
-heap-arrays *[size]*	Puts automatic arrays and temporary arrays on the heap instead of the stack

Table 5.17: Intel Compiler Options

5.5.2 Tuning Tips

5.5.2.1 The Optimization Report To fully exploit the capabilities of an optimizing compiler it is usually necessary to re-structure the program code. The Intel Compiler can assist you in this process via various reporting functions. Besides the vectorization report (cf. Section 5.5.1 on page 48) and the parallelization report (cf. Section 6.1.3 on page 64), a general optimization report can be requested via the command line option **-opt-report**. You can control the level of detail in this report; e.g. **-opt-report 3** provides the maximum amount of optimization messages.

The amount of feedback generated by this compiler option can easily get overwhelming. Therefore, you can put the report into a file (**-opt-report-file**) or restrict the output to a certain compiler phase (**-opt-report-phase**) or source code routine (**-opt-report-routine**).

5.5.2.2 Interprocedural Optimization Traditionally, optimization techniques have been limited to single routines because these are the units of compilation in FORTRAN. With interprocedural optimization, the compiler extends the scope of applied optimizations to multiple routines, potentially to the program as a whole. With the flag **-ip**, interprocedural optimization can be turned on for a single source file, i.e. the possible optimizations cover all routines in that file. When using the **-O2** or **-O3** flags, some single-file interprocedural optimizations are already included.

If you use **-ipo** instead of **-ip**, you turn on multi-file interprocedural optimization. In this case, the compiler does not produce the usual object files, but mock object files which include information used for the optimization.

The **-ipo** option may considerably increase the link time. Also, we often see compiler bugs with this option. The performance gain when using **-ipo** is usually moderate, but may be dramatic in object-oriented programs. Do not use **-ipo** for producing libraries because object files are not portable if **-ipo** is on.

5.5.2.3 Profile-Guided Optimization (PGO) When trying to optimize a program during compile/link time, a compiler can only use information contained in the source code itself or otherwise supplied to it by the developer. Such information is called "static" because it is passed to the compiler before the program has been built and hence does not change during runtime of the program. With Profile-Guided Optimization, the compiler can additionally gather information during program runs (dynamic information).

You can instrument your code for Profile-Guided Optimization with the **-prof-gen** flag. When the executable is run, a profile data file with the .dyn suffix is produced. If you now compile the source code with the **-prof-use** flag, all the data files are used to build an optimized executable.

5.5.3 Debugging

The Intel compiler offers several options to help you find problems with your code:

- **-g**: Puts debugging information into the object code. This option is necessary if you want to debug the executable with a debugger at the source code level (cf. Chapter 7 on page 74). Equivalent options are: **-debug**, **-debug full**, and **-debug all**.
- **-warn**: (FORTRAN only) Turns on all warning messages of the compiler.
- **-O0**: Disables any optimization. This option accelerate the compilations during the development/debugging stages.
- **-gen-interfaces**: (FORTRAN only) Creates an interface block (a binary .mod file and the corresponding source file) for each subroutine and function.

- **-check**: (FORTRAN only) Turns on runtime checks (cf. Chapter 7.2 on page 75).
- **-traceback**: Tells the compiler to generate extra information in the object file to provide source file traceback information when a severe error occurs at run time.
- **-ftrapuv**: Initializes stack local variables to an unusual value to aid error detection. This helps to find uninitialized local variables.

5.6 Oracle Compilers

On the Linux-based nodes, the Oracle[66] Studio 12.3 development tools are now in production mode and available after loading the appropriate module with the *module* command (refert to section 4.3.2 on page 31). They include the FORTRAN 95, C and C++ compilers. If necessary you can use other versions of the compilers by modification of the search path through loading the appropriate module with the *module* command (refer to section 4.3.2 on page 31).

```
$ module switch studio studio
```

Accordingly you can use preproduction releases of the compiler, if they are installed. You can obtain the list of all available versions by *module avail studio*.

We recommend that you always recompile your code with the latest production version of the used compiler due to performance reasons and bug fixes. Check the compiler version that you are currently using with the compiler option **-v**.

The compilers are invoked with the commands

```
$ cc, c89, c99, f90, f95, CC
```

and since Studio 12 additional Oracle-specific names are available

```
$ suncc, sunc89, sunc99, sunf90, sunf95, sunCC
```

You can get an overview of the available compiler flags with the option **-flags**.
We strongly recommended using the same flags for both compiling and linking.

Since the Sun Studio 7 Compiler Collection release, a separate FORTRAN 77 compiler is not available anymore. **f77** is a wrapper script used to pass the necessary compatibility options, like **-f77**, to the f95 compiler. This option has several suboptions. Using this option without any explicit suboption list expands to **-ftrap=%none -f77=%all**, which enables all compatibility features and also mimics FORTRAN 77's behavior regarding arithmetic exception trapping. We recommend adding **-f77 -ftrap=common** in order to revert to f95 settings for error trapping, which is considered to be safer. When linking to old f77 object binaries, you may want to add the option **-xlang=f77** at the link step. For information about shared memory parallelization refer to chapter 6.1.4 on page 65.

5.6.1 Frequently Used Compiler Options

Compute-intensive programs should be compiled and linked (!) with the optimization options which are contained in the environment variable $FLAGS_FAST.[67]

Since the Studio compiler may produce 64bit binaries as well as 32bit binaries and the default behavior is changing across compiler versions and platforms, we recommend setting the bit width explicitly by using the $FLAGS_ARCH64 or $FLAGS_ARCH32 environment variables.

The often-used option **-fast** is a macro expanding to several individual options that are meant to give the best performance with one single compile and link option. Note, however, that the expansion of the **-fast** option might be different across the various compilers, compiler releases, or compilation platforms. To see to which options a macro expands use the **-v** or **-#**

[66] formerly Sun

[67] Currently, on Linux the environment variables $FLAGS_FAST and $FLAGS_FAST_NO_FPOPT contain flags which optimize for the Intel Nehalem CPU's. On older chips, there may be errors with such optimized binaries due to lack of SSE4 units. Please read the compiler man page carefully to find out the best optimization flag for the chips you want your application to run on.

options. On our Nehalem machines this looks like:

```
$ CC -v -fast $PSRC/cpsp/pi.cpp -c
### command line files and options (expanded):
### -v -xO5 -xarch=sse4_2 -xcache=32/64/8:256/64/8:8192/64/16 -xchip=nehalem
-xdepend=yes -fsimple=2 -fns=yes -ftrap=%none -xlibmil -xlibmopt
-xbuiltin=%all -D__MATHERR_ERRNO_DONTCARE -nofstore -xregs=frameptr -Qoption
CC -iropt -Qoption CC -xcallee64 /rwthfs/rz/SW/HPC/examples/cpsp/pi.cpp -c
-Qoption ube -xcallee=yes
```

The compilers on x86 do not use automatic prefetching by default. Turning prefetching on with the **-xprefetch** option might offer better performance. Some options you might want to read up on are: **-xalias_level**, **-xvector**, **-xspfconst** and **-xprefetch**. These options only offer better performance in some cases and are therefore not included in the **-fast** macro.

Note: High optimization can have an influence on floating point results due to different **rounding errors**. To keep the order of the arithmetic operations, additional options **-fsimple=0** or **-xnolibmopt** can be added, which, however, may reduce the execution speed; see the $FLAGS_FAST_NO_FPOPT environment variable.

On the x86 nodes the **rounding precision** mode can be modified when compiling a program with the option[68] **-fprecision=single | double | extended**. The following code snippet demonstrates the effect:

Listing 3: $CC $FLAGS_ARCH32 $PSRC/pis/precision.c; a.out

```c
#include <stdio.h>
int main (int argc, char **argv)
{
    double f = 1.0, h = 1.0;
    int i;
    for (i = 0; i < 100; i++)
    {
       h = h / 2;
       if (f + h == f) break;
    }
    printf ("f: %e h: %e mantissa bits: %d\n", f, h, i);
    return 0;
}
```

Results	x86 32bit, no SSE2	other
1.000000e+00 5.960464e-08 23	-fprecision=single	n.a.
1.000000e+00 1.110223e-16 52	-fprecision=double	(*default*)
1.000000e+00 5.421011e-20 63	-fprecision=extended (*default*)	n.a.

Table 5.18: Results of different rounding modes

The results are collected in table 5.18 on page 53. The mantissa of the floating point numbers will be set to 23, 52 or 63 bits respectively. If compiling in 64bit or in 32bit with the usage of SSE2 instructions, the option **-fprecision** is ignored and the mantissa is always set to 52 bits.

The Studio FORTRAN compiler supports unformatted file sharing between big-endian and little-endian platforms (see chapter 5.4 on page 48) with the option **-xfilebyteorder=*endianmaxalign*:*spec*** where *endian* can be one of **little**, **big** or **native**, *maxalign* can be **1**, **2**, **4**, **8** or **16** specifying the maximum byte alignment for the target platform, and *spec* is a filename, a FORTRAN IO unit number, or **%all** for all files. The default is

[68] *Note*: this works only if the program is compiled in 32bit and does not use SSE2 instructions. The man page of Oracle compiler does not say this clear.

-xfilebyteorder=native:%all, which differs depending on the compiler options and platform. The different defaults are listed in table 5.19 on page 54.

32 bit addressing	64 bit addressing	architecture
`little4:%all`	`little16:%all`	x86
`big8:%all`	`big16:%all`	UltraSPARC

Table 5.19: Endianness options

The *default data type mappings* of the FORTRAN compiler can be adjusted with the **-xtypemap** option. The usual setting is **-xtypemap=real:32,double:64,integer:32**. The *REAL* type for example can be mapped to 8 bytes with **-xtypemap=real:64,double:64,integer:32**.

The option **-g** writes *debugging information* into the generated code. This is also useful for runtime analysis with the Oracle (Sun) Performance Analyzer that can use the debugging information to attribute time spent to particular lines of the source code. Use of **-g** does not substantially impact optimizations performed by the Oracle compilers. On the other hand, the correspondence between the binary program and the source code is weakened by optimization, making debugging more difficult. To use the Performance Analyzer with a *C++* program, you can use the option **-g0** in order not to prevent the compiler of inlining. Otherwise performance might drop significantly.

5.6.2 Tuning Tips

The option **-xunroll=n** can be used to advise the compiler to unroll loops.

Conflicts caused by the mapping of storage addresses to cache addresses can be eased by the creation of buffer areas (*padding*) (see compiler option **-pad**).

With the option **-dalign** the memory access on 64-bit data can be accelerated. This alignment permits the compiler to use single 64-bit load and store instructions. Otherwise, the program has to use two memory access instructions. If **-dalign** is used, every object file has to be compiled with this option.

With this option, the compiler will assume that double precision data has been aligned on an 8 byte boundary. If the application violates this rule, the runtime behavior is undetermined, but typically the program will crash. On well-behaved programs this should not be an issue, but care should be taken for those applications that perform their own memory management, switching the interpretation of a chunk of memory while the program executes. A classical example can be found in some (older) FORTRAN programs in which variables of a COMMON block are not typed consistently.

The following code will break, i.e. values other than 1 are printed, when compiled with the option **-dalign**:

Listing 4: f90 -dalign $PSRC/pis/badDalignFortran.f90; a.out

```
Program verybad
     call sub1
     call sub2
end Program
subroutine sub1
   integer a, b, c, d
   common / very_bad / a, b, c, d
   d=1
end subroutine sub1
subroutine sub2
   integer a, d
   real*8 x
   common / very_bad / a, x, d
   print *, d
end subroutine sub2
```

Note: The option **-dalign** is actually *required* for FORTRAN MPI programs and for programs linked to other libraries like the Oracle (Sun) Performance Library and the NAG libraries.

Inlining of routines from the same source file:
-xinline=*routine1,routine2,...*
However, please remember that in this case automatic inlining is disabled. It can be restored through the %auto option. We therefore recommend the following: **-xinline=%auto,*routine_list***.

With optimization level -xO4 and above, this is automatically attempted for functions / subroutines within the same source file. If you want the compiler to perform inlining across various source files at linking time, the option **-xipo** can be used. This is a compile and link option to activate interprocedural optimization in the compiler. Since the 7.0 release, **-xipo=2** is also supported. This adds memory-related optimizations to the interprocedural analysis.

In C and C++ programs, the use of pointers frequently limits the compiler's optimization capability. Through compiler options **-xrestrict** and **-xalias_level=...** it is possible to pass on additional information to the C-compiler. With the directive
`#pragma pipeloop(0)`
in front of a *for* loop it can be indicated to the C-compiler that there is no data dependency present in the loop. In FORTRAN the syntax is
`!$PRAGMA PIPELOOP=0`
Attention: These options (**-xrestrict** and **-xalias_level**) and the *pragma* are based on certain assumptions. When using these mechanisms incorrectly, the behavior of the program becomes undefined. Please study the documentation carefully before using these options or directives.

Program kernels with numerous branches can be further optimized with the profile feedback method. This two-step method starts with compilation using this option added to the regular optimization options **-xprofile=collect:*a.out***. Then the program should be run for one or more data sets. During these runs, runtime characteristics will be gathered. Due to the instrumentation inserted by the compiler, the program will most likely run longer. The second phase consists of recompilation using the runtime statistics **-xprofile=use:*a.out***. This produces a better optimized executable, but keep in mind that this is only beneficial for specific scenarios.

When using the **-g** option and optimization, the Oracle compilers introduce **comments** about loop optimizations into the object files. These comments can be printed with the command
`$ $PSRC/pex/541|| er_src serial_pi.o`
A comment like *Loop below pipelined with steady-state cycle count...* indicates that software

pipelining has been applied, which in general results in better performance. A person knowledgeable of the chip architecture will be able to judge by the additional information whether further optimizations are possible.

With a combination of `er_src` and grep, successful subroutine inlining can also be easily verified

```
$ $PSRC/pex/541|| er_src *.o |grep inline
```

5.6.3 Interval Arithmetic

The Oracle FORTRAN and C++ compilers support interval arithmetic. In FORTRAN this is implemented by means of an intrinsic INTERVAL data type, whereas C++ uses a special class library.

The use of interval arithmetic requires the use of appropriate numerical algorithms. For more information, refer to http://download.oracle.com/docs/cd/E19422-01/819-3695/ web pages.

5.7 GNU Compilers

On Linux, a version of the GNU compilers is always available because it is shipped with the operating system, although this system-default version may be heavily outdated. Please use the **module**[69] command to switch to a non-default GNU compiler version.

The GNU FORTRAN/C/C++ compilers can be accessed via the environment variables $CC, $CXX, $FC (if the gcc module is the last loaded module) or directly by the commands **gcc** | **g++** | **g77** | **gfortran**.

The corresponding manual pages are available for further information. The FORTRAN 77 compiler understands some FORTRAN 90 enhancements, when called with the parameters **-ff90 -ffree-form**. Sometimes the option **-fno-second-underscore** helps in linking. The FORTRAN 95 Compiler **gfortran** is available since version 4.

5.7.1 Frequently Used Compiler Options

Compute-intensive programs should be compiled and linked (!) with the optimization options which are contained in the environment variable $FLAGS_FAST. For the GNU compiler 4.4, $FLAGS_FAST currently evaluates to

```
$ echo $FLAGS_FAST
-O3 -ffast-math -mtune=native
```

These flags have the following meaning:

- **-O3**: The **-Ox** options control the number and intensity of optimization techniques the compiler tries to apply to the code. Each of these techniques has individual flags to turn it on, the **-Ox** flags are just summary options. This means that **-O** (which is equal to **-O1**) turns some optimizations on, **-O2** a few more, and **-O3** even more than **-O2**.
- **-ffast-math**: With this flag the compiler tries to improve the performance of floating point calculations while relaxing some correctness rules. **-ffast-math** is a summary option for several flags concerning floating point arithmetic.
- **-mtune=native**: Makes the compiler tune the code for the machine on which it is running. You can supply this option with a specific target processor; please consult the GNU compiler manual for a list of available CPU types. If you use **-march** instead of **-mtune**, the generated code might not run on all cluster nodes anymore, because the compiler is free to use certain parts of the instruction set which are not available on all

[69] refer to chapter 4.3.2 on page 31

processors. Hence, **-mtune** is the less aggressive option and you might consider switching to **-march** if you know what you are doing.

Other options which might be of particular interest to you are:

- **-fopenmp**: Enables OpenMP support (GCC 4.2 and newer versions). Please refer to Section 6.1 on page 62 for information about OpenMP parallelization.
- **-ftree-parallelize-loops=N**: Turns on auto-parallelization and generates an executable with N parallel threads (GCC 4.3 and newer versions). Please refer to Section 6.1 on page 62 for information about auto-parallelizing serial code.

5.7.2 Debugging

The GNU compiler offers several options to help you find problems with your code:

- **-g**: Puts debugging information into the object code. This option is necessary if you want to debug the executable with a debugger at the source code level (cf. Chapter 7 on page 74).
- **-Wall**: Turns on lots of warning messages of the compiler. Despite its name, this flag does not enable all possible warning messages, because there is
- **-Wextra**: which turns on additional ones.
- **-Werror**: Treats warnings as errors, i.e. stops the compilation process instead of just printing a message and continuing.
- **-O0**: Disables any optimization. This option speeds up the compilations during the development/debugging stages.
- **-pedantic**: Is picky about the language standard and issues warnings about non-standard constructs. **-pedantic-errors** treats such problems as errors instead of warnings.

