The RWTH SunFire SMP-Cluster

User's Guide, Version 3.2

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1 Introduction

This primer gives you a quick start in using the new Sun Fire SMP-Cluster at the Aachen University. It describes the hardware architecture, selected aspects of the operating environment, a few software tools, and helpful references for further information. The software tools include:

- The **Sun ONE Studio 8 Development Tools** NEW
- **Sun HPC ClusterTools Version 5.0**, Sun's MPI implementation and environment now fully supports MPI version 2. NEW
- **TotalView Version 6.3**, Etnus' latest parallel debugger version now supports Sun's latest compilers and the debugging of programs using the 64 bit addressing mode. Debugging MPI programs has also been considerably improved with the HPC ClusterTools Version 5.0. Debugging of OpenMP programs is possible in combination with the KAP/Pro Toolset's Guide compilers. NEW
- **VampirTrace Version 3.0** and **Vampir Version 3.0**, Pallas' tools for runtime analysis of MPI programs work well with HPC ClusterTools Version 5.0**.** (MPI2 is not yet fully supported) NEW
- KAP/Pro Toolset Version 4.0, KAI's OpenMP tools including
- the KCC C++ Compiler Version 4.0 which is part of the KAP/Pro Toolset
- some details about the **Solaris 9** operating system (It will successively be installed on all the Sun Fire systems and particularly effects the runtime behaviour of the Sun Fire 15 K systems RWTH)

Site-specific sections are marked with RWTH**.**

Please check our web pages for more up-to-date information and the latest version of this document:

http://www.rz.rwth-aachen.de/hpc/
http://www.rz.rwth-aachen.de/computing/info/sun/primer/

For interactive access to the cluster, login to

cluster-sun.rz.RWTH-Aachen.DE

Please join the **`rzcluster`** mailing list, if you want to be informed on a regular basis:

http://MailMan.RWTH-Aachen.DE/mailman/listinfo/rzcluster

Do not hesitate to send criticisms or suggestions to

hpc@rz.rwth-aachen.de

Have fun using the new Sun Fire SMP-Cluster!

2 Hardware

2.1 Configuration RWTH

The Sun SMP-Cluster currently consists of

- 16 Sun Fire 6800 nodes with 24 UltraSPARC-III Cu processors and 24 GB of shared memory each and of
- 4 Sun Fire 15K nodes with 72 UltraSPARC-III Cu processors and 144 GB of shared memory each.

All 672 CPUs have a 900 MHz clock cycles with an accumulated peak performance of 1,2 TFlop/s and a total main memory capacity of 960 GB.

All compute nodes are equipped with local scratch (**`TMP`**) and system file systems. They also have access to a common NFS file system for small long-term user data (**`HOME`**) and to another common file system for large medium-term work files (**`WORK`**).

In the future all compute nodes will have direct access to all shared filesystems via a fast storage area network (SAN) using the QFS file system. High IO bandwidth will be achieved by striping multiple RAID systems.

All SMP compute nodes are connected to each other by Gigabit Ethernet. In 1Q2003 the proprietary high-speed Sun Fire Link networks have been installed to form two clusters of 8 Sun Fire 6800 systems each. In september 2003 the Sun Fire Link connection between the 4 Sun Fire 15K systems has been installed.

Finally all nodes will be upgraded with UltraSPARC-IV processors.

2.2 Processors

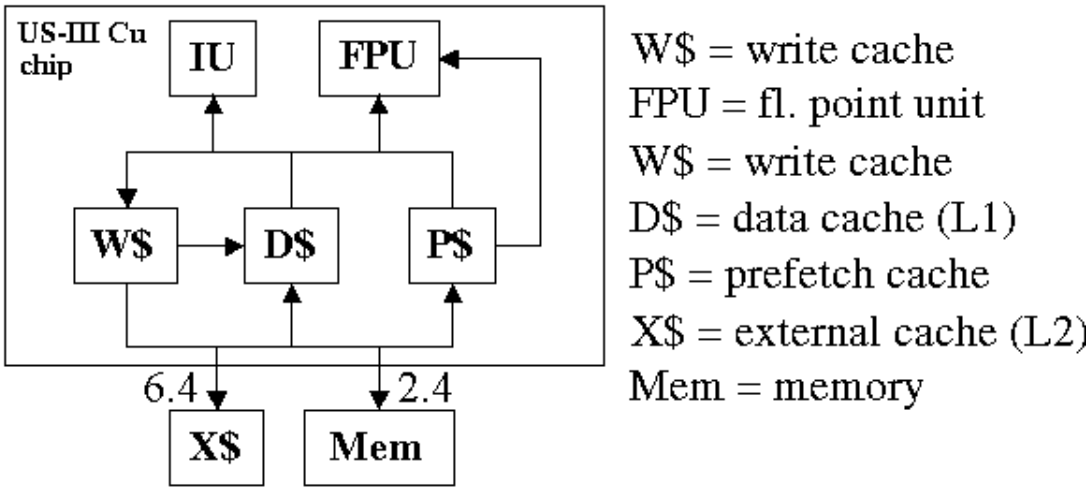
The UltraSPARC-III Cu processor (US-III Cu) is a superscalar 64-bit processor with two cache levels:

Level 1 (on chip):

- 64 KB for data and 32 KB for instructions
  (4-way associative, 32 byte cache-lines, write-through, no-write allocate, pseudo random replacement strategy, 2 clock cycles latency. Modified cache lines are written back immediately into the L2 cache and a cache line is not fetched before a write operation)
- 2 KB prefetch cache, for an accelerated load of floating point numbers
  (4-way associative, 64 byte cache lines, 32 byte subblocks, LRU replacement strategy)
- 2 KB write cache
  (4-way associative, 64 byte cache lines, 32 byte subblocks, LRU replacement strategy)

Level 2 (off chip):

- 8 MB for data and instructions
  (2-way associative (900 MHz), 512 Byte cache lines with 64 byte subblocks, approx. 12 clock cycles latency, 6.4 GB/s bandwidth, write-back; write-allocate strategy. Modified cache lines are not written back until they are pushed out of the cache and before a write the whole subblock has to be fetched from memory.)



The most important information about the current processors can be acquired with the instruction

```
$ fpversion
```

Each clock period the processor can initiate 2 integer operations or an integer and a memory operation, one floating point addition and one floating point multiplication. Thus the peak performance in Mflop/s is twice the clock rate in MHz. In suitable computing kernels, like the well-known Linpack benchmark or a matrix multiplication, 70-90% of this rate will be actually attainable.

2.3 Memory

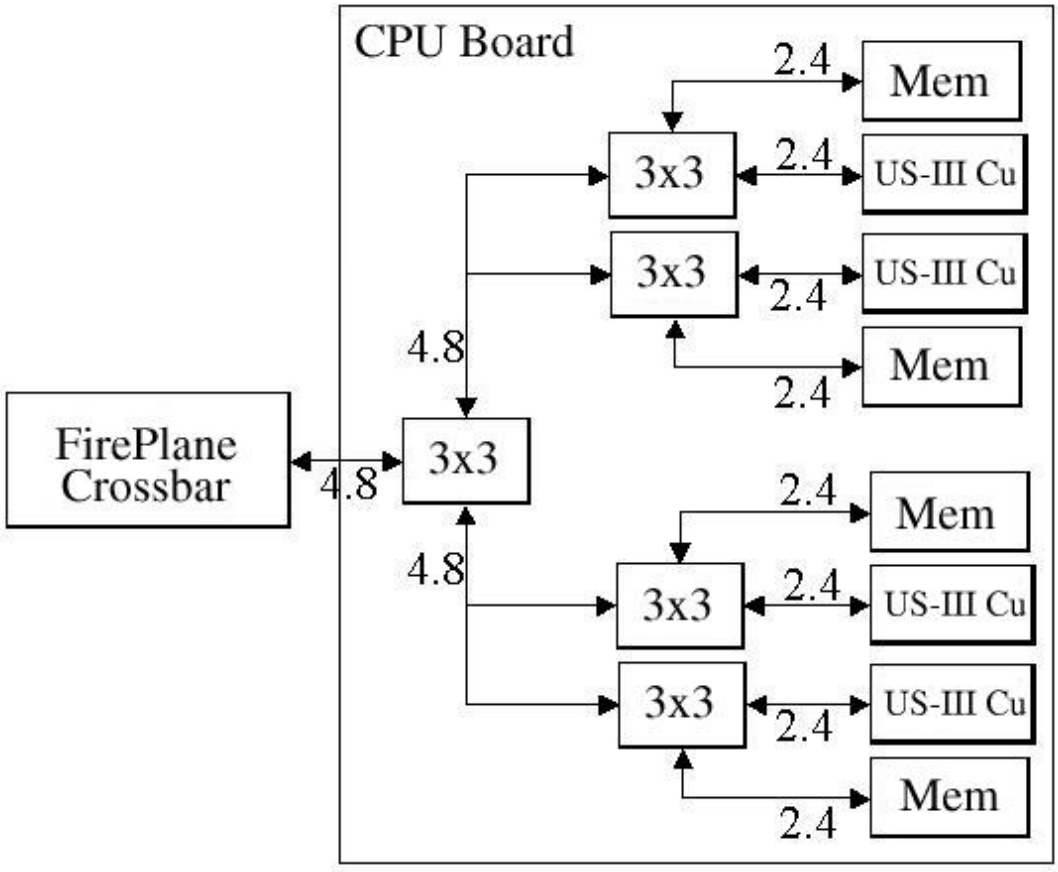
Each CPU board contains 4 processors and their external (L2) caches together with their local interleaved memory.

In the Sun Fire 6800, 6 of these boards are coupled with a crossbar. The memory bandwidth amounts to theoretically 2.4 GB/s for a single processor and -- due to snoop bus limitations -- 9.6 GB/s for all 24 processors of a SMP node.

In the Sun Fire 15K, 18 CPU boards are interconnected with a crossbar and the cache coherency is handled by a combination of snooping within each board and directory-based cache coherency between the boards.

From the programmer's point of view, the Fire 6800 thereby offers a " flat " memory system with a limited bandwidth (9.6 GB/s), i.e. all memory cells approximately have the same distance to each processor (latency about 270 ns), whereas data locality plays a more important role in the Fire 15K (cc-NUMA architecture).

The latency to get data from memory on the same board is approximately 270 ns. The Fire 15K's latency for fetching remote data will be at least 330 ns and in extreme cases, however, up to about 600 ns. Theoretically the total memory bandwidth will be between 43.2 GB/s (worst case) and 172.8 GB/s (only local accesses). Data locality will be supported by the upcoming version of the Solaris 9 operating system.