5.8 PGI Compilers

Use the `module` command to load the compilers of The Portland Group into your environment. The PGI C/C++/Fortran 77/Fortran 90 compilers can be accessed by the commands **pgcc | pgCC | pgf77 | pgf90**. Please refer to the corresponding manual pages for further information. Extensible documentation is available on The Portland Group's website.[70] The following options provide a good starting point for producing well-performing machine code with these compilers:

- **-fastsse**: Turns on high optimization including vectorization.
- **-Mconcur** (compiler and linker option): Turns on auto-parallelization.
- **-Minfo**: Makes the compiler emit informative messages including those about successful and failed attempts to vectorize and/or auto-parallelize code portions.
- **-mp** (compiler and linker option): Turns on OpenMP.

Of those PGI compiler versions installed on our HPC-Cluster, the 11.x releases include support for Nvidia's CUDA architecture via the PGI Accelerator directives and CUDA Fortran. The following options enable this support and must be supplied during compile and link steps. (The option **-Minfo** described above is helpful for CUDA code generation, too.)

[70] http://www.pgroup.com

- **-ta=nvidia**: Enables PGI accelerator code generation for a GPU.
- **-ta=nvidia,cc20**: Enables PGI accelerator code generation for a GPU supporting Compute Capability 2.0 or higher.
- **-Mcuda**: Enables CUDA FORTRAN for a GPU supporting Compute Capability 1.3 or higher.
- **-Mcuda=cc20**: Enable CUDA FORTRAN for a GPU supporting Compute Capability 2.0 or higher.

If you need more information on our GPU Cluster please refer to 2.4 on page 15

In order to read or write big-endian binary data in FORTRAN programs you can use the compiler option **-Mbyteswapio**. You can use the option **-Ktrap** when compiling the main function/program in order to enable error trapping. For information about shared memory parallelization with the PGI compilers refer to chapter 6.1.6 on page 68.

The PGI compiler offers several options to help you find problems with your code:

- **-g**: Puts debugging information into the object code. This option is necessary if you want to debug the executable with a debugger at the source code level (cf. Chapter 7 on page 74).
- **-O0**: Disables any optimization. This options speeds up the compilations during the development/debugging stages.
- **-w**: Disable warning messages.

5.9 Time Measurements

For real-time measurements, a high-resolution timer is available. However, the measurements can supply reliable, reproducible results only on an (almost) empty machine. Make sure you have enough free processors available on the node. The number of processes which are ready to run[71] plus the number of processors needed for the measurement has to be less or equal to the number of processors. On ccNUMA CPU's like Nehalem, be aware about processor placement and binding, refer to 3.1.1 on page 24.

User CPU time measurements have a lower precision and are more time-consuming. In case of parallel programs, real-time measurements should be preferred anyway!

The *r_lib* library offers two timing functions, **r_rtime** and **r_ctime**. They return the real time and the user CPU time as double precision floating point numbers. For information on how to use r_lib refer to 9.8 on page 92.

Depending on the operating system, programming language, compiler or parallelization paradigm, different functions are offered to measure the time. To get a listing of the file you can use

```
$ cat $PSRC/include/realtime.h
```

If you are using OpenMP the *omp_get_wtime()* function is used in background, and for MPI the *MPI_Wtime()* function. Otherwise some operating system dependent functions are selected by the corresponding C preprocessor definitions. The time is measured in seconds as double precision floating point number.

Alternatively, you can use all the different time measurement functions directly.

Linux example in C:

```
#include <sys/time.h>
struct timeval tv;
```

[71] You can use the **uptime** command on Linux to check the load

```
double second;
gettimeofday(&tv, (struct timezone*)0);
second = ((double)tv.tv_sec + (double)tv.tv_usec / 1000000.0);
```

In FORTRAN you also can use the **gettimeofday** Linux function, but it must be wrapped. An example is given in listings 5 on page 59 and 6 on page 59. After the C wrapper and the Fortran code are compiled, link and let the example binary run:

```
$ $FC rwthtime.o use_gettimeofday.o
$ ./a.out
```

Listing 5: $CC -c $PSRC/psr/rwthtime.c

```
#include <sys/time.h>
#include <stdio.h>
/* This timer returns current clock time in seconds. */
double rwthtime_() {
    struct timeval tv;
    int ierr;
    ierr = gettimeofday(&tv, NULL) ;
    if (ierr != 0 ) printf("gettimeofday ERR:, ierr=%d\n",ierr);
    return ((double)tv.tv_sec + (double)tv.tv_usec / 1000000.0);
}
```

Listing 6: $FC -c $PSRC/psr/use_gettimeofday.f90

```
PROGRAM t1
IMPLICIT NONE
REAL*8 rwthtime
WRITE (*,*) "Wrapped gettimeofday: ", rwthtime()
END PROGRAM t1
```

The Oracle Studio compiler has a built-in time measurement function *gethrtime*. Linux FORTRAN example with Oracle Studio compiler:

```
INTEGER*8 gethrtime
REAL*8 second
second = 1.d-9 * gethrtime()
```

In FORTRAN, there is an intrinsic time measurement function called **SYSTEM_CLOCK**. The time value returned by this function can overflow, so take care about it.

5.10 Memory Usage

To get an idea of how much physical memory your application needs, you can use the wrapper command **r_memusage**. We advise you to start and then stop it with CRTL+C or using the –**kill** parameter after some seconds/minutes, because for many applications most of the memory is allocated at the beginning of their run time. You can round up the displayed memory peak value and use it as parameter to the batch system. For example:

```
$  r_memusage hostname
[...]
memusage:  peak usage:  physical memory:  0.5 MB
```

For MPI applications you have to insert the wrapper just before the executable:

```
$ $MPIEXEC $FLAGS_MPI_BATCH r_memusage hostname
[...]
memusage:  rank 0:  peak usage:  physical memory:  0.5 MB
memusage:  rank 1:  peak usage:  physical memory:  0.5 MB
```

For a more detailed description of r_memusage use the following command:

```
$ r_memusage -man
```

5.11 Memory Alignment

The standard memory allocator *malloc()* allocates the memory not aligned to the beginning of the addres space and thus to any system boundary, e.g. start of a memory page. In some cases (e.g. transferring data using InfiniBand on some machines) the unaligned memory is being processed slower than memory aligned to some magic number (usually a power of two). Aligned memory can be allocated using *memalign()* instead of *malloc()*, however this is tedious, needs change of program code and recompilation (C/C++) and is not available at all in Fortran (where system memory allocation is wrapped to calls of Fortran *ALLOCATE()* by compiler's libraries).

Another way is to wrap the calls to *malloc()* to *memalign()* using a wrapper library. This library is provided to the binary by LD_PRELOAD environment variable. We provide the *memalign32* script which implement this, leading all allocated memory being aligned by 32. Example:

```
$  memalign32 sleep 1
```

For MPI programs you have to insert the wrapper just before the executable:

```
$  $MPIEXEC $FLAGS_MPI_BATCH memalign32 a.out
```

Note: Especially if memory is allocated in (very) small chunks, the aligned allocation lead to memory waste and thus can lead to significant increase of the memory footprint.

Note: We cannot give a guarantee that the application will still run correctly if using *memalign32* script. Use at your own risk!

5.12 Hardware Performance Counters

Hardware Performance Counters are used to measure how certain parts, like floating point units or caches, of a CPU or memory system are used. They are very helpful in finding performance bottlenecks in programs.
The Xeon processor core offers 4 programmable 48-bit performance counters.

5.12.1 Linux

At the moment we offer the following interfaces for accessing the counters:

- Intel VTune Amplifier (see chapter 8.2.1 on page 82)
- Oracle (Sun) Collector (see chapter 8.1 on page 79)
- Vampir (ch. 8.3.2 on page 85) and Scalasca (ch. 8.3.3 on page 85) (over PAPI Library)

- likwid-perfctr form LIKWID toolbox (see chapter 8.5 on page 86)

Note: At present, the kernel module for use with Intel VTune is available on a few specific machines.

6 Parallelization

Parallelization for computers with shared memory (SM) means the automatic distribution of loop iterations over several processors (automatic parallelization), the explicit distribution of work over the processors by compiler directives (OpenMP) or function calls to threading libraries, or a combination of those.

Parallelization for computers with distributed memory (DM) is done via the explicit distribution of work and data over the processors and their coordination with the exchange of messages (Message Passing with MPI).

MPI programs run on shared memory computers as well, whereas OpenMP programs usually do not run on computers with distributed memory. As a consequence, MPI programs can use virtually all available processors of the HPC-Cluster, whereas OpenMP programs can use up to 128 processors of a Bull SMP (BCS) node. For large applications the hybrid parallelization approach, a combination of coarse-grained parallelism with MPI and underlying fine-grained parallelism with OpenMP, might be attractive in order to efficiently use as many processors as possible.

Please note that long-running computing jobs should not be started interactively. Please use the batch system (see chapter 4.4 on page 34), which determines the distribution of the tasks to the machines to a large extent.

We offer examples using the different parallelization paradigms. Please refer to chapter 1.3 on page 10 for information how to use them.

6.1 Shared Memory Programming

OpenMP[72] is the de facto standard for shared memory parallel programming in the HPC realm. The OpenMP API is defined for FORTRAN, C, and C++ and consists of compiler directives (resp. pragmas), runtime routines and environment variables.

In the *parallel regions* of a program several *threads* are started. They execute the contained program segment redundantly until they hit a *worksharing construct*. Within this construct, the contained work (usually **do**- or **for**-loops, or **task** constructs since OMPv3.0) is distributed among the threads. Under normal conditions all threads have access to all data (shared data). But pay attention: If data, which is accessed by several threads, is modified, then the access to this data must be protected with *critical regions* or *OpenMP locks*.

Besides, *private* data areas can be used where the individual threads hold their local data. Such private data (in OpenMP terminology) is only visible to the thread owning it. Other threads will not be able to read or write private data.

Hint: In a loop that is to be parallelized the results must not depend on the order of the loop iterations! Try to run the loop backwards in serial mode. The results should be the same. This is a necessary, though not sufficient condition, to parallelize a loop correctly!

Note: For cases in which the stack area for the worker threads has to be increased, OpenMP 3.0 introduced the OMP_STACKSIZE environment variable. Appending a lower case V denotes the size to be interpreted in MB. The shell builtins **ulimit -s xxx** (zsh shell, specification in kilobytes) or **limit s xxx** (C-shell, in kilobytes) only affect the initial (master) thread.

The number of threads to be started for each parallel region may be specified by the environment variable OMP_NUM_THREADS which is set to 1 per default on our HPC-Cluster. The OpenMP standard does not specify the number of concurrent threads to be started if OMP_NUM_THREADS is not set. In this case, the Oracle and PGI compilers start only a single thread, whereas the Intel and GNU compilers start as many threads as there are processors available. Please always set the OMP_NUM_THREADS environment variable to a reasonable value. We especially warn against setting it to a value greater than the number of processors available on the machine on which the program is to be run. On a loaded system fewer threads

[72] http://www.openmp.org, http://www.compunity.org

may be employed than specified by this environment variable because the dynamic mode may be used by default. Use the environment variable OMP_DYNAMIC to change this behavior.

If you want to use nested OpenMP, the environment variable OMP_NESTED=TRUE has to be set. Beginning with the OpenMP v3.0 API, the new runtime functions OMP_THREAD_LIMIT and OMP_MAX_ACTIVE_LEVELS are available that control nested behavior and obsolete all the old compiler-specific extensions.
Note: Not all compilers support nested OpenMP.

6.1.1 Automatic Shared Memory Parallelization of Loops (Autoparallelization)

All compilers installed on our HPC-Cluster can parallelize programs (more precisely: loops) automatically, at least in newer versions. This means that upon request they try to transform portions of serial FORTRAN/C/C++ code into a multithreaded program. Success or failure of autoparallelization depends on the compiler's ability to determine if it is safe to parallelize a (nested) loop. This often depends on the area of the application (e.g. finite differences versus finite elements), programming language (pointers and function calls may make the analysis difficult) and coding style.

The flags to turn this feature on differ among the various compilers. Please refer to the subsequent sections for compiler-specific information. The environment variable FLAGS_AUTOPAR offers a portable way to enable autoparallelization at compile/link time. For the Intel, Oracle, and PGI compilers, the number of parallel threads to start at runtime may be set via OMP_NUM_THREADS, just like for an OpenMP program. Only with the GNU compiler the number of threads is fixed at compile/link time.

Usually some manual code changes are necessary to help the compiler to parallelize your serial loops. These changes should be guided by compiler feedback; increasing the compiler's verbosity level therefore is recommended when using autoparallelization. The compiler options to do this as well as the feedback messages themselves are compiler-specific, so again, please consult the subsequent sections.

While autoparallelization tries to exploit multiple processors within a machine, automatic vectorization (cf. section 5.5 on page 48) makes use of instruction-level parallelism within a processor. Both features can be combined if the target machine consists of multiple processors equipped with vector units as it is the case on our HPC-Cluster. This combination is especially useful if your code spends a significant amount of time in nested loops and the innermost loop can successfully be vectorized by the compiler while the outermost loop can be autoparallelized. It is common to autoparallelization and autovectorization that both work on serial, i.e. not explicitly parallelized code, which usually must be re-structured to take advantage of these compiler features.

Table 6.20 on page 63 summarizes the OpenMP compiler options. For the currently loaded compiler, the environment variables FLAGS_OPENMP and FLAGS_AUTOPAR are set to the corresponding flags for OpenMP parallelization and autoparallelization, respectively, as is explained in section 5.2 on page 45.

Compiler	FLAGS_OPENMP	FLAGS_AUTOPAR
Oracle	-xopenmp	-xautopar -xreduction
Intel	-openmp	-parallel
GNU	-fopenmp (4.2 and above)	(empty)[74]
PGI	-mp -Minfo=mp	-Mconcur -Minline

Table 6.20: Overview of OpenMP and autoparallelization compiler options

[74] Although the GNU compiler has an autoparallelization option, we intentionally leave the FLAGS_AUTOPAR environment variable empty, see 6.1.5.2 on page 68.

6.1.2 Memory Access Pattern and NUMA

Today's modern computer systems have a NUMA architecture (see chapter 2.1.1 on page 12). The memory access pattern is crucial if a shared memory parallel application should not only run multithreaded, but also perform well on NUMA computers. The data accessed by a thread should be located locally in order to avoid performance penalties of remote memory access. A typical example for a bad bad memory access pattern is to initialize all data from *one* thread (i.e. in a serial program part) before using the data with *many* threads. Due to the standard *first-touch* memory allocation policy in current operating systems, all data initialized from one thread is placed in the local memory of the current processor node. All threads running on a different processor node have to access the data from that memory location over the slower link. Furthermore, this link may be overloaded with multiple simultaneous memory operations from multiple threads. You should initialize the in-memory data in the same pattern as it will be used during computation.

6.1.2.1 Numamem

With the **numamem** script you can analyze the memory placement of an application. To get a sampling of the memory placement start your program

- using numamem as a wrapper:
  `$ numamem <opt> ./a.out <args>`
- or analyse a running program:
  `$ numamem -p process id`

For MPI programs insert the wrapper just before the executable:
`$ $MPIEXEC $FLAGS_MPI_BATCH numamem <opt> ./a.out <args>`

Command line options of the **numamem** script are given in the table 6.21 on page 64.

Option	Description
`-s <time>`	sampletime in seconds [default 10]
`-o <file name>`	Write an CSV file *out.csv* (or for MPI *out<rank>.csv*) [default None]
`-p <process id>`	analyse a running program using its *<process id>*
`-q`	quiet mode (don't print to stdout) [default off]

Table 6.21: Parameters of **numamem** script

6.1.3 Intel Compilers

The Intel FORTRAN/C/C++ compilers support OpenMP[75] via the compiler/linker option **-openmp**. This includes nested OpenMP and tasking, too. If OMP_NUM_THREADS is not set, an OpenMP program built with the Intel compilers starts as many threads as there are processors available. The worker threads' stack size may be set using the environment variable KMP_STACKSIZE, e.g.
`$ KMP_STACKSIZE=megabytesM`

Dynamic adjustment of the number of threads and support for nested parallelism is turned off by default when running an executable built with the Intel compilers. Please use the environment variables OMP_DYNAMIC and OMP_NESTED, respectively, to enable those features.

[75] Intel has open-sourced the production OpenMP runtime under a BSD license to support tool developers and others: http://openmprtl.org

6.1.3.1 Thread binding Intel compilers provide an easy way for thread binding: Just set the environment variable KMP_AFFINITY to **compact** or **scatter**, e.g.

```
$ export KMP_AFFINITY=scatter
```

Setting it to **compact** binds the threads as closely as possible, e.g. two threads on different cores of one processor chip. Setting it to **scatter** binds the threads as far away as possible, e.g. two threads, each on one core on different processor sockets. Explicitly assigning OpenMP threads to a list of OS proc IDs is also possible with the **explicit** keyword. For details, please refer to the compiler documentation on the Intel website. The default behavior is to not bind the threads to any particular thread contexts; however, if the operating system supports affinity, the compiler still uses the OpenMP thread affinity interface to determine machine topology. To get a machine topology map, specify

```
$ export KMP_AFFINITY=verbose,none
```

6.1.3.2 Autoparallelization The autoparallelization feature of the Intel compilers can be turned on for an input file with the compiler option **-parallel**, which must also be supplied as a linker option when an autoparallelized executable is to be built. The number of threads to be used at runtime may be specified in the environment variable OMP_NUM_THREADS, just like for OpenMP. We recommend turning on serial optimization via -O2 or -O3 when using **-parallel** to enable automatic inlining of function/subroutine calls within loops which may help in automatic parallelization.

You may use the option **-par-report** to make the compiler emit messages about loops which have been parallelized. If you want to exploit the autoparallelization feature of the Intel compilers it is also very helpful to know which portions of your code the compiler tried to parallelize, but failed. Via **-par-report3** you can get a very detailed report about the activities of the automatic parallelizer during compilation. Please refer to the Intel compiler manuals about how to interpret the messages in such a report and how to subsequently re-structure your code to take advantage of automatic parallelization.

6.1.4 Oracle Compilers

The Oracle FORTRAN/C/C++ compilers support OpenMP via the compiler/linker option **-xopenmp**. This option may be used together with automatic parallelization (enabled by **-xautopar**), but loops within OpenMP parallel regions are no longer subject to autoparallelization.

The **-xopenmp** option is used as an abbreviation for a multitude of options; the FORTRAN 95 compiler for example expands it to **-mp=openmp -explicitpar -stackvar -D_OPENMP -O3**. Please note that all local data of subroutines called from within parallel regions is put onto the stack. A subroutine's stack frame is destroyed upon exit from the routine. Therefore local data is not preserved from one call to the next. As a consequence, FORTRAN programs must be compiled with the **-stackvar** option.

The behavior of unused worker threads between parallel regions can be controlled with the environment variable SUNW_MP_THR_IDLE. The possible values are **spin |sleep |*n*s |*n*ms**. The worker threads wait either actively (busy waiting) and thereby consume CPU time, or passively (idle waiting) and must then be woken up by the system or, in a combination of these methods, they actively wait (spin) and are put to sleep ***n*** seconds or milliseconds later. With fine-grained parallelization, active waiting, and with coarse-grained parallelization, passive waiting is recommended. Idle waiting might be advantageous on an (over)loaded system.

Note: The Oracle compilers' default behavior is to put idle threads to sleep after a certain time out. Those users that prefer the old behavior (before Studio 10), where idle threads spin,

can use SUNW_MP_THR_IDLE=spin to change the behavior. Please be aware that having threads spin will unnecessarily waste CPU cycles.

Note: The environment variable SUNW_MP_GUIDED_WEIGHT can be used to set the weighting value used by **libmtsk** for-loops with the *guided* schedule. The libmtsk library uses the following formula to compute the chunk sizes for *guided* loops:
`chunk_size=num_unassigned_iterations/(weight*num_threads)`
where *num_unassigned_iterations* is the number of iterations in the loop that have not yet been assigned to any thread, *weight* is a floating-point constant (default 2.0) and *num_threads* is the number of threads used to execute the loop. The value specified for SUNW_MP_GUIDED_WEIGHT must be a positive, non-zero floating-point constant.

We recommend to set SUNW_MP_WARN=TRUE while developing, in order to enable additional warning messages of the OpenMP runtime system. Do not, however, use this during production because it has performance and scalability impacts.

We also recommend the use of the option **-vpara** (FORTRAN) or **-xvpara** (C), which might allow the compiler to catch errors regarding incorrect explicit parallelization at compile time. Furthermore the option **-xcommonchk** (FORTRAN) can be used to check the consistency of *thread-private* declarations.

6.1.4.1 Thread binding

The SUNW_MP_PROCBIND environment variable can be used to bind threads in an OpenMP program to specific virtual processors (denoted with logical IDs). The value specified for SUNW_MP_PROCBIND can be one of the following:

- The string **true** or **false**
- A list of one or more non-negative integers separated by one or more spaces
- Two non-negative integers, **n1** and **n2**, separated by a minus ("-"); n1 must be less than or equal to n2 (means "all IDs from n1 to n2")

Logical IDs are consecutive integers that start with **0**. If the number of virtual processors available in the system is **n**, then their logical IDs are **0, 1, ..., n-1**.

Note: The thread binding with SUNW_MP_PROCBIND currently does not care about binding in operating system e.g. by **taskset**. This may lead to unexpected behavior or errors if using both ways to bind the threads simultaneously.

6.1.4.2 Automatic Scoping

The Oracle compiler offers a highly interesting feature, which is not part of the current OpenMP specification, called *Automatic Scoping*. If the programmer adds one of the clauses *default(__auto)* or *__auto(list-of-variables)* to the OpenMP *parallel* directive, the compiler will perform the data dependency analysis and determine what the scope of all the variables should be, based on a set of scoping rules. The programmer no longer has to declare the scope of all the variables (*private*, *firstprivate*, *lastprivate*, *reduction* or *shared*) explicitly, which in many cases is a tedious and error-prone work. In case the compiler is not able to determine the scope of a variable, the corresponding parallel region will be serialized. However, the compiler will report the result of the autoscoping process so that the programmer can easily check which variables could not be automatically scoped and add suitable explicit scoping clauses for just these variables to the OpenMP parallel directive.

Add the compiler option **-vpara** to get warning messages and a list of variables for which autoscoping failed. Add the compiler option **-g** to get more details about the effect of autoscoping with the **er_src** command.

```
$ $PSRC/pex/610|| f90 -g -O3 -xopenmp -vpara -c $PSRC/psr/jacobi_autoscope.f95
$ $PSRC/pex/610|| er_src jacobi_autoscope.o
```

Find more information about autoscoping in http://download.oracle.com/docs/cd/E19059-01/stud.9/817-6703/5_autoscope.html

6.1.4.3 Autoparallelization The option to turn on autoparallelization with the Oracle compilers is **-xautopar** which includes **-depend -O3** and in case of FORTRAN also **-stackvar**. In case you want to combine autoparallelization and OpenMP[76], we strongly suggest using the **-xautopar -xopenmp** combination. With the option **-xreduction**, automatic parallelization of reductions is also permitted, e.g. accumulations, dot products etc., whereby the modification of the sequence of the arithmetic operation can cause different rounding error accumulations.

Compiling with the option **-xloopinfo** makes the compiler emit information about the parallelization. If the number of loop iterations is unknown during compile time, code is produced which decides at runtime whether a parallel execution of the loop is more efficient or not (alternate coding). With automatic parallelization it is furthermore possible to specify the number of used threads by the environment variable OMP_NUM_THREADS.

6.1.4.4 Nested Parallelization The Oracle compilers' OpenMP support includes nested parallelism. You have to set the environment variable OMP_NESTED=TRUE or call the runtime routine **omp_set_nested()** to enable nested parallelism.

Oracle Studio compilers support the OpenMP v3.0 as of version 12, so it is recommended to use the new functions OMP_THREAD_LIMIT and OMP_MAX_ACTIVE_LEVELS to control the nesting behavior (see the OpenMP API v3.0 specification).[77]

6.1.5 GNU Compilers

As of version 4.2, the GNU compiler collection supports OpenMP with the option **-fopenmp**. The OpenMP v3.0 support is as of version 4.4 included.

The default thread stack size can be set with the variable GOMP_STACKSIZE (in kilobytes), or via the OMP_STACKSIZE environment variable. For more information on GNU OpenMP project refer to web pages:

http://gcc.gnu.org/projects/gomp/

http://gcc.gnu.org/onlinedocs/libgomp/

6.1.5.1 Thread binding CPU binding of the threads can be done with the GOMP_CPU_AFFINITY environment variable. The variable should contain a space- or comma-separated list of CPUs. This list may contain different kind of entries: either single CPU numbers in any order, a range of CPUs (M-N), or a range with some stride (M-N:S). CPU numbers are zero-based. For example, GOMP_CPU_AFFINITY="0 3 1-2 4-15:2" will bind the initial thread to CPU 0, the second to CPU 3, the third to CPU 1, the fourth to CPU 2, the fifth to CPU 4, the sixth through tenth to CPUs 6, 8, 10, 12, and 14 respectively and then start assigning back to the beginning of the list. GOMP_CPU_AFFINITY=0 binds all threads to

[76] The Oracle(Sun)-specific MP pragmas have been deprecated and are no longer supported. Thus the **-xparallel** option is obsolete now. Do not use this option.

[77] However, the older Oracle(Sun)-specific variables SUNW_MP_MAX_POOL_THREADS and SUNW_MP_MAX_NESTED_LEVELS are still supported.

- SUNW_MP_MAX_POOL_THREADS specifies the size (maximum number of threads) of the thread pool. The thread pool contains only non-user threads – threads that the libmtsk library creates. It does not include user threads such as the main thread. Setting SUNW_MP_MAX_POOL_THREADS to 0 forces the thread pool to be empty, and all parallel regions will be executed by one thread. The value specified should be a non-negative integer. The default value is 1023. This environment variable can prevent a single process from creating too many threads. That might happen e.g. for recursively nested parallel regions.
- SUNW_MP_MAX_NESTED_LEVELS specifies the maximum depth of active parallel regions. Any parallel region that has an active nested depth greater than SUNW_MP_MAX_NESTED_LEVELS will be executed by a single thread. The value should be a positive integer. The default is 4. The outermost parallel region has a depth level of 1.

CPU 0. A defined CPU affinity on startup cannot be changed or disabled during the runtime of the application.

6.1.5.2 Autoparallelization Since version 4.3 the GNU compilers are able to parallelize loops automatically with the option **-ftree-parallelize-loops=<*threads*>**. However, the number of threads to use has to be specified at compile time and cannot be changed at runtime.

6.1.5.3 Nested Parallelization OpenMP nesting is supported using the standard OpenMP environment variables. *Note*: The support for OpenMP v3.0 nesting features is available as of version 4.4 of GCC compilers.

6.1.6 PGI Compilers

To build an OpenMP program with the PGI compilers, the option **-mp** must be supplied during compile and link steps. Explicit parallelization via OpenMP compiler directives may be combined with automatic parallelization (cf. 6.1.6.2 on page 68), although loops within parallel OpenMP regions will not be parallelized automatically. The worker thread's stack size can be increased via the environment variable **MPSTKZ=*megabytes*M**, or via the OMP_STACKSIZE environment variable.

Threads at a barrier in a parallel region check a semaphore to determine if they can proceed. If the semaphore is not free after a certain number of tries, the thread gives up the processor for a while before checking again. The MP_SPIN variable defines the number of times a thread checks a semaphore before idling. Setting MP_SPIN to **-1** tells the thread never to idle. This can improve performance but can waste CPU cycles that could be used by a different process if the thread spends a significant amount of time before a barrier.

Note: Nested parallelization is NOT supported.[78]

Note: The environment variables OMP_DYNAMIC does not have any effect.[79]

Note: OpenMP v3.0 standard is supported, including all the nesting-related routines. However, due to lack of nesting support, these routines are dummies only. For more information refer to http://www.pgroup.com/resources/openmp.htm or http://www.pgroup.com/resources/docs.htm.

6.1.6.1 Thread binding The PGI compiler offers some support for NUMA architectures with the option **-mp=numa**. Using NUMA can improve performance of some parallel applications by reducing memory latency. Linking **-mp=numa** also allows to use the environment variables MP_BIND, MP_BLIST and MP_SPIN. When MP_BIND is set to *yes*, parallel processes or threads are bound to a physical processor. This ensures that the operating system will not move your process to a different CPU while it is running. Using MP_BLIST, you can specify exactly which processors to attach your process to. For example, if you have a quad socket dual core system (8 CPUs), you can set the blist so that the processes are interleaved across the 4 sockets (MP_BLIST=2,4,6,0,1,3,5,7) or bound to a particular (MP_BLIST=6,7).

6.1.6.2 Autoparallelization Just like the Intel and Oracle compilers, the PGI compilers are able to parallelize certain loops automatically. This feature can be turned on with the option **-Mconcur[=*option*[,*option*,...]]** which must be supplied at compile and link time.

Some options of the **-Mconcur** parameter are:

- **bind** Binds threads to cores or processors.

[78] Refer to p. 170 (p. 190 in the PDF file) in http://www.pgroup.com/doc/pgifortref.pdf
All other shared-memory parallelization directives have to occur within the scope of a parallel region. Nested PARALLEL... END PARALLEL directive pairs are not supported and are ignored.

[79] Refer to p. 182 (p. 202 in the PDF file) ibidem.

- **levels:*n*** Parallelizes loops nested at most **n** levels deep (the default is **3**).
- **numa|nonuma** Uses (doesn't use) thread/processor affinity for NUMA architectures. **-Mconcur=numa** will link in a **numa** library and objects to prevent the operating system from migrating threads from one processor to another.

Compiler feedback about autoparallelization is enabled with **-Minfo**. The number of threads started at runtime may be specified via OMP_NUM_THREADS or NCPUS. When the option **-Minline** is supplied, the compiler tries to inline functions, so even loops with function calls may be successfully parallelized automatically.

6.2 Message Passing with MPI

MPI (Message-Passing Interface) is the de-facto standard for parallelization on distributed memory parallel systems. Multiple processes explicitly exchange data and coordinate their work flow. MPI specifies the interface but not the implementation. Therefore, there are plenty of implementations for PCs as well as for supercomputers. There are free implementations available as well as commercial ones, which are particularly tuned for the target platform. MPI has a huge number of calls, although it is possible to write meaningful MPI applications just employing some 10 of these calls.

Like the compiler environment flags, which were set by the compiler modules, we also offer MPI environment variables in order to make it easier to write platform-independent makefiles. Since the compiler wrappers and the MPI libraries relate to a specific compiler, a compiler module has to be loaded *before* the MPI module.

Some MPI libraries do not offer a C++ or a FORTRAN 90 interface for all compilers, e.g. the Intel MPI does not offer such interfaces for the Oracle compiler. If this is the case there will be an info printed while loading the MPI module.

- MPIEXEC – The MPI command used to start MPI applications, e.g. mprun or mpiexec.
- MPIFC, MPICC, MPICXX – Compiler driver for the last-loaded compiler module, which automatically sets the include path and also links the MPI library automatically.
- FLAGS_MPI_BATCH – Options necessary for executing in batch mode .

This example shows how to use the variables.

```
$ $PSRC/pex/620|| $MPICXX -I$PSRC/cpmp $PSRC/cpmp/pi.cpp -o a.out
$ $PSRC/pex/620|| $MPIEXEC -np 2 a.out
```

6.2.1 Interactive "mpiexec" Wrapper

On Linux we offer dedicated machines for interactive MPI tests. These machines will be used automatically by our interactive **mpiexec** and **mpirun** wrapper. The goal is to avoid overloading the front end machines with MPI tests and to enable larger MPI tests with more processes.

The interactive wrapper works transparently so you can start your MPI programs with the usual MPI options. In order to make sure that MPI programs do not hinder each other the wrapper will check the load on the available machines and choose the least loaded ones. The chosen machines will get one MPI process per available processor. However, this default setting may not work for jobs that need more memory per process than there is available per core. Such jobs have to be spread to more machines. Therefore we added the **-m** *<processes per node>* option, which determines how many processes should be started per node. You can get a list of the mpiexec wrapper options with

```
$ mpiexec --help
```

which will print the list of mpiexec wrapper options, some of which are shown in table 6.22 on page 70, followed by help of native mpiexec of loaded MPI module.

--help | -h	prints this help and the help information of normal mpiexec
--show | -v	prints out which machines are used
-d	prints debugging information about the wrapper
--mpidebug	prints debugging information of the MPI lib, only Open MPI, needs TotalView
-n, -np <np>	starts <np> processes
-m <nm>	starts exactly <nm> processes on every host (except the last one)
-s, --spawn <ns>	number of processes that can be spawned with MPI_spawn; (np+ns) processes can be started in total
--listcluster	prints out all available clusters
--cluster <clname>	uses only cluster <clname>
--onehost	starts all processes on one host
--listonly	just writes the machine file, without starting the program
MPIHOSTLIST	specifies which file contains the list of hosts to use; if not specified, the default list is taken
MPIMACHINELIST	if --listonly is used, this variable specifies the name of the created host file, default is $HOME/host.list
--skip (<cmd>)	*(advanced option)* skips the wrapper and executes the <cmd> with given arguments. Default <cmd> with openmpi is **mpiexec** and with intelmpi is **mpirun**.

Table 6.22: The options of the interactive mpiexec wrapper

Passing environment variables from the master, where the MPI program is started, to the other hosts is handled differently by the MPI implementations.

We recommend that if your program depends on environment variables, you let the master MPI process read them and broadcast the value to all other MPI processes.

The following sections show how to use the different MPI implementations without those predefined module settings.

6.2.2 Open MPI

Open MPI (http://www.openmpi.org) is developed by several groups and vendors.

To set up the environment[80] for the Open MPI use

```
$ module load openmpi
```

This will set environment variables for further usage. The list of variables can be obtained with

```
$ module help openmpi
```

The compiler drivers are **mpicc** for C, **mpif77** and **mpif90** for FORTRAN, **mpicxx** and **mpiCC** for C++. To start MPI programs, **mpiexec** is used.

We strongly recommend using the environment variables $MPIFC, $MPICC, $MPICXX and $MPIEXEC set by the module system in particular because the compiler driver variables are set according to the latest loaded compiler module. Example:

```
$ $MPIFC -c prog.f90
$ $MPIFC prog.o -o prog.exe
$ $MPIEXEC -np 4 prog.exe
```

[80] Currently a version of Open MPI is the standard MPI in the cluster environment, so the corresponding module is loaded by default.

Refer to the manual page for a detailed description of **mpiexec**. It includes several helpful examples.

For quick reference we include some options here, see table 6.23 on page 71.

Open MPI provide a lot of tunables which may be adjusted in order to get more performance for an actual job type on an actual platform. We set some Open MPI tunables by default, usually using $OMPI* environment variables.

Option	Description
-n <#	Number of processes to start.
-H <**host1,..,hostN**>	Synonym for **-host**. Specifies a list of execution hosts.
-machinefile <**machinefile**>	Where to find the machinefile with the execution hosts.
-mca <**key**> <**value**>	Option for the Modular Component Architecture. This option e.g. specifies which network type to use.
-nooversubscribe	Does not oversubscribe any nodes.
-nw	Launches the processes and do not wait for their completion. mpiexec will complete as soon as successful launch occurs.
-tv	Launches the MPI processes under the TotalView debugger (old style MPI launch)
-wdir <**dir**>	Changes to the directory <dir> before the user's program executes.
-x <**env**>	Exports the specified environment variables to the remote nodes before executing the program.