2.4 Network RWTH

Gigabit Ethernet is used to interconnect SMP nodes. Furthermore, two tightly coupled clusters of 8 Fire 6800 systems each have been formed and one cluster of 4 Fire 15K systems will be formed in the near future with proprietary high-speed Sun Fire Link networks. With Sun's version of MPI, a latency of 4 micro seconds and a bandwidth of about 2 GB/s can be obtained between 2 nodes compared to a latency of at least 100 us and a maximum bandwidth of about 100 MB/s when using the Gigabit Ethernet. It takes at least 8 simultaneous transfers to saturate the Fire Link connection between two nodes. NEW

3 Operating System

The Solaris Operating Environment is an operating system of the UNIX family.

The current version on about half of the Sun Fire machines is Solaris 8, and Solaris 9 on the other half. We will completely migrate to Solaris 9 soon. RWTH

The command

```
$ uname -r
```

will print out the corresponding SunOS release level 5.8 or 5.9.

NEW Solaris 9 will introduce the multiple page size support and the memory placement option (MPO) which is particularly important for the Sun Fire 15K systems.

By default Solaris organizes all data in pages of 8 KB. Programs with a large memory requirement and/or programs which access memory randomly or with non-unit strides might profit from using a large page size (reduction of TLB misses). This can be done by using the **ppgsz** command. Example:

```
$ man ppgsz    # manual page
$ ppgsz -o heap=4M,stack=4M a.out # program start
```

As an alternative environment variables can be used:

```
$ LD_PRELOAD=mpss.so.1    MPSSHEAP=4M   \
  MPSSSTACK=4M    a.out
```

A new command-line option, **-xpagesize**, enables the running program to set the preferred stack and heap page size at program startup (Studio 8 compilers). For example, **-xpagesize=4M** sets the preferred Solaris 9 operating environment stack and heap page sizes to 4 megabytes. Choose from a set of preset values. Stack or heap page sizes can be set individually with **-xpagesize_stack** and **-xpagesize_heap**. (Note that this feature is not available on Solaris 7 and Solaris 8 environments. A program compiled with this flag will fail to link these environments.) See the f95 man page for details.

All dynamically or locally allocated data, as well as uninitialized Fortran COMMON Blocks will be allocated on large pages (4 MB in the above example), if enough consecutive memory is available. You may check the running program with the command (Solaris 9)

```
$ pmap -s pid  # address space map of a process
```

The Sun Fire 15K machines have a non uniform memory access (cc-NUMA) architecture. Thus processors have a quicker access to data on a memory chip on the same CPU board than to that residing on a different board. Whereas Solaris 8 allocates data uniformly on all boards, MPO in Solaris 9 tries to place data (pages) on the same board as the processor, which touches the data first (**first touch policy**). If you prefer to distribute the data across the boards, you can start your prgram with the environment variables

```
$ LD_PRELOAD=madv.so.1 MADV=access_many a.out
```

See the madv.so.1 and **`madvise`** manual pages for further information. MPO is nicely described in a detailed whitepaper, which is available on the Sun web site at http://www.sun.com/servers/wp/docs/mpo_v7_CUSTOMER.pdf.

3.1 Addressing Modes

Solaris 8 and 9 are 64-bit UNIX operating systems. Programs can be compiled and linked in 32-bit mode (default) or 64-bit mode. This affects memory addressing (usage of 32- or 64-bit pointers) and has no influence on the precision of floating point numbers (4- or 8-byte real numbers). Programs needing more than 4 GB memory, have to use the 64-bit addressing mode. The switches for UltraSPARC-III Cu specific compilation and linking are

`-xarch=v8plusb`	`32-bit`
`-xarch=v9b`	`64-bit`

Note: **`long int`** data and pointers in C programs are stored with 8 bytes when using 64-bit addressing mode.

3.2 Batch Job Administration RWTH

Batchjobs are handled by the **Sun GridEngine** (formerly **Codine**).

Job scripts can be submitted to the batch system with the line command

```
$ qsub [options] [scriptfile | - [script_args] ]
```

or through the graphical user interface

```
$ qmon
```

The attributes of queued jobs can be modified with

```
$ qalter [options]
```

Jobs can be deleted with

```
$ qdel job_id
```

Status information can be inquired with

```
$ qstat -f | -j job_id | -u user
```

On overview of the current batch job load of the entire Sun Fire cluster can be obtained with the utility

```
$ jobinfo RWTH
```

The most important **parameters of `qsub`** are:

-o [*hostname*:]*path*	standard output file
-e [*hostname*:]*path*	standard error file
-j y|n	merge error outputs into standard output
-l *resource=value,...*	specification of the necessary resources (see below)
-N *name*	job name
-pe *parallel_environment ntask*	processor count for the MPI environment (see below)
-v *variable*[=*value*]	set environment variables
-w v	only check the job parameters, do not submit (this does currently not work in combination with the **-pe** parameter)
-r n	no restart, in case of a system crash
-hold_jid *job_id,...*	start after the termination of the indicated job
-M mail_address	notification mail address
-m b | e | a | s | n	send notification mail at job begin | end | abort | suspend | send no mail

The most important **resource parameters** are (see **`qsub`**-parameter **`-l`**):

-l hostname=*hostname*	computer name. Normally the use of this parameter is not recommended.
-l h_rt=*hh*:*mm*:*ss*	required real time [[hours:]minutes:]seconds Default: 0:10:00 Maximum: 24:00:00
-l h_vmem=*xxxX*	virtual memory specification in bytes, KB, MB oder GB e.g. vmem=10M default: vmem=1M
-l num_proc=*nthread*	in case of shared memory parallelization: specification of the number of threads
-l ostype=sunos	start on the SunFire compute nodes.
-l solaris8 **-l solaris9**	during the migration period from Solaris 8 to Solaris 9 these resource parameters may be used. Normally the use of these parameters is not recommended.
-l march=sf-15k **-l march=sf-6800**	jobs can be directed to the Sun Fire 15K or to the Sun Fire 6800 nodes. Normally the use of these parameters is not recommended.
-l *software*=#_*of_licenses*	the need for software licenses has to be specified. Currently the available licensed packages are: abaqus, ansys, cfx4, cfx5, gamess, gaussian, g98, linda, marc, matlab, tascflow The number of licenses normally equals 1.
-l hw_counters ***NEW***	Specify this resource, if you want to collect performance information (**collect** command).

MPI-Jobs have to be submitted into one of the following "**parallel environments**". The number of MPI processes has to be specified (***nproc***)

-pe mpi_sunos_* *nproc*	the MPI job will be started on any of the Sun Fire machines
-pe mpi_sunos_6800 *nproc*	the MPI job will be started on Sun Fire 6800 nodes only
-pe mpi_sunos_15k *nproc*	the MPI job will be started on Sun Fire 15K nodes only
-pe mpi_sunos_1host *nproc*	all processes of the MPI job will be started on any one Sun Fire node.All MPI communication will use the common main memory.

The parameters can also be indicated as comment lines, starting with the characters "#$", in the beginning of the job scripts. Command line parameters have higher precedence than the imbedded script flags.

Submitting a serial job:

```
$ qsub -o $HOME/aus.txt -j y -l ostype=sunos \
-l h_rt=00:15:00 -l h_vmem=500M scriptfile
```

This corresponds to

```
#!/usr/bin/ksh
#$ -o $HOME/aus.txt
#$ -j y
#$ -l h_rt=00:15:00
#$ -l h_vmem=500M
#$ -l ostype=sunos

cd workdir
program
```

Example of a batch job script for starting a Sun MPI program:

(The environment variable **MPRUN_FLAGS** is predefined by the batch system in order to direct the MPI processes to the reserved machines. The limits are per process limits, so in total 5 times 500 MB will be reserved.)

```
#!/usr/bin/ksh
#$ -N MPI-Test-Job
#$ -l h_rt=00:15:00
#$ -l h_vmem=500M
#$ -pe mpi_sunos_* 5
#$ -l ostype=sunos
cd workdir
mprun program
```

Example of a batch job script starting an OpenMP or an autoparallel program:

(The environment variable **OMP_NUM_THREADS** is predefined by the batch system in order to start as many threads as processors have been reserved. 500 MB will be reserved on one node for all 5 threads.)

```
#!/usr/bin/ksh
#$ -N OpenMP-Test-Job
#$ -l h_rt=00:15:00
#$ -l h_vmem=500M
#$ -l num_proc=6
#$ -l ostype=sunos
cd workdir
program
```

Hybrid Programs use a combination of MPI and OpenMP, where each MPI process is multi-threaded. Example of a batch job script starting a hybrid program:

(The environment variables **MPRUN_FLAGS** and **OMP_NUM_THREADS** are predefined by the batch system. In this example 5 groups of 4 CPUs will be reserved.)

```
#!/usr/bin/ksh
#$ -N Hybrid-Test-Job
#$ -l h_rt=00:15:00
#$ -l h_vmem=500M
#$ -l num_proc=4
#$ -pe mpi_sunos_15k 5
#$ -l ostype=sunos
cd workdir
mprun program
```

3.3 Defaults of the User Environment RWTH

The login shell is the korn shell (**ksh**). It's prompt is symbolized by the dollar sign. Accordingly numerous initialization scripts follow this syntax. They must be started with

```
$ . scriptfile
```

Environment variables are set with

```
$ export variable=value
```

This corresponds to the C shell command

```
% setenv variable value
```

If you prefer to use a different shell, start any necessary initialization scripts before you change to your preferred shell.

```
$ . init_script
$ exec csh
%
```

The C shell prompt is indicated with an "percentage" symbol.

For the use of the Sun ONE Studio 8 Compiler Collection environment and HPC ClusterTools, the environment variables **PATH** and **MANPATH** are already adapted in the user profile:

```
$ export PATH=${PATH}:\
     /opt/SUNWspro/bin:/optSUNWhpc/bin
$ export MANPATH=${MANPATH}:\
     /opt/SUNWspro/man:/optSUNWhpc/man
```

3.4 User File Management RWTH

Every user owns directories on shared file systems for small, long-term user files (**$HOME=/home/*username***) and for large, medium-term workfiles (**$WORK=/work/*username***). The **$HOME** data will be saved regularly.

A directory for local scratch files (**$TMP=/tmp/*username/login_pid***) is accessible only on the respective node and will be automatically created before and deleted after the terminal session or the batch job.