Table 6.23: Open MPI mpiexec options

6.2.3 Intel MPI

Intel provides a commercial MPI library based on **MPICH2** from Argonne National Labs. It may be used as an alternative to Open MPI.

On Linux, Intel MPI can be initialized with the command

```
$ module switch openmpi intelmpi
```

This will set up several environment variables for further usage. The list of these variables can be obtained with

```
$ module help intelmpi
```

In particular, the compiler drivers **mpiifort**, **mpifc**, **mpiicc**, **mpicc**, **mpiicpc** and **mpicxx** as well as the MPI application startup scripts **mpiexec** and **mpirun** are included in the search path.[81] The compiler drivers **mpiifort**, **mpiicc** and **mpiicpc** use the Intel Compilers whereas **mpifc**, **mpicc** and **mpicxx** are the drivers for the GCC compilers. The necessary include directory $MPI_INCLUDE and the library directory $MPI_LIBDIR are selected automatically by these compiler drivers.

We strongly recommend using the environment variables $MPIFC, $MPICC, $MPICXX and $MPIEXEC set by the module system for building and running an MPI application. Example:

```
$ $MPIFC -c prog.f90
$ $MPIFC prog.o -o prog.exe
$ $MPIEXEC -np 4 prog.exe
```

The Intel MPI can basically be used in the same way as the Open MPI, except of the Open MPI-specific options, of course. You can get a list of options specific to the startup script of Intel MPI by

[81] Currently, these are not directly accessible, but obscured by the wrappers we provide.

```
$ $MPIEXEC -h
```

6.3 Hybrid Parallelization

The combination of MPI and OpenMP and/or autoparallelization is called *hybrid parallelization*. Each MPI process may be multi-threaded. In order to use hybrid parallelization the MPI library has to support it. There are four stages of possible support:

0. single – multi-threading is not supported.
1. funneled – only the main thread, which initializes MPI, is allowed to make MPI calls.
2. serialized – only one thread may call the MPI library at a time.
3. multiple – multiple threads may call MPI, without restrictions.

You can use the **MPI_Init_thread** function to query multi-threading support of the MPI implementation. Read more on this web page:
http://www.mpi-forum.org/docs/mpi22-report/node260.htm

In listing 7 on page 72 an example program is given which demonstrates the switching between threading support levels in case of a Fortran program. This program can be used to test if a given MPI library supports threading.

Listing 7: $MPIFC $PSRC/pis/mpi_threading_support.f90; a.out

```
1  PROGRAM tthr
2  USE MPI
3  IMPLICIT NONE
4  INTEGER :: REQUIRED, PROVIDED, IERROR
5  REQUIRED = MPI_THREAD_MULTIPLE
6  PROVIDED = -1
7  !  A call to MPI_INIT has the same effect as a call to
8  !  MPI_INIT_THREAD with a required = MPI_THREAD_SINGLE.
9  !CALL MPI_INIT(IERROR)
10 CALL MPI_INIT_THREAD(REQUIRED, PROVIDED, IERROR)
11 WRITE (*,*) MPI_THREAD_SINGLE, MPI_THREAD_FUNNELED, &
12 & MPI_THREAD_SERIALIZED, MPI_THREAD_MULTIPLE
13 WRITE (*,*) REQUIRED, PROVIDED, IERROR
14 CALL MPI_FINALIZE(IERROR)
15 END PROGRAM tthr
```

6.3.1 Open MPI

The Open MPI community site announces untested support for thread-safe operations.[82] The support for threading is disabled by default.

We provide some versions of Open MPI with threading support enabled.[83] These versions have the letters **mt** in the module names, e.g. **openmpi/1.6.5mt**. However, due to less-tested status of this feature, use it at own risk.

Note: The actual Open MPI version (1.6.x) is known to silently disable the InfiniBand transport iff the highest **multiple** threading level is activated. In this case the hybride program runs over IPoIB transport, offerung much worse performance than expected. Please be aware of this and do not use the **multiple** threading level without a good reason.

[82] http://www.open-mpi.org/faq/?category=supported-systems#thread-support
[83] Configured and compiled with *–enable-mpi-threads* option.

6.3.2 Intel MPI

Unfortunately, *Intel MPI* is not thread-safe by default.

To provide full MPI support inside parallel regions the program must be linked with the option *-mt_mpi* (Intel and GCC compilers) or *-lmpi_mt* instead of *-lmpi* (other compilers).

Note: If you specify one of the following options for the Intel Fortran Compiler, the thread-safe version of the library is used automatically:

1. -openmp
2. -parallel
3. -threads
4. -reentrancy
5. -reentrancy threaded

The **funneled** level is provided by default by the thread-safe version of the Intel MPI library. To activate other levels, use the **MPI_Init_thread** function.

7 Debugging

If your program is having strange problems, there's no need for immediate despair - try leaning back and thinking hard first:

- Which were the latest changes that you made? (A source code revision system e.g. SVN, CVS or RCS might help.)
- Reduce the optimization level of your compilation.
- Choose a smaller data set. Try to build a specific test case for your problem.
- Look for compiler messages and warnings.
- Use tools for a static program analysis (see chapter 7.1 on page 74).
- Try a dynamic analysis with appropriate compiler options (see chapter 7.2 on page 75).
- Reduce the number of CPUs in a parallel program; try a serial program run, if possible.
- Use a debugger like TotalView (see chapter 7.3.1 on page 76). Use the smallest case which shows the error.
- In case of an OpenMP program, use a thread-checking tool like the Oracle Thread Analyzer (see chapter 7.4.1 on page 77) or the Intel Inspector (see chapter 7.4.2 on page 78).
- If it is an OpenMP program, try to compile without optimization, e.g. with **-g -O0 -xopenmp=noopt** for the Oracle compilers.
- In case of an MPI program, use a parallel debugger like TotalView. Try another MPI implementation version and/or release.
- Try a different compiler. Maybe you have run into a compiler bug.

7.1 Static Program Analysis

First, an exact static analysis of the program is recommended for error detection. Today's compilers are quite smart and can detect many problems. Turn on a high verbosity level while compiling and watch for compiler warnings. Please refer to Chapter 5 for various compiler options regarding warning levels.

Furthermore, the tools listed in table 7.24 on page 74 can be used for static analysis.

lint	syntax check of C programs, distributed with Oracle Studio compilers (*module load studio*)
cppcheck	syntax check of C++ programs, downloadable at http://sourceforge.net/projects/cppcheck/
ftnchek	syntax check of FORTRAN 77 programs (with some FORTRAN 90 features), directly available at our cluster
Forcheck	Fortran source code analyzer and programming aid (commercial) http://www.forcheck.nl/
***plus*FORT**	a multi-purpose suite of tools for analyzing and improving Fortran programs (commercial) http://www.polyhedron.com/pf-plusfort0html

Table 7.24: Static program analysis tools

Sometimes program errors occur only with high (or low) compiler optimization. This can be a compiler error or a program error. If the program runs differently with and without compiler

optimizations, the module causing the trouble can be found by systematic bisecting. With this technique, you compile half of the application with the *right* options and the other half with the *wrong* options. If the program then fails, you will know which part causes the problem. Likewise, if the program runs fine afterwards, repeat the process for the part of the program causing the failure.

7.2 Dynamic Program Analysis

Many compilers offer options to perform runtime checks of the generated program, e.g. array bound checks or checks for uninitialized variables. Please study the compiler documentation and look for compiler options which enable additional runtime checks. Please note that such checks usually cause a slowdown of your application, so do not use them for production runs.

The **Intel Fortran** compiler allows you to turn on various runtime checks with the **-check** flag. You may also enable only certain conditions to be checked (e.g. **-check bounds**), please consult the compiler manual for available options.

The **Oracle Fortran** compiler does array bound checking with the option **-C** and global program analysis with the option **-Xlist**. Compiling with **-xcheck=init_local** initializes local variables to a value that is likely to cause an arithmetic exception if it is used before it is assigned by the program. Memory allocated by the ALLOCATE statement will also be initialized in this manner. SAVE variables, module variables, and variables in COMMON blocks are not initialized. Floating point errors like division by zero, overflows and underflows are reported with the option **-ftrap=%all**.

The Oracle compilers also offer the option **-xcheck=stkovf** to detect stack overflows at runtime. In case of a stack overflow a core file will be written that can then be analyzed by a debugger. The stack trace will contain a function name indicating the problem.

The **GNU C/C++** compiler offers the option **-fmudflap** to trace memory accesses during runtime. If an illegal access is detected, the program will halt. With **-fbounds-check** the array bound checking can be activated.

To detect *common errors with dynamic memory allocation*, you can use the library **libefence** (Electric Fence). It helps to detect two common programming bugs: software that overruns the boundaries of a *malloc()* memory allocation, and software that touches a memory allocation that has been released by *free()*. If an error is detected, the program stops with a segmentation fault and the error can easily be found with a debugger. To use the library, link with **-lefence**. You might have to reduce the memory consumption of your application to get a proper run. Furthtermore, note that for MPI programs, the Intel-MPI is the only MPI that is working with the efence library in our environment. Using other MPIs will cause error messages. For more information see the manual page (**man libefence**).

Memory leaks can be detected using TotalView (see chapter A.1.8 on page 98), the sampling collector (**collect -H**, see chapter 8.1 on page 79) or the open source instrumentation framework Valgrind (please refer to http://valgrind.org).

If a program with optimization delivers other results than without, floating point optimization may be responsible. There is a possibility to test this by optimizing the program carefully. Please note that the environment variables $FLAGS_FAST and $FLAGS_FAST_NO_FPOPT containing different sets of optimization flags for the last-loaded compiler module. If you use $FLAGS_FAST_NO_FPOPT flag instead of $FLAGS_FAST, the sequence of the floating point operations is not changed by the optimization, perhaps increasing the runtime.

Besides, you have to consider that on the x86 platform floating point calculations do not necessarily conform to IEEE standard by default, so rounding effects may differ between platforms.

7.3 Debuggers

A Debugger is a tool to control and look into a running program. It allows a programmer to follow the program execution step by step and see e.g. values of variables. It is a powerful tool for finding problems and errors in a program.

For debugging, the program must be translated with the option **-g** and optimization should be turned off to facilitate the debugging process. If compiled with optimization, some variables may not be visible while debugging and the mapping between the source code and the executable program may not be accurate.

A core dump can be analyzed with a debugger, if the program was translated with **-g**. Do not forget to increase the core file size limit of your shell if you want to analyze the core that your program may have left behind.

```
$ ulimit -c unlimited
```

But please do not forget to purge core files afterwards!

Note: You can easily find all the core files in your home dir with the following command:

```
$ find $HOME -type f -iname "core*rz.RWTH-Aachen.DE*"
```

In general we recommend using a full-screen debugger like TotalView or Oracle Studio to

- start your application and step through it,
- analyze a core dump of a prior program run,
- attach to a running program.

In some cases, e.g. in batch scripts or when debugging over a slow connection, it might be preferable to use a line mode debugger like **dbx** or **gdb**.

7.3.1 TotalView

The state-of-the-art debugger TotalView from Rogue Wave Software[84] can be used to debug serial and parallel FORTRAN, C and C++ programs. You can choose between different versions of TotalView with the module command.[85] From version 8.6 on, TotalView comes with the ReplayEngine. The ReplayEngine allows backward debugging or reverting computations in the program. This is especially helpful if the program crashed or miscomputed and you want to go back and find the cause.

In the appendix A on page 96, we include a TotalView *Quick Reference Guide*. We recommend a careful study of the *User Guide* and *Reference Guide* (http://www.roguewave.com/support/product-documentation/totalview.aspx) to find out about all the near limitless skills of TotalView debugger. The module is loaded with:

```
$ module load totalview
```

7.3.2 Oracle Solaris Studio

Oracle Solaris Studio includes a complete Integrated Development Environment (IDE) which also contains a full screen debugger for serial and multi-threaded programs. Furthermore, it provides a standalone debugger named *dbx* that can also be used by its GUI *dbxtool*.

In order to start a debugging session, you can attach to a running program with

```
$ module load studio
$ dbxtool - pid
```

or analyze a core dump with

[84] Etnus was renamed to TotalView Technologies which now belongs to Rogue Wave Software: http://www.roguewave.com/

[85] see chapter 4.3.2 on page 31

```
$ dbxtool - corefile
```
(if you know the name of your executable, you can also use this name instead of the dash (-)) or start the program under the control of the debugger with
```
$ $PSRC/pex/730|| dbxtool a.out
```

7.3.3 gdb

gdb is a powerful command line-oriented debugger. The corresponding manual pages as well as online manuals are available for further information.

7.3.4 pgdbg

pgdbg is a debugger with a GUI for debugging serial and parallel (multithreaded, OpenMP and MPI) programs compiled with the PGI compilers. To use it, first load the PGI module and then run the debugger:
```
$ module load pgi
$ pgdbg
```

7.3.5 Allinea ddt

Allinea **ddt** (Distributed Debugging Tool) is a debugger with a GUI for serial and parallel programs. It can be used for multithreaded, OpenMP and MPI applications. Furthermore, since version 2.6 it can handle GPGPU programs written with NVIDIA Cuda. For non-GPU programs, you should enable the check box *Run without CUDA support*. The module is located in the `DEVELOP` category and can be loaded with:
```
$ module load ddt
```
For full documentation please refer to: http://content.allinea.com/downloads/userguide.pdf
Note: If DDT is running in the background, e.g. using &:
```
$ ddt &
```
then this process may get stuck (some SSH versions cause this behaviour when asking for a password). If this happens to you, go to the terminal and use the fg or similar command to make DDT a foreground process, or run DDT again, without using &.

7.4 Runtime Analysis of OpenMP Programs

If an OpenMP program runs fine using a single thread but not multiple threads, there is probably a data sharing conflict or data race condition. This is the case if e.g. a variable which should be private is shared or a shared variable is not protected by a lock.

The presented tools will detect data race conditions during runtime and point out the portions of code which are not thread-safe.
Recommendation:
Never put an OpenMP code into production before having used a thread checking tool.

7.4.1 Oracle's Thread Analyzer

Oracle (Sun) integrated the Thread Analyzer, a data race detection tool, into the Studio compiler suite. The program can be instrumented while compiling, so that data races can be detected at runtime. The Thread Analyzer also supports nested OpenMP programs.

Make sure you have the version 12 or higher of the studio module loaded to set up the environment. Add the option **-xinstrument=datarace** to your compiler command line. Since additional functionality for thread checking is added the executable will run slower and need more memory. Run the program under the control of the **collect**[86] command
```
$ $PSRC/pex/740|| $CC $FLAGS_OPENMP -xinstrument=datarace $PSRC/C-omp-pi/pi.c
```

[86] more details are given in the analyzer section 8.1 on page 79

```
-lm $FLAGS_DEBUG
$ $PSRC/pex/740|| collect -r on a.out
```

You have to use more than one thread while executing, since only *occurring* data races are reported. The results can be viewed with **tha**, which contains a subset of the analyzer functionality, or the **analyzer**.

```
$ $PSRC/pex/740|| tha tha.1.er
```

7.4.2 Intel Inspector

The Intel Inspector tool is an easy to use thread and memory debugger for serial and parallel applications and is able to verify the correctness of multithreaded programs. It is bundled into the Intel Parallel Studio and provides a graphical and also command line interfaces (GUI and CLI). On Linux, you can run it by:

```
$ module load intelixe
$ inspxe-gui
```

To get a touch of how to use the command line interface type

```
$ inspxe-cl -help
```

More information may be found online:
http://software.intel.com/en-us/articles/intel-inspector-xe-documentation

8 Performance / Runtime Analysis Tools

This chapter describes tools that are available to help you assess the performance of your code, identify potential performance problems, and locate the part of the code where most of the execution time is spent.

Runtime analysis is no trivial matter and cannot be sufficiently explained in the scope of this document. An introduction to some of the tools described in this chapter will be given at workshops in Aachen and other sites in regular intervals. If you need help using these tools or if you need assistance when tuning your code, please contact the HPC group via the Service Desk: servicedesk@itc.rwth-aachen.de

The following chart provides an overview of the available tools and their field of use:

	Call Graph Based Analysis	Cache and Memory Analysis	OpenMP and Threading Analysis	MPI Analysis	Hardware Performance Counter
Oracle Performance Analyzer	x	x	x	x	x
Intel Amplifier XE (VTune)	x	x	x		x
Intel Trace Analyzer and Collector	x		x	x	x
Vampir	x		x	x	x
Scalasca	x		x	x	x
likwid-perfctr		x	x	x	x

Table 8.25: Performance Analysis Tools

8.1 Oracle Sampling Collector and Performance Analyzer

The Oracle Sampling Collector and the Performance Analyzer are a pair of tools that you can use to collect and analyze performance data for your serial or parallel application. The **collect** command line program gathers performance data by sampling at regular time intervals and by tracing function calls. The performance information is gathered in so-called experiment files, which can then be displayed with the **analyzer** GUI or the **er_print** command line after the program has finished. Since the collector is part of the Oracle compiler suite, the *studio compiler module* has to be loaded. However, you can analyze programs compiled with any x86-compatible compiler; the GNU or Intel compiler for example work as well.

8.1.1 The Oracle Sampling Collector

At first it is recommended to compile your program with the **-g** option (debug information enabled), if you want to benefit from source line attribution and the full functionality of the analyzer. When compiling C++ code with the *Oracle compiler* you can use the **-g0** option instead, if you want to enable the compiler to expand inline functions for performance reasons.

Link the program as usual and then start the executable under the control of the *Sampling Collector* with the command

```
$ $PSRC/pex/810|| collect a.out
```

or with the analyzer GUI (select *Collect Experiment* in the *File* menu).

By default, profile data will be gathered every 10 milliseconds and written to the experiment file **test.1.er**. The filename number will be automatically incremented on subsequent experiments. In fact the experiment file is an entire directory with a lot of information. You can manipulate these with the regular Linux commands, but it is recommended to use the *er_mv, er_rm, er_cp* utilities to move, remove or copy these directories. This ensures for example that time stamps are preserved.

The **-g** *experiment_group*.**erg** option bundles experiments to an experiment group. The result of an experiment group can be displayed with the Analyzer (see below)

```
$ analyzer experiment_group
```

By selecting the options of the collect command, many different kinds of performance data can be gathered. Just invoking **collect -h** will print a complete list including available hardware counters. The most useful combinations of raw hardware counters are joined in "Aliased HW counters" on top of the list. Various hardware-counter event-types can be chosen for collecting. The maximum number of theoretically simultaneously usable counters on available hardware platforms varies (e.g. 7 on Intel Nehalem). However, it is hardly possible to use more than 4 counters in the same measurement because some counters use the same resources and thus conflict with each other. Favorite choices are given in table 8.27 on page 81 for Nehalem and Westmere CPUs.

This example counts the floating point operations on different units in addition to the clock profiling on Nehalem processors:

```
$ $PSRC/pex/811|| collect -p on -h cycles,on,fp_comp_ops_exe.x87,on,\\
fp_comp_ops_exe.mmx,on,fp_comp_ops_exe.sse_fp a.out
```

The most important collect options are listed in table 8.26 on page 80.

-p on | off | hi | lo	Clock profiling ('hi' needs to be supported on the system)
-H on | off	Heap tracing
-m on | off	MPI tracing
-h *counter0*,on,...	Hardware Counters
-j on | off	Java profiling
-S on | off | *seconds*	Periodic sampling (default interval: 1 sec)
-o *experimentfile*	Output file
-d *directory*	Output directory
-g *experimentgroup*	Output file group
-L *size*	Output file size limit [MB]
-F on | off	Follows descendant processes
-C *comment*	Puts comments in the notes file for the experiment

Table 8.26: Collect options

8.1.2 Sampling of MPI Programs

Sampling of MPI programs is something for toughies, because of additional complexity dimension. Nevertheless it is possible with **collect** in at least two ways:

Wrap the MPI binary Use *collect* to measure each MPI process individually:

```
$ mpiexec <opt> collect <opt> a.out <opt>
```

This technique is no longer supported to collect MPI trace data, but it can still be used for all other types of data. Each process write its own trace, thouch resulting in multiple **test.∗.er** profiles. These profiles can be vieved separately or alltogether, giving an overview over the whole application run.

-h cycles,on,insts,on	Cycle count, instruction count. The quotient is the CPI rate (clocks per instruction). The MHz rate of the CPU multiplied with the instruction count divided by the cycle count gives the MIPS rate. Alternatively, the MIPS rate can be obtained as the quotient of instruction count and runtime in seconds.. In general high MIPS values are "good", but on bad-scaling parallel programs high MIPS values are a sign of busy waiting (spinning).
-h fp_comp_ops_exe.x87,on, fp_comp_ops_exe.mmx,on, fp_comp_ops_exe.sse_fp	Floating point counters on different execution units. The sum divided by the runtime in seconds gives the FLOPS rate. However, FLOPS rate is measured by LIKWID (see chapter 8.5 on page 86) much easier.
-h cycles,on,dtlbm,on	A high rate of DTLB misses indicates an unpleasant memory access pattern of the program. Large pages might help.
-h l3h,on,l3m,on -h l2h,on,l2m,on -h dch,on,dcm,on	L3 cache hits (w/o Snoop) and misses L2 cahce hits and misses L1 D-cache hits and misses

Table 8.27: Some hardware counter available for profiling with **collect** on Nehalem CPUs

We found out that all processes must run on localhost in order to get the profiled data. Example (run 2 MPI processes on localhost with 2 threads each, look for instructions and cycles harware counter):

```
$ $PSRC/pex/813|| OMP_NUM_THREADS=2 mpiexec -np 2 -H ‘hostname‘ collect -h cycles,on,insts,on a.out; analyzer test.*.er
```

Wrap the *mpiexec* Use *collect* for MPI profiling to manage collection of the data from the constituent MPI processes, collect MPI trace data, and organize the data into a single "founder" experiment, with "subexperiments" for each MPI process:

```
$ collect <opt> -M <MPI> mpiexec <opt> - a.out <opt>
```

MPI profiling is based on the open source VampirTrace 5.5.3 release. It recognizes several VampirTrace environment variables. For further information on the meaning of these variables, see the VampirTrace 5.5.3 documentation.

Use the **-M** option to set the version of MPI to be used; selectable values are OMPT, CT, OPENMPI, MPICH2, MVAPICH2, INTEL. As clear from the names, for Open MPI the 'OPENMPI' value and for Intel MPI the 'INTEL' value are to be used.

Also here all processes must run on localhost in order to get the profiled data.

Open MPI example (as above, but additionally collect the MPI trace data):

```
$ $PSRC/pex/814|| OMP_NUM_THREADS=2 collect -h cycles,on,insts,on -M OPENMPI mpiexec -np 2 -H ‘hostname‘ -- a.out; analyzer test.1.er
```

Intel MPI example (same as above)

```
$ $PSRC/pex/815|| OMP_NUM_THREADS=2 collect -h cycles,on,insts,on -M INTEL mpiexec -np 2 -H ‘hostname‘ -- a.out; analyzer test.1.er
```

When *collect* is run with a large number of MPI processes, the amount of experiment data might become overwhelming. Try to start your program with as few processes as possible.

8.1.3 The Oracle Performance Analyzer

Collected experiment data can be evaluated with the **analyzer** GUI:

```
$ $PSRC/pex/810|| analyzer test.1.er
```

A program call tree with performance information can be displayed with the locally developed utility **er_view**:
```
$ $PSRC/pex/810.1|| er_view test.1.er
```
There is also a command line tool **er_print**. Invoking **er_print** without options will print a command overview. Example:
```
$ $PSRC/pex/810.2|| er_print -fsummary test.1.er | less
```

If no command or script arguments are given, **er_print** enters interactive mode to read commands from the input terminal. Input from the input terminal is terminated with the quit command.

8.2 Intel Tools

The Intel Corporation offers a variety of goods in the software branch, including many very useful tools, compilers and libraries. However, due to agile marketing division, you never can be sure what the name of a particular product today is and what it will be the day after tomorrow. We try to catch up this evolution. But don't panic if you see some outdated and/or shortened names.

The Intel **Studio** product bundles[87] provides an integrated development, performance analysis and tuning environment, with features like highly sophisticated compilers and powerful libraries, monitoring the hardware performance counters, checking the correctness of multi-threaded programs.

The basic components are:

- Intel Composer (ch. 5.5 on page 48), including Intel MKL (ch. 9.3 on page 88),
- Intel MPI Library (see chapter 6.2.3 on page 71),
- Intel Trace Analyzer and Collector (see chapter 8.2.2 on page 83),
- Intel Inspector (ch. 7.4.2 on page 78)
- Intel VTune Amplifier (see chapter 8.2.1 on page 82)
- Intel Parallel Advisor (not yet described here).

All tools but VTune Amplifier can be used with no restrictions. All tools are designed to work with binaries built with the Intel compilers, but in general other compilers can be used as well. In order for the tools to show performance data in correlation to your programs source code, you need to compile with debug information (**-g**).

8.2.1 Intel VTune Amplifier

The Intel VTune Amplifier is a powerful threading and performance optimization tool for Fortran, C/C++, ASM and more.

It has its own GUI as well as CLI and provides a whole bunch of predefined analysis types. It is also possible to define own analysis types.

Load the VTune Amplifier module and start the GUI:
```
$ module load intelvtune
$ amplxe-gui
```
Many predefined analysis types like

- Basic Hotspots

[87] ... bearing a lot of names: *Parallel Studio*, *Parallel Studio 2011*, *Parallel Studio XE*, *Cluster Toolkit*, *Cluster Studio*, *Cluster Studio XE*, *Cluster Studio XE 2013* - the area of collection is still open!

- Advanced Hotspots
- Concurrency
- Locks and Waits

are available on any machine in the HPC-Cluster.

The *hardware counter based analysis*[88] like

- General Exploration
- CPU Specific Analysis (Bandwidth, ...)

requires special settings. These settings are only implemented on the **cluster-linux-tuning** front end. Therefore, interactive hardware counter based experiments can be done on this front end only.

For longish test runs you are kindly invited to use the batch system. You can run Intel VTune Amplifier in the batch in two ways:

- start an interactive GUI session (see ch. 4.4.1 on page 42) and start the GUI as above;
- define an analysis via CLI[89] in a batch job; after the job has finished examine the output files using the GUI on a front end.

Note: for activating the hardware counter support (needed for *hardware counter based analysis*) you have to add this option to your batch job:
`#BSUB -app vtune`
This option also set your job to be exclusive - mind the resource consumption!

Batch job examples (with hardware counter support):

- via GUI, interactive - **$PSRC/pis/LSF/GUI_VTune.sh**
- via CLI, analyse after job run - **$PSRC/pis/LSF/serial_job_CLI_VTune.sh**

or online at https://doc.itc.rwth-aachen.de/display/CC/intelvtune

For details on how to use **VTune Amplifier** please contact the HPC Group or attend one of our regular workshops.

8.2.2 Intel Trace Analyzer and Collector (ITAC)

The Intel Trace Collector (ITC) is primarily designed to investigate MPI applications. The Intel Trace Analyzer (ITA) is a graphical tool that analyzes and displays the trace files generated by the ITC. Both ITC and ITA are quite similar to Vampir (8.3.2 on page 85).

The tools help to understand the behavior of the application and to detect inefficient communication and performance problems. Please note that these tools are designed to be used with Intel or GNU compilers in conjunction with Intel MPI.

On Linux, initialize the environment with
`$ module load intelitac`.

[88] There is no need to be registered in a special group (as described in previous releases of this document) to use VTune Amplifier with hardware counters anymore.

[89] The most convenient way to define the CLI command is by using the special service of the **amplxe-gui** GUI: after you choose the analysis type, binary to run, options and so on, click on *Command Line...* button right down in the window.

Profiling of dynamically linked binaries without recompilation: This mode is applicable to programs which use Intel MPI. In this mode, only MPI calls will be traced, which often is sufficient for general investigation of the communication behaviour.

Run the program under the control of ITC by using the **-trace** command line argument of the Intel **mpiexec**. A message from the Trace Collector should appear indicating where the collected information is saved in form of an "*.stf*"-file. Use the ITA GUI to analyze this trace file. On Linux, start the Analyzer GUI with

```
$ traceanalyzer <somefile>.stf.
```

Example:

```
$ $PSRC/pex/890|| $MPIEXEC -trace -np 2 a.out || traceanalyzer a.out.stf
```

There also exists a command line interface of the Trace Analyzer on Linux. Please refer to the manual.

Compiler-driven Subroutine Instrumentation allows you to trace the whole program additionally to the MPI library. In this mode the user-defined non-MPI functions are traced as well. Function tracing can easily generate huge amounts of trace data, especially for function-call intensive and object-oriented programs. For the Intel compilers, use the flag **-tcollect** to enable the collecting. The switch accepts an optional argument to specify the collecting library to link. For example, for non-MPI applications you can select **libVTcs**: **-tcollect=VTcs**. The default value is **VT**.

Use the **-finstrument-function** flag with GNU Compilers to compile the object files that contain functions to be traced. ITC is then able to obtain information about the functions in the executable.

Run the compiled binary the usual way. After the program terminates, you get a message from the Trace Collector which says where the collected information is saved (an **.stf** file). This file can be analyzed with the ITA GUI in an usual way.

Linux Example (generate about 3GB of data!):

```
$ $PSRC/pex/891|| $MPICC -tcollect pi.c || $MPIEXEC -trace -np 2 a.out ||
traceanalyzer a.out.stf
```

There are a lot of other features and operating modes, e.g. binary instrumentation with **itcpin**, tracing of non-correct programs (e.g. containing deadlocks), tracing MPI File IO and more.

More documentation on ITAC may be found in */opt/intel/itac/<VERSION>/doc* and at http://www.intel.com/cd/software/products/asmo-na/eng/cluster/tanalyzer/index.htm.

8.3 VI-HPS Tools

The Virtual Institute - High Productivity Supercomputing (VI-HPS)[90] is an union of notable partner institutions, each with a strong record of high-performance computing research. The mission is to improve the quality and accelerate the development process of simulation programs. For this purpose integrated state-of-the-art programming tools for high-performance computing are developed. A range of these tools is available in the HPC-Cluster and located mainly on the UNITE category of the module system:

```
$ module load UNITE
```

The VI-HPS Tools Guide[91] is updated regularly and contains a brief description of all VI-HPS tools. We do not want to double this document here thus we describe only some tools in very brief manner.

[90] http://www.vi-hps.org/

[91] http://www.vi-hps.org/upload/material/general/ToolsGuide.pdf

8.3.1 Score-P

The Score-P measurement infrastructure is a tool for profiling, event tracing, and online analysis. Load it from the UNITE module category by
```
$ module load scorep
```

Instrumentation: To perform automatic instrumentation, simply replace your compiler command with the appropriate Score-P wrapper, for example:

`$CC` → `scorep $CC` `$CXX` → `scorep $CXX` `$FC` → `scorep $FC`
If your application uses MPI, you have to specify the MPI-compiler-wrapper for *Score-P* to ensure correct linking of the MPI libraries, e.g. `$MPICC` → `scorep $MPICC` for C code.

Measurement: An instrumented binary can then be executed as usually and will generate measurement data during its execution. There are several environment variables to control the behavior of the measurement facility within the binary. *Note:* Tracing (default: OFF) can cause substantial additional overhead and may produce lots of data, which will ultimately perturb your application runtime behavior during measurement.

Please refer to the *Score-P* documentation[92] for more details.

Analysis: Use Vampir, Scalasca or other tools.

8.3.2 Vampir

Vampir is a tool for the visualization of data collected by the instrumentation and measurement package *scorep*[93].

To start the Vampir GUI and open a trace file with the *Vampir*:
```
$ module load vampir
$ vampir tracefilename.otf2
```

Example in C, summing up usage of Score-P and Vampir:
```
$ $PSRC/pex/860|| scorep $MPICC $FLAGS_DEBUG $PSRC/cmj/*.c
$ $PSRC/pex/860|| $MPIEXEC -np 4 -H ‘hostname‘ -x SCOREP_EXPERIMENT_DIRECTORY=tracing
-x SCOREP_ENABLE_TRACING=1 -x SCOREP_ENABLE_PROFILING=0 a.out
$ $PSRC/pex/860|| vampir tracing/traces.otf2
```

Take a look at the tutorials: http://www.vampir.eu/tutorial

8.3.3 Scalasca

Scalasca is a performance analysis tool suite designed to spot typical performance problems in parallel applications with large counts of processes or threads. Scalasca displays a large number of metrics in a tree view, describing your application run. Scalasca presents different classes of metrics to you: generic, MPI-related and OpenMP-related ones.

Load Scalasca (and Cube) from the UNITE module category by
```
$ module load scalasca
```

Instrumentation: Use Score-P, see 8.3.1 on page 85. The `skin` also known as `scalasca -instrument` is deprecated in favour of `scorep` instrumentater.

[92] https://silc.zih.tu-dresden.de/scorep-current/pdf/scorep.pdf
[93] The *vampirtrace* is deprecated.

Execution: Use `scalasca -analyze` (short `scan`) as prefix to $MPIEXEC to control the Score-P measurement environment during the execution of the target application.

Visualization: To start analysis of your trace data call `square` *scalascaDataDirectory* where *scalascaDataDirectory* is the directory created during your program execution. This will bring up the `cube` GUI and display performance data about your application. Please refer to the documentation[94] for more details.

Example in C, summing up all steps:

```
$ $PSRC/pex/870|| scorep $MPICC $FLAGS_DEBUG $PSRC/cmj/*.c
$ $PSRC/pex/870|| scan $MPIEXEC "-show -H ‘hostname‘" -np 4 a.out
$ $PSRC/pex/870|| square scorep_a_4_sum
```

8.3.4 MUST

MUST[95] is a runtime error detection tool for MPI applications. It detects usage errors of the MPI at runtime and reports them to the user. It provides a wide range of correctness checks, including MPI deadlock detection, resource leak detection, datatype matching, and detection of communication buffer overlaps.

Take a look at the tutorial[96] in the PPCES event[97] series.

Load MUST from the UNITE module category by

```
$ module load must
```

Example in C:

```
$ $PSRC/pex/875|| $MPICC $FLAGS_DEBUG $PSRC/cmj/*.c
$ $PSRC/pex/875|| mustrun -np 4 -H ‘hostname‘ a.out
$ $PSRC/pex/875|| konqueror MUST_Output.html
```

8.4 Runtime Analysis with gprof

With **gprof**, a runtime profile can be generated. The program must be translated and linked with the option **-pg**. During the execution a file named **gmon.out** is generated that can be analyzed by

```
$ gprof program
```

With **gprof** it is easy to find out the number of the calls of a program module, which is a useful information for inlining.

Note: *gprof* assumes that all calls of a module are equally expensive, which is not always true. We recommend using the Callers-Callees info in the Oracle Performance Analyzer to gather this kind of information as it is much more reliable. However, gprof is useful to get the *exact* function call counts.

8.5 LIKWID

LIKWID ("Like I Knew What I'm Doing") is a set of easy to use command line tools to support optimization. It is targeted towards performance oriented programming in a Linux environment, does not require any kernel patching, and is suitable for Intel and AMD processor architectures. Multithreaded and even hybrid shared/distributed-memory parallel code is supported.