4 Programming/Tuning

4.1 Sun Compilers

The Sun ONE Studio 8 Development Tools are now in production mode and the default compilers. They include the Sun Fortran 95 7.1, Sun C 5.5 and Sun C++ 5.5 compilers. If necessary you can use the previous version of the compilers by modification of the search path with the following commands ***RWTH***

```
$ . studio7.init    # previous compiler
```

We recommend that you always recompile your code with the latest production compiler for performance reasons and bug fixes.

Check the compiler version which you are currently using with the option

```
-V
```

or with the command

```
$ dumpstabs object_file
```

Online information in addition to the manual pages can be found by directing your browser to the local file

```
file:///opt/SUNWspro/docs/index.html
```

or to the website

```
http://docs.sun.com/db/coll/771.2
```

Particularly the new features are described in

```
http://docs.sun.com/source/816-452/1.html
```

The compilers are invoked with the commands

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

The appropriate manual pages are available. You can get an overview of the available compiler flags with the option

```
-flags
```

It is in general recommended to use the same flags for compiling and for linking.

NEW From Studio 7 on, there no longer is a separate Fortran 77 compiler available. But there is an additional option in the new Fortran95 compiler improving the compatibility to Fortran 77

```
-f77
```

which has several suboptions. Using this option without any suboption list expands to

```
-ftrap=%none -f77=%all
```

which enables all compatibility features at the same time and also mimics the Fortran 77's behavior regarding arithmetic exception trapping. We recommend to add

```
-f77 -ftrap=common
```

in order to revert to the `f95` 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.

Detailed information about compatibility issues between Fortran 77 and Fortran 95 can be found in

http://docs.sun.com/source/816-2457/5_f77.html

Compute intensive program parts can be translated and linked with the optimization options (US-III Cu)

`-fast -xarch=v9b` (64 bit addressing) or

`-fast -xarch=v8plusb` (32 bit addressing)

`-fast` is a macro expanding to several individual options, which are meant to give you the best performance with one single compile and link (!) option. Note however that the expansion of **`-fast`** might be different across the various compilers and can change between different compiler releases.

At present (Studio 8) **`-fast`** with the Fortran 95 compiler corresponds to the following list (see *manual page*):

```
-O5 -xarch=native -xpad=local -xvector=yes
-xprefetch=auto,explicit -dalign -fsimple=2
-fns=yes -ftrap=common -xlibmil  -xlibmopt
-xdepend=yes -fround=nearest
```

with the C compiler:

```
-fns -fsimple=2 -fsingle -ftrap=%none -
xalias_level=basic -xarch=native -xbuiltin=%all
-xdepend -xlibmil -xmemalign=8s
-xprefetch=auto,explicit -xO5
```

and with the C++ compiler:

```
-xO5 -xarch=native -xmemalign=8s -fsimple=2
-fns=yes -ftrap=%none -xlibmil -xlibmopt
-xbuiltin=%all
```

For further optimization by the C-compiler the following options can be added:

```
-xvector -xspfconst
```

and for further optimization by the C++-compiler the following options can be added:

```
-xalias_level -xvector -xspfconst
-xprefetch=auto,explicit
```

The generated code can be specifically tuned for the 900 Mhz-UltraSPARC-III Cu processor (US-III Cu) by specifying

```
-xchip=ultra3cu -xcache=64/32/4:8192/512/2 \
      -xarch=v8plusb      (32-bit addressing mode)
-xchip=ultra3cu -xcache=64/32/4:8192/512/2 \
      -xarch=v9b          (64-bit addressing mode)
```

In general it is recommended to specify the precise architecture flags for linkage as well (**-xarch=v8plusb** / **v9b** for the UltraSPARC-III Cu processor), so that the optimal run time libraries are used.

You can get a survey of the compiler flags used by adding the option

```
-v (Fortran and C++)
-# (C)
```

The compiler supports inlining of function and subroutine calls. With optimization level -xO4 and above, this is attempted for functions/subroutines within the same source file. The programmer can also specify which functions/subroutines should be inlined, by specifying these with the following option

-xinline=*routine_list*

Note however 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*

If one wishes to have the compiler perform inlining across various source files, the -xipo option can be used. This is a compile and link option. With the 7.0 release, -xipo=2 is also supported. This adds memory related optimizations to the interprocedural analysis.

Program kernels with numerous branches can be further optimized with the profile feedback method. This two step method starts with a compile 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, run-time characteristics will be gathered.

The second phase consists of a re-compile, using the run-time statistics:

-xprofile=use:*a.out*

This will then hopefully give a better optimized executable, but keep in mind this is of benefit for specific scenario's only.

NOTE: High optimization can have an influence on floating points results due to different **rounding errors**. In order not to change the order of the arithmetic operations by the optimization, a further option can be added, which reduces the execution speed however:

```
-fast -fsimple=0 -xnolibmopt (Fortran)
```

The option

```
-g
```

produces **debugging information**. This is also useful for run-time analysis with the Performance Analyzer, which 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 new Sun compilers. Meanwhile, the correspondence between the binary program and the source code is weakened by optimization, making debugging more difficult.

The Fortran compiler prints a lot of information (compiler messages, cross reference list, etc.) about the program in a separate **listing file** when compiling with the option

```
$ f90 -Xlist ... program.f
$ cat  program.lst
```

The **default data mappings** of the Fortran compiler can be adjusted with the **-typemap** option. The normal setting is

```
-typemap=real:32,double:64,integer:32 ...
```

For example with

```
$ f90 -typemap=real:64,double:64,integer:32 ...
```

the REAL type can be mapped to 8 bytes.

When using the **-g** option, the latest Sun compilers introduce comments about loop optimizations into the object files, which can be output by the command

```
$ er_src progname.o
```

A comment like

```
Loop below pipelined with steady-state cycle
count..
```

indicates that modulo scheduling (aka software pipelining) has been applied, which in general gives better performance.

An expert of the chip architecture will be able to judge by the additional information, if further optimizations are possible.

With the help of the er_src command a successful subroutine inlining can also be easily verified:

```
$ er_src *.o | grep inline
```

NOTE: The compiler options are interpreted from left to the right. In the case of contradictory options the right most dominates.

4.2 The KCC C++ Compiler by KAI RWTH

KCC is an excellent C++ compiler by Kuck & Associates. KCC translates C++ programs to an intermediate C code, which then can be compiled by a native C compiler. KCC is imbedded in the **guidec++** OpenMP compiler.

The most important KCC flags are

+K3	maximum optimization
-O<n> resp. **-fast**	optimization level of the back-end C compiler (will be passed through)
-k or **-keep_gen_c**	do not delete the generated intermediate C code. The C code stored into **<filename>.int.c** might be interesting, but it is hard to read.
-v	verbose mode
--backend ...	pass the following option to the back end compiler
-c, -o	will be passed through as well.

4.3 Interval Arithmetic

The Sun Fortran and C++ compilers support interval arithmetic by an intrinsic **INTERVAL** data type and the UltraSPARC-III Cu processor supports fast switching of the rounding mode of floating point operations.
The use of interval arithmetic requires the use of appropriate numerical algorithms.

4.4 Tuning Tips

Compiler options, compiler directives, programming techniques and last but not least the Sun performance library with highly optimized routines can be used for accelerating programs.

Recently an excellent book covering this topic particularly on UltraSPARC computers has been published:

> **Rajat Garg and Ilya SharapovTechniques for Optimizing Applications: High Performance Computing,ISBN:0-13-093476-3, published by Prentice-Hall PTR/Sun Press.**

Contiguous memory access is critical for reducing cache and TLB misses. This has a direct impact on the addressing of multidimensional fields or structures. Therefore Fortran arrays should be processed in columns and C and C++ arrays in rows. When using structures, all structure components should be processed in quick succession. Frequently this can be achieved by the technique of the *loop interchange*.
The limited memory bandwidth of RISC processors like the UltraSPARC III is a severe bottleneck for many scientific applications. With *prefetching* data can be loaded in advance from the memory into the cache and into the registers. This can be supported automatically by hard- and software but also by explicitly adding prefetch directives resp. calls.

The re-use of cache contents is very important, in order to reduce the number of memory accesses. If possible block algorithms should be used e.g. from the optimized Sun performance library described below.

Cache behavior of programs can be improved frequently by the techniques of *loop*

fission (=*loop splitting*), by *loop fusion* (=*loop collapsing*), by *loop unrolling* (see option **xunroll=n**), by loop blocking, the strip mining and by combinations of these methods. 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 must use more than one instruction for each memory access. However this option must be applied to each routine.

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 run-time behaviour 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. A large INTEGER COMMON -block is allocated, but later on this is declared to be a DOUBLE PRECISION COMMON -block of half the size. Under such circumstances, a misalignment of data can easily happen.

NOTE: The **-dalign** options is actually *required* for Fortran MPI programs and for programs linked to other libraries like the Sun Performance Library and the NAG libraries.

The compiler optimization can be improved by integrating frequently called small subroutines into the calling subroutines (*inlining*). The expense for the subroutine call will be avoided thereby.

-xinline=*routine1,routine2,...*
(*Inlining* of routines from the same source file)

-xO4 -xcrossfile
(*Inlining* of routines from other files in the same compiler call)

-xipo
(*Inlining* of routines from other files in different compiler calls)

In C and C++ programs the use of pointers frequently obstructs the possibility for optimization by the compiler. Through compiler options

-xrestrict and **-xalias_level=...**

it is possible to give 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.

Word of caution. These options and the pragma make certain assumption. When using these mechanisms incorrectly, the behaviour of the program becomes undefined. Please study the documentation carefully before using these options or

directives.

4.5 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. At least the number of runnable processes (use **uptime** command) plus the number of processors needed for the measurement has to be by far less than the number of processors available on the compute node.

Example in C

```
#include <sys/time.h>
/* Real time in nanoseconds as long long int */
double second;
second = (double) gethrtime() * 1.0E-9;
```

and in Fortran

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

CPU time measurements have a smaller precision and are more time costly. For measuring large time intervals they are quite suitable.

In case of parallel programs, real time measurements should by made anyway!

After linking a library supplied by the computing center:

```
-L/usr/local_rwth/lib -lr_lib RWTH
```

the functions **r_rtime** and **r_ctime** are available. They return the real time and the CPU time, respectively, as double precision floating point numbers.

4.6 Hardware Performance Counters

The UltraSPARC-III Cu chip offers 2 programmable 32-bit performance counters for counting various hardware events.