[94] http://www.scalasca.org/software/scalasca-2.x/documentation.html
[95] http://www.itc.rwth-aachen.de/MUST and http://www.vi-hps.org/tools/must.html
[96] https://doc.itc.rwth-aachen.de/download/attachments/20056127/2016-03-17_PPCES_Correctness_Tools.pdf
[97] https://www.itc.rwth-aachen.de/ppces

The usage of LIKWID requires special permissions. You need to be added to the **likwid** group (via the Service Desk servicedesk@itc.rwth-aachen.de).

The LIKWID module is loaded with:

```
$ module load likwid
```

The most relevant LIKWID tools are:

- **likwid-features** can display and alter the state of the on-chip hardware prefetching units in Intel x86 processors.
- **likwid-topology** probes the hardware thread and cache topology in multicore, multi-socket nodes. Knowledge like this is required to optimize resource usage like, e.g., shared caches and data paths, physical cores, and ccNUMA locality domains in parallel code. Example:
  `$ likwid-topology -g`
- **likwid-perfctr** measures performance counter metrics over the complete runtime of an application or, with support from a simple API, between arbitrary points in the code. Although it is possible to specify the full, hardware-dependent event names, some predefined event sets simplify matters when standard information like memory bandwidth or Flop counts is needed.
- **likwid-pin** enforces thread-core affinity in a multi-threaded application "from the outside", i.e. without changing the source code. It works with all threading models that are based on POSIX threads, and is also compatible with hybrid (MPI + threads, e.g. OpenMP) programming. Sensible use of *likwid-pin* requires correct information about thread numbering and cache topology, which can be delivered by *likwid-topology* (see above). Example:
  `$ likwid-pin -c 0,4-6 ./a.out`

  You can pin with the following numberings:

  1. Physical numbering of OS.
  2. Logical numbering inside node. e.g. `-c N:0-3`
  3. Logical numbering inside socket. e.g. `-c S0:0-3`
  4. Logical numbering inside last level cache group. e.g. `-c C0:0-3`
  5. Logical numbering inside NUMA domain. e.g. `-c M0:0-3`

  You can also mix domains separated by `@` letter, e.g. `-c S0:0-3@S1:0-3`

  If you ommit the `-c` option *likwid-pin* will use all processors available on the node with physical cores first. It will also set the OMP_NUM_THREADS environment variable with as many threads as specified in your pin expression if OMP_NUM_THREADS is not set in your environment.

For each tool a man page and built-in help (accessible by `-h` flag) is available.

9 Application Software and Program Libraries

9.1 Application Software

You can find a list of available application software and program libraries form several ISVs at https://doc.itc.rwth-aachen.de/display/CC/Installed+software

As for the compiler and MPI suites, we also offer environment variables for the mathematical libraries to make usage and switching easier. These are **FLAGS_MATH_INCLUDE** for the include options and **FLAGS_MATH_LINKER** for linking the libraries. If loading more than one mathematical module, the last loaded will overwrite and/or modify these variables. However (almost) each module sets extra variables that will not be overwritten.

9.2 BLAS, LAPACK, BLACS, ScaLAPACK, FFT and other libraries

If you want to use BLAS, LAPACK, BLACS, ScaLAPACK or FFT you are encouraged to read the chapters about optimized libraries: Intel MKL (recommended, see 9.3 on page 88), Oracle (Sun) Performance Library (see 9.4 on page 89), ACML (see 9.5 on page 90). The optimized libraries usually provide very good performance and do not only include the above-mentioned but also some other libraries.

Alternatively, you are free to use the native Netlib implementations - just download the source and install the libraries in your home.

Note: The self-compiled versions from Netlib usually provide lower performance than the optimized versions.

9.3 MKL - Intel Math Kernel Library

The Intel Math Kernel Library (Intel MKL) is a library of highly optimized, extensively threaded math routines for science, engineering, and financial applications.

Intel MKL contains an implementation of BLAS, BLACS, LAPACK and ScaLAPACK, Fast Fourier Transforms (FFT) complete with FFTW[98] interfaces, Sparse Solvers (Direct - PARDISO, Iterative - FGMRES and Conjugate Gradient Solvers), Vector Math Library and Vector Random Number Generators. The Intel MKL contains a couple of OpenMP parallelized routines, and up to version 10.0.3.020 runs in parallel by default if it is called from a non-threaded program. Be aware of this behavior and disable parallelism of the MKL if needed. The number of threads the MKL uses is set by the environment variable **OMP_NUM_THREADS** or **MKL_NUM_THREADS**.

There are two possibilties for calling the MKL routines from C/C++.

1. **Using BLAS**
   You can use the Fortran-style routines directly. Please follow the Fortran-style calling conventions (call-by-reference, column-major order of data). Example:
   ```
   $ $PSRC/pex/950|| $CC $FLAGS_MATH_INCLUDE -c $PSRC/psr/useblas.c
   $ $PSRC/pex/950|| $FC $FLAGS_MATH_LINKER $PSRC/psr/useblas.o
   ```

2. **Using CBLAS**
   Using the BLAS routines with the C-style interface is the preferred way because you don't need to know the exact differences between C and Fortran and the compiler is able to report errors before runtime. Example:
   ```
   $ $PSRC/pex/950.1|| $CC $FLAGS_MATH_INCLUDE -c $PSRC/psr/usecblas.c
   $ $PSRC/pex/950.1|| $CC $FLAGS_MATH_LINKER $PSRC/psr/usecblas.o
   ```

[98] http://www.fftw.org/

Please refer to Chapter *Language-specific Usage Options* in the Intel MKL User's Guide[99] for details with mixed language programming.

Starting with version 11 of Intel compiler, a version of MKL is included in the compiler distribution and the environment is initialized if the compiler is loaded.

To use Intel MKL with another compiler, load this compiler at last and then load the MKL environment. To initialize the Intel MKL environment, use
`$ module load LIBRARIES; module load intelmkl`.

This will set the environment variables **FLAGS_MKL_INCLUDE** and **FLAGS_MKL_LINKER** for compiling and linking, which are the same as the **FLAGS_MATH_..** if the MKL module was loaded last. These variables let you use at least the BLAS and LAPACK routines of Intel MKL.

To use other capabilities of Intel MKL, please refer to the Intel MKL documentation:
http://software.intel.com/en-us/articles/intel-math-kernel-library-documentation
The Intel MKL Link Line Advisor may be great help in linking your program:
http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor

The BLACS and ScaLAPACK routines use either Open MPI or Intel MPI, thus you have to compile using MPI compiler wrappers. We introduced **FLAGS_MKL_SCALAPACK_LINKER** environment variable for simplification of linking a program which uses BLACS or ScaLAPACK with Intel, GCC and PGI compilers. Example:

```
$ $PSRC/pex/950.2|| $MPICC $FLAGS_MATH_INCLUDE -c ex1.f
$ $PSRC/pex/950.2|| $MPIFC $FLAGS_MATH_LINKER $FLAGS_MKL_SCALAPACK_LINKER ex1.o
```

9.4 The Oracle (Sun) Performance Library

The Oracle (Sun) Performance Library is part of the Oracle Studio software and contains highly optimized and parallelized versions of the well-known standard public domain libraries available from Netlib http://www.netlib.org: LAPACK version 3, BLAS, FFTPACK version 4 and VFFTPACK version 2.1 from the field of linear algebra, Fast Fourier transforms and solution of sparse linear systems of equations (Sparse Solver **SuperLU**, see http://crd.lbl.gov/~xiaoye/SuperLU/).

The studio module sets the necessary environment variables.

To use the Oracle performance library link your program with the compiler option **-xlic_lib=sunperf**. The performance of FORTRAN programs using the BLAS-library and/or intrinsic functions can be improved with the compiler option **-xknown_lib=blas,intrinsics**. The corresponding routines will be inlined if possible.

The Performance Library contains parallelized sparse BLAS routines for matrix-matrix multiplication and a sparse triangular solver. Linpack routines are no longer provided. It is strongly recommended to use the corresponding LAPACK routines instead.

Many of the contained routines have been parallelized using the shared memory programming model. Compare the execution times! To use multiple threads set the **OMP_NUM_THREADS** variable accordingly.

```
$ $PSRC/pex/920|| export OMP_NUM_THREADS=4;
$ $PSRC/pex/920|| $CC $FLAGS_MATH_INCLUDE $FLAGS_MATH_LINKER $PSRC/psr/useblas.c
```

The number of threads used by the parallel Oracle Performance Library can also be controlled by a call to its **use_threads(n)** function, which overrides the OMP_NUM_THREADS value.

Nested parallelism is not supported; Oracle Performance Library calls made from a parallel region will not be further parallelized.

[99] http://software.intel.com/sites/products/documentation/hpc/mkl/mkl_userguide_lnx/index.htm

9.5 ACML - AMD Core Math Library

The AMD Core Math Library (ACML) incorporates BLAS, LAPACK and FFT routines that are designed for performance on AMD platforms, but the ACML works on Intel processors as well. There are OpenMP parallelized versions of this library, are recognizable by an *_mt* appended to the version string. If you use the OpenMP version don't forget to use the OpenMP flags of the compiler while linking.

To initialize the environment, use
`$ module load LIBRARIES; module load acml`. This will set the environment variables **FLAGS_ACML_INCLUDE** and **FLAGS_ACML_LINKER** for compiling and linking, which are the same as the **FLAGS_MATH_..** if the ACML module was loaded last.

Example:

```
$ $PSRC/pex/941|| $CC $FLAGS_MATH_INCLUDE -c $PSRC/psr/useblas.c
$ $PSRC/pex/941|| $FC $FLAGS_MATH_LINKER $PSRC/psr/useblas.o
```

However, given the current dominance of Intel-based processors in the cluster, we do not recommend using ACML and propose to use the Intel MKL instead.

9.6 NAG Numerical Libraries

The NAG Numerical Libraries provide a broad range of reliable and robust numerical and statistical routines in areas such as optimization, PDEs, ODEs, FFTs, correlation and regression, and multivariate methods, to name just a few.

The following NAG Numerical Components are available:

1. NAG **C** Library: A collection of over 1,000 algorithms for mathematical and statistical computation for C/C++ programmers. Written in C, these routines can be accessed from other languages, including C++ and Java.

2. NAG **Fortran** Library: A collection of over 1,600 routines for mathematical and statistical computation. This library remains at the core of NAG's product portfolio. Written in Fortran, the algorithms are usable from a wide range of languages and packages including Java, MATLAB, .NET/C# and many more.

3. NAG **SMP** Library: A numerical library containing over 220 routines that have been optimized or enhanced for use on Symmetric Multi-Processor (SMP) computers. The NAG SMP Library also includes the full functionality of the NAG Fortran Library. It is easy to use and link due to identical interface to the NAG Fortran Library. On his part, the NAG SMP library uses routines from the BLAS/LAPACK library.

4. NAG **SMP for the Xeon Phi Coprocessor** Library: developed in conjunction with Intel to harness the performance of the Intel Xeon Phi coprocessor. Many of the algorithms in this Library are tuned to run significantly faster on the coprocessor both in offload or native modes.

5. NAG **Parallel** Library: A high-performance computing library consisting of 180 routines that have been developed for distributed memory systems. The interfaces have been designed to be as close as possible to equivalent routines in the NAG Fortran Library. The components of the NAG Parallel Library hide the message passing (MPI) details in underlying tiers (BLACS, ScaLAPACK).

6. NAG **Toolbox for *MATLAB***: A large and comprehensive numerical toolkit that both complements and enhances MATLAB. The NAG Toolbox for MATLAB contains over 1500 functions that provide solutions to a vast range of mathematical and statistical problems.

To use the NAG components you have to load the LIBRARIES module environment first:
```
$ module load LIBRARIES
```
To find out which versions of NAG libraries are available, use
```
$ module avail nag
```
To set up your environment for the appropriate version, use the **module load** command, e.g. for the NAG FORTRAN library (Mk23):
```
$ module load nag/fortran_mark23
```
This will set the environment variables **FLAGS_MATH_INCLUDE**, **FLAGS_MATH_LINKER** and also **FLAGS_NAG_INCLUDE**, **FLAGS_NAG_LINKER**.

Example:
```
$ $PSRC/pex/970|| $FC $FLAGS_MATH_INCLUDE $FLAGS_MATH_LINKER $PSRC/psr/usenag.f
```

Note: All above mentioned libraries are installed as 64bit versions only.

Note: All libraries usually needs in turn an implementation of a BLAS/LAPACK library. If using the Intel compiler, the enclosed implementation of Intel MKL will be used automatically if you use the **FLAGS_MATH_INCLUDE** and **FLAGS_MATH_LINKER** flags. If using the GCC compiler, please load also the ACML module (see chapter 9.5 on page 90) and use the **FLAGS_MATH_INCLUDE** and **FLAGS_MATH_LINKER** environment variables.

The **FLAGS_NAG_INCLUDE** and **FLAGS_NAG_LINKER** variables provide a possibility of using NAG libraries with other BLAS/LAPACK implementations than mentioned.

Note: The **smp_Phi** library will work with Intel compiler on hosts with MIC devices only. Compile for host+MIC (offload) in the same way as when using **smp** library using the **FLAGS_MATH_INCLUDE** and **FLAGS_MATH_LINKER** flags.
When cross-compiling for MIC device, link the **smp_Phi** library statically, e.g.
```
$  $FC $FLAGS_MATH_INCLUDE test.f90 -mmic -mkl -Bstatic
-L/rwthfs/rz/SW/NAG/mmu/smp_Phi/intel_64_mark23/lib/mic -lnagsmp
```
Set the **NAG_KUSARI_FILE** envvar on the MIC device to the same value as on the host before starting cross-compiled binary.

Note: The **parallel** library needs an implementation of a BLACS/ScaLAPACK and those need a MPI library. If using the Intel compiler, the enclosed implementation of Intel MKL will be used automatically to provide BLACS/ScaLAPACK if you use the **FLAGS_MATH_INCLUDE** and **FLAGS_MATH_LINKER** flags. However, the MKL implementation of BLACS/ScaLAPACK is known to run with Intel MPI only, so you have to switch your MPI by typing **module switch openmpi intelmpi** *before* loading the NAG **parallel** library. The usage of any another compiler and/or BLACS/ScaLAPACK library with the NAG **parallel** library is in principle possible but not supported through the modules now.

Note: The NAG Toolbox for MATLAB is tightly integrated into appropriate MATLAB versions, so you do not need to load any additional modules.

Would You Like To Know More? http://www.nag.co.uk/numeric/numerical_libraries.asp

9.7 TBB - Intel Threading Building Blocks

Intel Threading Building Blocks is a runtime-based threaded parallel programming model for C++ code. It consists of a template-based runtime library to help you to use the performance of multicore processors. More information can be found at http://www.threadingbuildingblocks.org/.

A release of TBB is included into Intel compiler releases and thus no additional module needs to be loaded.

For other compilers (e.g. GCC), load the standalone TBB version form LIBRARIES area:
```
$ module load LIBRARIES; module load inteltbb
```
Use the environment variables $LIBRARY_PATH and $CPATH for compiling and linking. To link TBB set the **-ltbb** flag. With **-ltbb_debug** you may link a version of TBB

which provides some debug help.

Linux Example:

```
$ $PSRC/pex/961|| $CXX -O2 -DNDEBUG -I$CPATH -o ParSum ParallelSum.cpp -ltbb
$ $PSRC/pex/961|| ./ParSum
```

Use the debug version of TBB:

```
$ $PSRC/pex/962|| $CXX -O0 -g -DTBB_DO_ASSERT $CXXFLAGS -I$CPATH -o
ParSum_debug ParallelSum.cpp -ltbb_debug
$ $PSRC/pex/962|| ./ParSum_debug
```

9.8 R_Lib

The r_lib is a Library that provides useful functions for time measurement, processor binding and memory migration, among other things. It can be used under Linux. An r_lib library version for Windows is under development.

Example:

```
$ $PSRC/pex/960|| $CC -L/usr/local_rwth/lib64 -L/usr/local_rwth/lib -lr_lib
-I/usr/local_rwth/include $PSRC/psr/rlib.c
```

The following sections describe the available functions for C/C++ and Fortran.

9.8.1 Timing

double r_ctime(void) - returns user and system CPU time of the running process and its children in seconds
double r_rtime(void) - returns the elapsed wall clock time in seconds
char* r_time(void) - returns the current time in the format hh:mm:ss
char* r_date(void) - returns the current date in the format yy.mm.dd

Example in C

```
#include "r_lib.h"
/* Real and CPU time in seconds as double */
double realtime, cputime;
realtime = r_rtime();
cputime = r_ctime();
```

and in Fortran

```
! Real and CPU time in seconds
REAL*8 realtime, cputime, r_rtime, r_ctime
realtime = r_rtime()
cputime = r_ctime()
```

Users' CPU time measurements have a lower precision and are more time-consuming. In case of parallel programs, real-time measurements should be preferred anyway!

9.8.2 Processor Binding

The following calls automatically bind processes or threads to empty processors.
void r_processorbind(int p) - binds current thread to a specific CPU
void r_mpi_processorbind(void) - binds all MPI processes
void r_omp_processorbind(void) - binds all OpenMP threads
void r_ompi_processorbind(void) - binds all threads of all MPI processes

Print out current bindings:
void r_mpi_processorprint(int iflag)
void r_omp_processorprint(int iflag)
void r_ompi_processorprint(int iflag)

9.8.3 Memory Migration

int r_movepages(caddr_t addr, size_t len) - Moves data to the processor where the calling process/thread is running. *addr* is the start address and *len* the length of the data to be moved in byte.
int r_madvise(caddr_t addr, size_t len, int advice) - If the advise equals 7, the specified data is moved to the thread that uses it next.