The **cputrack** command (see **man cputrack**), the **cpc-library** (see **man cpc**), the portable PCL-library or the Performance **Analyzer** (see chapter 7) can be used to access these counters.

The command

```
$ cputrack -h
```

lists the names of the countable events. A simple application can be seen in the shell script

```
/usr/local_rwth/bin/mflops RWTH
```

Just call

```
$ /usr/local_rwth/bin/mflops a.out RWTH
```

to count the number of floating points instructions during the execution of **a.out** in MFlop/s.

```
$ man cpc_bind_event
```

displays an example program using the cpc library.

The portable performance counter library (PCL) profits from the cpc library. It can be linked by

```
$ f90 -L/usr/local_rwth/lib -lpcl -lcpc ...
```

A more elegant way of obtaining performance information is the use of the **collect** command and the **er_print** utility or the **analyzer** GUI (see chapter 7).

5 Parallelization

Parallelization for computers with shared memory (SM) means either the automatic distribution of loop iterations on several processors or the explicit distribution of work on the processors by compiler directives and function calls (OpenMP) or a combination of both.

Parallelism for computers with distributed memory (DM) is done via the explicit distribution of work and data on 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 (normally) do not run on computers with distributed memory. As a consequence MPI programs can use all available processors of the SMP cluster, whereas OpenMP programs can use up to 24 processors of a Sun Fire 6800 node, or up to 72 Processors of a Sun Fire 15K 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 an attractive possibility, in order to use as many processors efficiently as possible.

5.1 Message passing with MPI

5.1.1 Sun MPI

Sun MPI is the Sun implementation of the MPI standard and is part of the Sun HPC ClusterTools software suite. At present, HPC ClusterTools 5.0 is installed.

The compiler drivers **mpf77**, **mpf90** , **mpcc** and **mpCC** and the instruction for starting an MPI application **mprun** are in the directory **/opt/SUNWhpc/bin**. The necessary include directory **/opt/SUNWhpc/include** and the library directory **/opt/SUNWhpc/lib** are picked up automatically by these compiler drivers.

Example (recommendation):

```
$ mpf90 -c -dalign ... *.f90
$ mpf90 -o a.out *.o -lmpi
$ mprun -np 4 a.out
```

Example (only for explanation):

```
$ f90 -I /opt/SUNWhpc/include -c -dalign ... *.f90
$ f90 -o a.out *.o -L/opt/SUNWhpc/lib -lmpi
$ /opt/SUNWhpc/bin/mprun -np 4 a.out
```

MPI programs can be started with the command

```
$ mprun [options] program
```

The command **mprun** has numerous flags for placing the MPI tasks on the compute nodes and for input and output control (see also **man mprun** and **mprun -h**).

5.1.1.1 Placing the MPI-Tasks with `mprun`

The following table contains the most important parameters of **mprun** for the distribution of the MPI tasks on the involved machines.

Please note however, that large computing jobs should not be started interactively, and that with use of batch jobs (see chapter 3), the GridEngine batch system determines the distribution of the MPI tasks on the machines to a large extent.

Small MPI test jobs can be started on the interactive node, where you use to logged in by just specifying

```
$ mprun -np n program
```

because the environment variable MPRUN_FLAGS is predefined in the user profile such that all MPI processes will be started on the current machine.

-J	Prints the job identification number
-np *n*	Start of exactly n MPI tasks
-np 0	Start of exactly one MPI task for each processor
-S -np *n*	Start n MPI tasks, but settle for one process per CPU if not enough CPUs are available.
-W -np *n*	Cyclic distribution of the MPI tasks on the processors, if the number of MPI tasks is larger than the number of the processors of the SMP node.
-np *n* ** **-l "sunc01 2, sunc02 3"	Explicit distributing of the ***n*** MPI tasks to the indicated SMP nodes. **Note**: capitalization is relevant
-np *n* -m *rankmapfile*	Explicit distribution of the ***n*** MPI tasks on SMP nodes listed in a file.
-np *n* -Ns	Start of exactly one MPI task on each of ***n*** SMP nodes.
-Zt *m* -np *n*	Start of ***n*** MPI tasks in groups of ***m*** on each of the involved nodes.
-Z *m* -np *n*	Start of ***n*** MPI tasks in groups of ***m***. Several groups on a sufficiently large SMP node are allowed.

5.1.1.2 Input and output control with `mprun`

Under normal conditions standard input (**`stdin`**) is passed to all MPI tasks by the **`mprun`**, command. Standard output (**`stdout`**) as well as standard error output (**`stderr`**) of all tasks are passed to the standard output of **`mprun`**.

By further options of the command **mprun** this behavior can be modified:

-D	The error outputs of the tasks are passed to the error output of the **mprun** command.
-N	All standard input and output is turned off.
-n	**/dev/null** is passed to the standard input. That can be useful for MPI jobs, which run in the background (e.g. as a batch job), so that they do not block, if they wait unintentionally for an input. In this case they will read an EOF.
-B	The output of the tasks is written to files named **out.*jid.rank***.
-o	The output is buffered line by line and the rank of the respective process is written on the beginning of each line.
-I "0r,1wl,2wl"	more precise controlling of the input and output. Only complete lines will be written.
-I "0r,1wt,2wt"	Only complete lines are output and all lines have the task rank placed in front.
-I "0r=input,\ 1wt=out.&J.&R,\ 2w=err.&J.&R"	All tasks read the same input file, but write in separate output and error output files

5.1.1.3 Handling MPI program runs

You can terminate a MPI job with the job identification number ***jid***
(see: **mprun -J**) by:

```
$ mpkill jid
```

The command **mpps** gives a list of the processes, that run under the control of the MPI run time system (**CRE=cluster run time environment**).

```
$ mpps -pef
```

The command **mpinfo** gives an overview of the configuration of all nodes attached to the CRE. Example:

```
$ mpinfo -N
```

5.1.1.4 Sun MPI environment variables

Numerous environment variables can govern the behavior of an MPI program and improve its performance.