9.8.4 Other Functions

char* r_getenv(char* envnam) - Gets the value of an environment variable.
int r_gethostname(char *hostname, int len) - Returns the hostname.
int r_getcpuid(void) - Returns processor ID.
void r_system(char *cmd) - Executes a shell command.
Details are described in the manual page (**man r_lib**). If you are interested in the r_lib sources please contact us.

9.9 HDF5

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of data types, and is designed for flexible and efficient I/O and for high volume and complex data. More information can be found at http://www.hdfgroup.org/HDF5/.

To initialize the environment, use

```
$ module load LIBRARIES; module load hdf5
```

This will set the environment variables **HDF5_ROOT**, **FLAGS_HDF5_INCLUDE** and **FLAGS_HDF5_LINKER** for compiling and linking,[100] and enhance the environment variables **PATH**, **LD_LIBRARY_PATH**, **FLAGS_MATH_**....

Example:

```
$ $PSRC/pex/990|| $MPIFC $FLAGS_MATH_INCLUDE -c $PSRC/psr/ex_ds1.f90
$ $PSRC/pex/990|| $MPIFC $FLAGS_MATH_LINKER ex_ds1.o
$ $PSRC/pex/994|| a.out
```

9.10 Boost

Boost provides free peer-reviewed portable C++ source libraries that work well with the C++ Standard Library. *Boost* libraries are intended to be widely useful, and usable across a broad spectrum of applications. More information can be found at http://www.boost.org/.

To initialize the environment, use

```
$ module load LIBRARIES; module load boost
```

This will set the environment variables **BOOST_ROOT**, **FLAGS_BOOST_INCLUDE** and **FLAGS_BOOST_LINKER** for compiling and linking, and enhance the environment variables **PATH**, **LD_LIBRARY_PATH**, **FLAGS_MATH_**....

Most Boost libraries are header-only: they consist entirely of header files containing templates and inline functions, and require no separately-compiled library binaries or special treatment when linking. Example:

```
$ $PSRC/pex/992|| $CXX $FLAGS_BOOST_INCLUDE $PSRC/psr/example.cpp -c
$ $PSRC/pex/992|| $CXX example.o -o example
$ $PSRC/pex/992|| echo 1 2 3 | ./example
```

[100] The *C++* interfaces are available for Open MPI only, please add **-lhdf5_cpp** to the link line.

However, these *Boost* libraries are built separately and must be linked explicitly:
atomic, chrono, context, date_time, exception, filesystem, graph, graph_parallel, iostreams, locale, math, mpi, program_options, python, random, regex serialization, signals, system, test, thread, timer, wave.

E.g. in order to link say the *Boost.MPI* library you have to add the **-lboost_mpi** flag to the link line and so forth.

Example:

```
$ $PSRC/pex/994|| $MPICXX $FLAGS_BOOST_INCLUDE $PSRC/psr/pointer_test.cpp -c
$ $PSRC/pex/994|| $MPICXX $FLAGS_BOOST_LINKER pointer_test.o -lboost_mpi
$ $PSRC/pex/994|| $MPIEXEC -np 2 a.out
```

9.11 ALPS project

The ALPS project (Algorithms and Libraries for Physics Simulations) is an open source effort aiming at providing high-end simulation codes for strongly correlated quantum mechanical systems as well as C++ libraries for simplifying the development of such code. ALPS strives to increase software reuse in the physics community. More information can be found at http://alps.comp-phys.org/

The ALPS software use MPI, HDF5 (chapter 9.9 on page 93), Boost (chapter 9.10 on page 93) and Intel MKL libraries.

To initialize the environment, use

```
$ module load LIBRARIES; module load hdf5 boost; module load alps
```

Note: you DO NOT NEED to load Intel MKL module if using the Intel compiler (default environment). Following environment variables will be set: **ALPS_ROOT**, **ALPS_HOME**, **FLAGS_ALPS_INCLUDE** and **FLAGS_ALSP_LINKER** for compiling and linking, and enhanced: **PATH**, **LD_LIBRARY_PATH**, **FLAGS_MATH_...**.

Alternatively, **cmake** may be used as described here:
http://alps.comp-phys.org/mediawiki/index.php/Tutorials:Alpsize-01_CMake

Or you use ALPS from Python:
http://alps.comp-phys.org/mediawiki/index.php/Tutorials:Code-01_Python

10 Miscellaneous

10.1 Useful Commands

csplit	Splits C programs
fsplit[102]	Splits FORTRAN programs
nm	Prints the name list of object programs
ldd	Prints the dynamic dependencies of executable programs
ld	Runtime linker for dynamic objects
readelf	Displays information about ELF format object files.
vmstat	Status of the virtual memory organization
iostat	I/O statistics
sar	Collects, reports, or saves system activity information
mpstat	Reports processor related statistics
lint[102]	More accurate syntax examination of C programs
dumpstabs[102]	Analysis of an object program (included in Oracle Studio)
pstack **pmap**	Analysis of the /proc directory
cat /proc/cpuinfo	Processor information
free	Shows how much memory is used
top	Process list
strace	Logs system calls
file	Determines file type
uname -a	Prints name of current system
ulimit -a	Sets/gets limitations on the system resources
which ***command***	Shows the full path of *command*
dos2unix, unix2dos	DOS to UNIX text file format converter and vice versa
screen	Full-screen window manager that multiplexes a physical terminal

[102] *Note*: The utilities **fsplit**, **lint**, **dumpstabs** are shipped with Oracle Studio compilers, thus you have to load the **studio** module to use them:
`$ module load studio`

A Debugging with TotalView - Quick Reference Guide

This quick reference guide describes briefly how to debug serial and parallel (OpenMP and MPI) programs written in C, C++ or FORTRAN 90/95, using the TotalView debugger from TotalView Technologies on the RWTH Aachen HPC-Cluster.

For further information about TotalView refer to the Users's Manual and the Reference Guide which can be found here: http://www.roguewave.com/support/product-documentation/totalview-family.aspx.

A.1 Debugging Serial Programs

A.1.1 Some General Hints for Using TotalView

- Click your middle mouse button to **dive** on things in order to get more information.
- Return (**undive**) by clicking on the *undive* button (if available), or by *View* →*Undive*.
- You can change all highlighted values (Press F2).
- If at any time the source pane of the process window shows disassembled machine code, the program was stopped in some internal routine. Select the first user routine in the **Stack Trace Pane** in order to see where this internal routine was invoked.

A.1.2 Compiling and Linking

Before debugging, compile your program with the option **-g** and without any optimization.

A.1.3 Starting TotalView

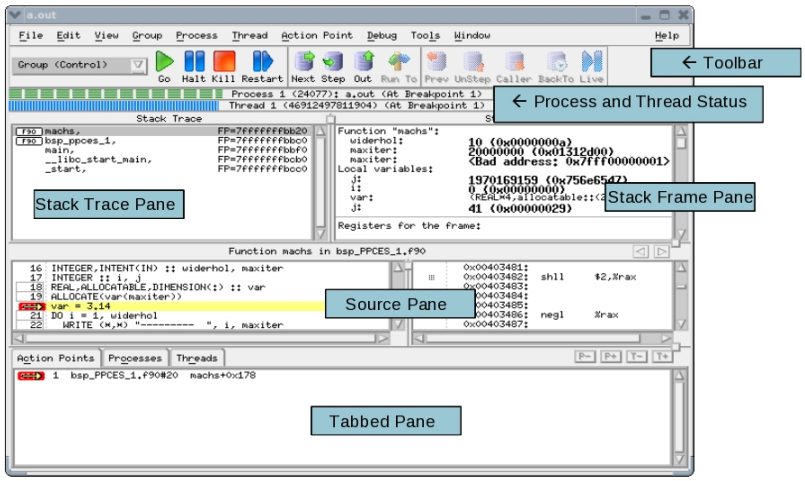
You can debug your program

1. either by starting TotalView with your program as a parameter
   `$ $PSRC/pex/a10|| totalview a.out [ -a options ]`
2. or by starting your program first and then attaching TotalView to it. In this case start
   `$ totalview`
   which first opens its *New Program* dialog. This dialog allows you to choose the program you want to debug.
3. You can also analyze the core dump after your program crashed by
   `$ totalview a.out core`

Start Parameters (runtime arguments, environment variables, standard IO) can be set in the *Process* →*Startup Parameters* ... menu.

After starting your program, TotalView opens the *Process Window*. It consists of

- the *Source Pane*, displaying your program's source code;
- the *Stack Trace Pane*, displaying the call stack;
- the *Stack Frame Pane*, displaying all the variables associated with the selected stack routine;
- the *Tabbed Pane*, showing the threads of the current process (*Threads* subpane), the MPI processes (*Processes* subpane), and listing all breakpoints, action points and evaluation points (*Action Points Threads* subpane);
- the *Status Bar*, displaying the status of current process and thread;
- the *Toolbar*, containing the action buttons.



A.1.4 Setting a Breakpoint

- If the right function is already displayed in the *Source Pane*, just click on a boxed line number of an executable statement once to *set a breakpoint*. Clicking again will *delete the breakpoint*.
- Search the function with the *View* →*Lookup Function* command first.
- If the function is in the current call stack, dive on its name in the *Stack Trace Pane* first.
- Select *Action Points* →*At Location* and enter the function's name.

A.1.5 Starting, Stopping and Restarting your Program

- Start your program by selecting *Go* on the icon bar and stop it by selecting *Halt*.
- Set a *breakpoint* and select *Go* to run the program until it reaches the line containing the breakpoint.
- Select a program line and click on *Run To* on the icon bar.
- Step through a program line by line with the *Step* and *Next* commands. *Step* steps into and *Next* jumps over function calls.
- Leave the current function with the *Out* command.
- To restart a program, select *Restart*.

A.1.6 Printing a Variable

- The values of simple actual variables are displayed in the *Stack Frame Pane* of the *Process Window*.
- You may use the *View* →*Lookup Variable* command.
- When you dive (middle click) on a variable, a separate *Variable Window* will be opened.
- You can change the variable type in the *Variable Window* (*type casting*).
- If you are displaying an array, the *Slice* and *Filter* fields let you select which subset of the array will be shown (examples: Slice: (3:5,1:10:2), Filter: > 30).
- One and two-dimensional arrays or array slices can be graphically displayed by selecting *Tools* →*Visualize* in the *Variable Window*.

- If you are displaying a structure, you can look at substructures by rediving or by selecting *Dive* after clicking on the right mouse button.

A.1.7 Action Points: Breakpoints, Evaluation Points, Watchpoints

- The program will stop when it hits a *breakpoint*.
- You can temporarily introduce some additional C or FORTRAN style program lines at an *Evaluation Point*. After creating a breakpoint, right-click on the *STOP* sign and select *Properties* →*Evaluate* to type in your new program lines. Examples are shown in table A.28 on page 98.

An additional print statement: (FORTRAN write is not accepted)	**printf ("x = %f\n", x/20)**
Conditional breakpoint:	**if (i == 20) $stop**
Stop after every 20 executions:	**$count 20**
Jump to program line 78:	**goto $78**
Visualize an array	**$visualize a**

Table A.28: Action point examples

- A *watchpoint* monitors the value of a variable. Whenever the content of this variable (memory location) changes, the program stops. To set a watchpoint, dive on the variable to display its *Variable Window* and select the *Tools* →*Watchpoint* command.

You can save / reload your action points by selecting *Action Point* →*Save All* resp. *Load All*.

A.1.8 Memory Debugging

TotalView offers different memory debugging features. You can guard dynamically allocated memory so that the program stops if it violates the boundaries of an allocated block. You can hoard the memory so that the program will keep running when you try to access an already freed memory block. Painting the memory will cause errors more probably; especially reading and using uninitialized memory will produce errors. Furthermore you can detect memory leaks.

- Enable the memory debugging tool before you start your program by selecting the *Debug* entry from the tools menu and click the *Enable memory debugging* button.
- Set a breakpoint at any line and run your program into it.
- Open the Memory Debugging Window: select *Debug* →*Open MemoryScape*.
- Select the *Memory Reports* →*Leak Detection* tab and choose *Source report* or *Backtrace report*. You will then be presented with a list of Memory blocks that are leaking.

Memory debugging of MPI programs is also possible. The Heap Interposition Agent (HIA) interposes itself between the user program and the system library containing malloc, realloc, and free. This has to be done at program start up and sometimes it does not work in MPI cases.

We recommend to use the newest MPI and TotalViev versions, the *Classic Launch* (cf. chapter A.2.2.1 on page 100) and to link the program against the debugging libraries[103] to make sure that it captured properly. Example:

```
$  $MPICC -g -o mpiprog mpiprog.c -L$TVLIB -ltvheap_64 -Wl,-rpath,$TVLIB
```

[103] http://www.roguewave.com/Portals/0/products/totalview-family/totalview/docs/8.10/wwhelp/wwhimpl/js/html/wwhelp.htm#href=User_Guides/LinkingYourApplicationWithAgent28.html

A.1.9 ReplayEngine

TotalView provides the possibility of reversely debugging your code by recording the execution history. The ReplayEngine restores the whole program states, which allows the developer to work back from a failure, error or even a crash. The ability of stepping forward and backward through your code can be very helpful and reduce the amount of time for debugging dramatically because you do not need to restart your application if you want to explore a previous program state. Furthermore the following replay items are supported:[104]

- Heap memory usage
- Process file and network I/O
- Thread context switches
- Multi-threaded applications
- MPI parallel applications
- Distributed applications
- Network applications

The following functionality is provided:

- First you need to activate the ReplayEngine: *Debug →Enable ReplayEngine*
- *GoBack* runs the program backwards to a previous *breakpoint*.
- *Prev* jumps backwards to the previous line (function call).
- *Unstep* steps backwards to the previous instruction within the function.
- *Caller* jumps backwards to the caller of the function.

A.1.10 Offline Debugging - TVScript

If interactive debugging is impossible, e.g. because the program has to be run in the batch system due to problem size, an interesting feature of the TotalView debugger called *TVScript* can be helpful. Use the **tvscript** shell command to define points of interest in your program and corresponding actions for TotalView to take. TVScript supports serial, multithreaded and MPI programming models and has full access to the memory debugging capabilities of TotalView. More information about TVScript can be found in Chapter 4 of the Reference Guide[105].

Example: Compile and run a Fortran program; print the current stack backtrace into the log file on the begining of subroutines “t1“ and “t2“

```
$ $PSRC/pex/a15|| $FC -g $PSRC/psr/TVScript_tst.f90; tvscript
-create_actionpoint ‘‘t1=>display_backtrace‘‘ -create_actionpoint
‘‘t2=>display_backtrace‘‘ a.out
```

MPI Programs also can be debugged with tvscript. Each process is debugged independently, but the whole output is written to the same log files. However, the records are still distinguishable, because the MPI rank is noted as well. Note that for each MPI process a license token is consumed, so the number of debuggable processes is limited. Optional parameters to underlying “mpiexec“ of the MPI library can be provided with the *-starter_ args* option.

[104] http://www.roguewave.com/products/totalview-family/replayengine/overview/features.aspx
[105] http://www.roguewave.com/support/product-documentation/totalview-family.aspx

If using tvscript in the batch, you must provide *both* the number of processes to start *and* $FLAGS_MPI_BATCH environment variable containing the host file. Example (runs also interactively): Launch "a.out" with 2 processes using Open MPI with aim to prints the value of variables "my_MPI_Rank" and "my_Host" if the line 10 in mpihelloworld.f90 is hit

```
$ $PSRC/pex/a17|| $MPIFC -g $PSRC/psr/mpihelloworld.f90; tvscript -mpi
``Open MPI`` -np 2 -starter_args ``$FLAGS_MPI_BATCH`` -create_actionpoint
``mpihelloworld.f90#10=>print my_MPI_Rank, print my_Host`` a.out
```

A.2 Debugging Parallel Programs

A.2.1 Some General Hints for Parallel Debugging

- Get familiar with using TotalView by debugging a serial toy program first.
- If possible, make sure that your serial program runs fine first.
- Debugging a parallel program is not always easy. Use as few MPI processes / OpenMP threads as possible. Can you reproduce your problem with only one or two processes / threads?
- Many typical multithreaded errors may not (or not comfortable) be found with a debugger (for example *race condition*) →Use threading tools, refer to chapter 7.4 on page 77

A.2.2 Debugging MPI Programs

More hints on debugging of MPI programs can be found in the TotalView Setting Up MPI Programs[106] Guide. The presentation[107] of Ed Hinkel at ScicomP 14 Meeting is interesting in the context of large jobs.

A.2.2.1 Starting TotalView

- There are two ways to start the debugging of MPI programs: *New Launch* and *Classic Launch*.

  The *New Launch* is the easy and intuitive way to start a debugging session. Its disadvantage is the inability to detach from and reattach to running processes. Start TotalView as for serial debugging and use the *Parallel* pane in the *Startup Parameters* window to enable startup of a parallel program run. The relevant items to adjust are the *Tasks* item (number of MPI processes to start) and the *Parallel System* item. The latter has to be set according to the MPI vendor used.

  The *Classic Launch* helps to start a debug session from command line without any superfluous clicks in the GUI. It is possible to attach to a subset of processes and to detach/reattach again. The arguments that are to be added to the command line of **mpiexec** depend on the MPI vendor. For Intel MPI and Open MPI use the flag **-tv** to enable the Classic Launch:
  `$ $PSRC/pex/a20|| $MPIEXEC -tv -np 2 a.out < input`

  When the GUI appears, type *g* for go, or click *Go* in the TotalView window.

  TotalView may display a dialog box stating: *Process ... is a parallel job. Do you want to stop the job now?* Click **Yes** to open the TotalView debugger window with the source window and leave all processes in a traced state or **No** to run the parallel application directly.

[106] http://www.idris.fr/su/Scalaire/vargas/tv/MPI.pdf
[107] http://www.spscicomp.org/ScicomP14/talks/hinkel-tv.pdf

You may switch to another MPI process by

- Clicking on another process in the root window
- Circulating through the attached processes with the **P-** or **P+** buttons in the process window

Open another process window by clicking on one of the attached processes in the root window with your right mouse button and selecting *Dive in New Window*.

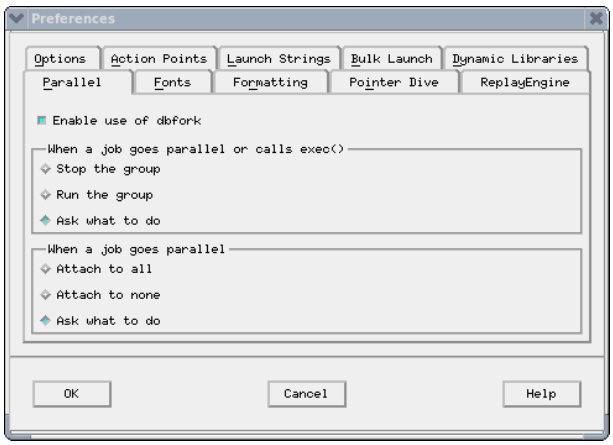
A.2.2.2 Debugging of large jobs Each MPI process consumes a TotalView license token. Due to the fact that RWTH has only 50 licenses, the number of debuggable processes is limited to this number.

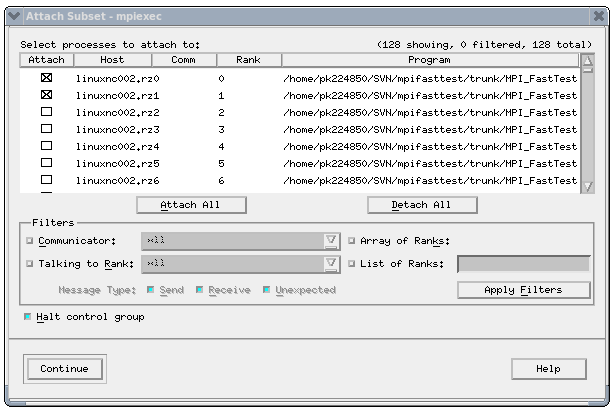
The best way to debug a MPI application is to debug using a limited (small) number of processes, ideally only one or two. The debug session is neat, communication pattern is simple and you save license tokens.

If the debugging with a small number of processes is impossible (e.g. because the error you are searching for occurs in a *large* job only), you can *attach to a subset of a whole job:* Open *"File"* →*"Preferences"* →*"Parallel"*, in the *"When a job goes parallel"* menu set the checkbox on *"Ask what to do"* (instead of *"Attach to all"*).

The next time a parallel job is started, a *"Attach Subset"* dialog box turns up. Choose a subset of processes in the menu. The program will start with the requested number of processes, whereas TotalView debugger connects to the chosen processes only.

It is possible to select a different subset of processes at any time during the debug session in the *"Group"* →*"Attach Subset"* dialog box.





A.2.2.3 Setting a Breakpoint By right-clicking on a breakpoint symbol you can specify its properties. A breakpoint will stop the whole process group (all MPI processes, default) or only one process. In case you want to synchronize all processes at this location, you have to change the breakpoint into a barrier by right clicking on a line number and selecting *Set Barrier* in the pull-down menu.

It is a good starting point to set and run into a barrier somewhere after the MPI initialization phase. After initially calling MPI_Comm_rank, the rank ID across the processes reveals whether the MPI startup went well. This can be done by right-clicking on the variable for the rank in the source pane, then selecting either Across Processes or Across Threads from the context menu.

A.2.2.4 Starting, Stopping and Restarting your Program

You can perform stop, start, step, and examine single processes or groups of processes. Choose *Group* (default) or *Process* in the first pull-down menu of the toolbar.

A.2.2.5 Printing a Variable

You can examine the values of variables of all MPI processes by selecting *View* →*Show Across* →*Processes* in a variable window, or alternatively by right-clicking on a variable and selecting *Across Processes*. The values of the variable will be shown in the array form and can be graphically visualized. One-dimensional arrays or array slices can also be shown across processes. The thread ID is interpreted as an additional dimension.

A.2.2.6 Message Queues

You can look into outstanding message passing operations (unexpected messages, pending sends and receives) with the *Tools* →*Message Queue*. Use *Tools* →*Message Queue Graph* for visualization - you will see pending messages and communication patterns. Find deadlocks by selecting *Options* →*Cycle Detection* in an opened *Message Queue Graph* window.

A.2.3 Debugging OpenMP Programs

A.2.3.1 Some General Hints for Debugging OpenMP Programs

Before debugging an OpenMP program, the corresponding serial program should run correctly. The typical OpenMP parallelization errors are data races, which are hard to detect in a debugging session because the timing behavior of the program is heavily influenced by debugging. You may want to use a thread-checking tool first (see chapter 7.4 on page 77).

Many compilers turn on optimization when using OpenMP by default. This default should be overwritten. Use e.g. the **-xopenmp=noopt** suboption for the Oracle compilers or **-openmp -O0** flags for the Intel compiler.

For the interpretation of the OpenMP directives, the original source program is transformed. The *parallel regions* are *outlined* into separate subroutines. *Shared* variables are passed as call parameters and *private* variables are defined locally. A parallel region cannot be entered stepwise, but only by running into a breakpoint. If you are using FORTRAN, check that the serial program does run correctly compiled with

- **-automatic** option (Intel **ifort** compiler) or
- **-stackvar** option (Oracle Studio **f95** compiler) or
- **-frecursive** option (GCC **gfortran** compiler) or
- **-Mrecursive** option (PGI **pgf90** compiler).

A.2.3.2 Compiling

Some options, e.g. the ones for OpenMP support, cause certain compilers to turn on optimization. For example, the Oracle-specific compiler switches **-xopenmp** and **-xautopar** automatically invoke high optimization (**-xO3**).
Compile with **-g** to prepare the program for debugging and do not use optimization if possible:

- Intel compiler: use **-openmp -O0 -g** switches
- Oracle Studio compiler: use **-xopenmp=noopt -g** switches
- GCC compiler: use **-fopenmp -O0 -g** switches
- PGI compiler: use **-mp -Minfo=mp -O0 -g** switches

A.2.3.3 Starting TotalView Start debugging your OpenMP program after specifying the number of threads you want to use

```
$ OMP_NUM_THREADS=nthreads totalview a.out
```

The parallel regions of an OpenMP program are outlined into separate subroutines. Shared variables are passed as call parameters to the outlined routine and private variables are defined locally. A parallel region cannot be entered stepwise, but only by running into a breakpoint.

You may switch to another thread by

- clicking on another thread in the root window or
- circulating through the threads with the **T-** or **T+** buttons in the process window.

A.2.3.4 Setting a Breakpoint By right-clicking on a breakpoint symbol, you can specify its properties. A breakpoint will stop the whole process (group) by default or only the thread for which the breakpoint is defined. In case you want to synchronize all processes at this location, you have to change the breakpoint into a barrier by right-clicking on a line number and selecting *Set Barrier* in the pull-down menu.

A.2.3.5 Starting, Stopping and Restarting your Program You can perform stop, start, step, and examine single threads or the whole process (group). Choose *Group* (default) or *Process* or *Thread* in the first pull-down menu of the toolbar.

A.2.3.6 Printing a Variable You can examine the values of variables of all threads by selecting *View* →*Show Across* →*Threads* in a variable window, or alternatively by right-clicking on a variable and selecting *Across Threads*. The values of the variable will be shown in the array form and can be graphically visualized. One-dimensional arrays or array slices can be also shown across threads. The thread ID is interpreted as an additional dimension.

B Beginner's Introduction to the Linux HPC-Cluster

This chapter contains a short tutorial for new users about how to use the RWTH Aachen Linux HPC-Cluster. It will be explained how to set up the environment correctly in order to build a simple example program. Hopefully this can easily be adapted to your own code. In order to get more information on the steps performed you need to read the referenced chapters.

The first step you need to perform is to log in[108] to the HPC-Cluster.

B.1 Login

You have to use the *secure shell protocol* (**ssh**) to log in. Therefore it might be necessary to install an ssh client on your local machine. If you are running Windows, please refer to chapter 4.1 on page 26 to get such an ssh client. Depending on the client you use, there are different ways to enter the necessary information. The name of the host you need to connect to is **cluster.rz.rwth-aachen.de** (other front end nodes can be found in table 1.1 on page 8) and your user name is usually your IdM ID.

On Unix or Linux systems, **ssh** is usually installed or at least included in the distribution. If this is the case you can open a terminal and enter the command

```
$ ssh -Y <username>@cluster.rz.rwth-aachen.de
```

After entering the password, you are logged in to the HPC-Cluster and see a shell prompt like this:

```
ab123456@cluster:~[1]$
```

The first word is your user name, in this case `ab123456`, separated by an "@" from the machine name `cluster`. After the colon the current directory is prompted, in this case `~` which is an alias for `/home/ab123456`. This is your home directory (for more information on available directories please refer to chapter 4.2 on page 28). Please note that your user name, contained in the path, is of course different from ab123456. The number in the brackets counts the entered commands. The prompt ends with the $ character. If you want to change your prompt, please take a look at chapter 4.3 on page 31.

You are now logged in to a Linux front end machine.

The cluster consists of interactively accessible machines and machines that are only accessible by batch jobs. Refer to chapter 4.4 on page 34. The interactive machines are not meant for time consuming jobs. Please keep in mind that there are other users on the system which are affected if the system gets overloaded.

B.2 The Example Collection

As a first step, we show you how to compile an example program from our Example Collection (chapter 1.3 on page 10). The Example Collection is located at `/rwthfs/rz/SW/HPC/examples`. This path is stored in the environment variable $PSRC.

To list the contents of the examples directory use the command *ls* with the content of that environment variable as the argument:

```
$ ls $PSRC
```

The examples differ in the parallelization paradigm used and the programming language which they are written in. Please refer to chapter 1.3 on page 10 or the README file for more information:

```
$ less $PSRC/README.txt
```

The examples need to be copied into your home directory (`~`) because the global directory is read-only. This is can be done using Makefiles contained in the example directories. Let's

[108] If you do not yet have an account for our cluster system you can create one in RWTH identity management system (IdM): http://www.rwth-aachen.de/selfservice

assume you want to run the example of a jacobi solver written in C++ and parallelized with OpenMP. Just do the following:

```
$ cd $PSRC/C++-omp-jacobi ; gmake cp
```

The example is copied into a subdirectory of your home directory and a new shell is started in that new subdirectory.

B.3 Compilation, Modules and Testing

Before you start compiling, you need to make sure that the environment is set up properly. Because of different and even contradicting needs regarding software, we offer the modules system to easily adapt the environment. All the installed software packages are available as modules that can be loaded and unloaded. The modules themselves are put into different categories to help you find the one you are looking for (refer to chapter 4.3.2 on page 31 for more detailed information).

Directly after login some modules are already loaded by default. You can list them with

```
$ module list
```

The output of this command looks like this:

```
$ module list
Currently Loaded Modulefiles:
1) DEVELOP        2) intel/16.0       3) openmpi/1.10.2
```

The default modules are in the category DEVELOP, which contains compilers, debuggers, MPI libraries etc. At the moment the Intel FORTRAN/C/C++ Compiler version 12 and Open MPI 1.4.3 are loaded by default. The list of available modules can be printed with

```
$ module avail
```

In this case, the command prints out the list of available modules in the DEVELOP category, because this category is loaded and the list of all other available categories. Let's assume that for some reason you'd like to use the GNU compiler instead of the Intel compiler for our C++/OpenMP example.[109]

All availble GCC versions can be listed by

```
$ module avail gcc
```

To use GCC version 6 do the following:

```
$ module switch intel gcc/6

Unloading openmpi 1.10.2                                [ OK ]
Unloading Intel Suite 16.0.2.181                        [ OK ]
Loading gcc 6.1.0                                       [ OK ]
Loading openmpi 1.10.2 for gcc compiler                 [ OK ]
```

Please observe how Open MPI is first unloaded, then loaded again. In fact, the loaded version of Open MPI is different from the unloaded version, because the loaded version is suitable for being used together with the GNU compiler whereas the unloaded is built to be used with the Intel compiler. The module system takes care of such dependencies.

Of course you can also load an additional module instead of replacing an already loaded one. For example, if you want to use a debugger, you can do a

```
$ module load totalview
```

In order to make the usage of different compilers easier and to be able to compile with the same command, several environment variables are set. You can look up the list of variables in chapter 5.2 on page 45.

[109] Usually, though, we'd recommend using the Intel, PGI or Oracle compilers for production because they offer better performance in most cases.

Often, there is more than one step needed to build a program. The **make** tool offers a nice way do define these steps in a *Makefile*. We offer such Makefiles for the examples, which use the environment variables. Therefore when starting

```
$ gmake
```

the example will be built and executed according to the specified rules. Have a look at the Makefile if you are interested in more details.

As the Makefile already does everything but explain the steps, the following paragraph will explain it step-by-step. You have to start with compiling the source files, in this case *main.cpp* and *jacobi.cpp*, with the C++ compiler:[110]

```
$ $CXX $FLAGS_DEBUG $FLAGS_FAST $FLAGS_OPENMP -DREAD_INPUT -c jacobi.cpp
main.cpp
```

This command invokes the C++ compiler stored in the environment variable $CXX, in this case *g++* as you are using the GNU compiler collection. The compiler reads both source files and puts out two object files, which contain machine code. The variables $FLAGS_DEBUG, $FLAGS_FAST, and $FLAGS_OPENMP contain compiler flags to, respectively, put debugging information into the object code, to optimize the code for high performance and to enable OpenMP parallelization. The *-D* option specifies C preprocessor directives to allow conditional compilation of parts of the source code. The command line above is equivalent to writing just the content of the variables:

```
$ g++ -g -O3 -ffast-math -mtune=native -fopenmp -DREAD_INPUT -c jacobi.cpp
main.cpp
```

You can print the values of variables with the *echo* command, which should print the line above

```
$ echo $CXX $FLAGS_DEBUG $FLAGS_FAST $FLAGS_OPENMP -DREAD_INPUT -c jacobi.cpp
main.cpp
```

After compiling the object files, you need to link them to an executable. You can use the linker *ld* directly, but it is recommended to let the compiler invoke the linker and add appropriate options e.g. to automatically link against the OpenMP library. You should therefore use the same compiler options for linking as you used for compiling. Otherwise the compiler may not generate all needed linker options. To link the objects to the program *jacobi.exe* you have to use

```
$ $CXX $FLAGS_DEBUG $FLAGS_FAST $FLAGS_OPENMP jacobi.o main.o -o jacobi.exe
```

Now, after having built the executable, you can run it. The example program is an iterative solver algorithm with built-in measurement of time and megaflops per second. Via the environment variable $OMP_NUM_THREADS you can specify the number of parallel threads with which the process is started. Because the *jacobi.exe* program needs input you have to supply an input file and start

```
$ export OMP_NUM_THREADS=1; ./jacobi.exe < input
```

After a few seconds you will get the output, including the runtime and megaflop rate, which depend on the load on the machine.

As you built a parallel OpenMP program it depends on the compiler with how many threads the program is executed if the environment variable $OMP_NUM_THREADS is not explicitly set. In the case of the GNU compiler the default is to use as many threads as processors are available.

As a next step, you can double the number of threads and run again:

```
$ export OMP_NUM_THREADS=2; ./jacobi.exe < input
```

Now the execution should have taken less time and the number of floating point operations per

[110] If you are not using one of our cluster systems the values of the environment variables $CXX, $FLAGS_DEBUG et cetera are probably not set and you cannot use them. However, as every compiler has its own set of compiler flags, these variables make life a lot easier on our systems because you don't have to remember or look up all the flags for all the compilers and MPIs.

second should be about twice as high as before.

B.4 Computation in batch mode

After compiling the example and making sure it runs fine, you want to compute. However, the interactive nodes are not suited for larger computations. Therefore you can submit the example to the batch queue (for detailed information see chapter 4.4 on page 34). It will be executed when a compute node is available.

To submit a batch job you have to use the command *bsub* which is part of the workload management system Platform LSF (refer to 4.4.1 on page 34). The **bsub** command needs several options in order to specify the required resources, e.g. the number of CPUs, the amount of memory to reserve or the runtime.

```
$ bsub -J TEST -o output.txt -n 2 -R "span[hosts=1]" -W 15 -M 700 -a openmp -u
<your_email_address> -N "module switch intel gcc/6; export OMP_NUM_THREADS=2;
jacobi.exe < input"
```
[111]

You will get an email when the job is finished if you enter your email address instead of *<your_email_address>*. The output of the job will be written to *output.txt* in the current directory.

The same job can be scripted in a file, say simplejob.sh, in which the options of *bsub* are saved with the magic cookie "#BSUB":

```
#!/usr/bin/env zsh
#BSUB -J TEST
#BSUB -o ouput.txt
#BSUB -n 2
#BSUB -W 15
#BSUB -M 700
#BSUB -a openmp
#BSUB -u <your_email_address>
#BSUB -N

module switch intel gcc/6
jacobi.exe < input
```

To submit a job, use

```
$ bsub < simplejob.sh
```

Please note the "<" in the command line. It is very important to pipe the script into the bsub executable, because otherwise none of the options specified with magic cookie will be interpreted.

You can also mix both ways to define options; the options set over commandline are preferred.

[111] This is not the recommended way to submit jobs, however you do not need a job script here. You can find several example scripts in chapter 4.4 on page 34. The used options are explained there as well.

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Notes