In the case of exclusive use of the involved SMP nodes, in particular if one processor in each node is kept free for system processes, which is typically the case in the RWTH batch environment, it's possible to accelerate a program with:

```
$ export MPI_SPIN=1
```

The MPI tasks wait then actively (busy waiting, spinning) for messages and keep their processor busy thereby.

In some cases (e.g. pingpong tests)

```
$ export MPI_POLLALL=0
```

accelerates the application (do not poll).

In case of problems more run time messages can be printed through

```
$ export MPI_SHOW_INTERFACES=3
$ export MPI_SHOW_ERRORS=1
$ export MPI_CHECK_ARGS=1
```

The current values of all MPI related environment variables will be listed at the program start with:

```
$ export MPI_PRINTENV=1
```

The Sun HPC ClusterTools Performance Guide contains many tips for the tuning of MPI applications (http://docs-pdf.sun.com/816-0656-10/816-0656-10.pdf).

NEW The new **HPC ClusterTools Version 5.0** includes a novel profiling tool **mpprof** which is easy to use and gives hints for setting additional environment variables which might improve the performance of a similar program run.

After enabling MPI profiling by setting the environment variable

```
$ export MPI_PROFILE=1
$ mprun -J -np n ... a.out
```

the MPI program run will write out profiling date for the MPI process ranks to a set of intermediate files, one file per process rank, as well as an index file pointing to the intermediate files. The **mpprof** command then generates a report of the performance characteristics of the MPI program

```
$ mpprof mpprof.index.cre.jid
```

with *jid* being the job ID of the cluster runtime environment (CRE) printed out with the **-J** option of the **mprun** command. The report also contains recommendations for settings or modifications of MPI environment variables. The process of profiling and modifying these variables can be iterated, until the performance is optimal and no further hints are given.

The collection of profiling data can be controlled by additional environment variables which are described in the manual page (**man mpprof**).

5.1.2 mpich RWTH

With the improved interoperability of the latest version 6.1 of the Totalview debugger and the upcoming HPC ClusterTools 5.0 we will no longer support **mpich** on the Sun platform. NEW

5.2 Shared memory programming with OpenMP

For shared memory programming OpenMP is becoming the de facto standard. The OpenMP API is defined for FORTRAN, C and C++ and consists of compiler directives, run time routines and environment variables.

In the *parallel regions* of a program several *threads* are started, that execute the contained program segment redundantly, until they hit a *worksharing construct*.

Within this construct, the contained work (usually **do**- or **for**-loops) is distributed among the threads. Under normal conditions all threads have access to all data (*shared* data). But pay attention: if data, accessed by several threads, is modified, then the access to this data must be protected in *critical regions*.

Also *private* data areas can be used, where the individual threads hold their temporary data. All local data of subroutines, which are called within parallel regions, are put on the stack, and thus don't keep their contents from one call to the next!

Therefore, Fortran programs must be translated with the option **`-stackvar.`** **`COMMON`** blocks, data in modules or **`SAVE`** statements must be used with caution (***thread safety***).

Attention! In many cases, the stack area for the slave threads must be increased by changing the environment variable **`STACKSIZE,`** or the stack area for the master thread must be increased with the (Korn shell) command **`ulimit`** (specification in KB). It is recommended to use the new compiler option (version 7.0)

```
-xcheck=stkovf
```

in order to detect stack overflow at runtime.

Hint: In a loop, which 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, but not a sufficient condition!)

The number of the threads to use is indicated by the environment variable **`OMP_NUM_THREADS.`**

Notes: If **`OMP_NUM_THREADS`** is not set, then Sun OpenMP starts only 1 thread (as opposed to the Guide compiler from the KAP/Pro Toolset which starts as many threads as there are processors available).

On a loaded system fewer threads may be employed than specified by this environment variable, because the dynamic mode is used by default (as opposed to the Guide compiler). Use the environment variable **`OMP_DYNAMIC`** to change this behaviour.

5.2.1 Sun-OpenMP

By adding the option

```
-xopenmp
```

the OpenMP directives (according to the latest OpenMP 2.0 specifications) are interpreted by the Fortran95 compiler. This option is an abbreviation for

```
-mp=openmp -explicitpar -stackvar -D_OPENMP -O3
```

Fortunately, the explicit parallelization can be combined with the automatic parallelization of the Fortran compiler. Loops within parallel OpenMP regions are no longer subject to automatic parallelization. Nested parallelization is not (yet) supported.

The C- and C++-compilers support OpenMP as well after adding the option

```
-xopenmp
```

Enabling OpenMP[tm] parallelization with the -xopenmp option makes a program potentially multi-threaded, but the **-D_REENTRANT** flag is not passed to the compiler. The lack of the **-D_REENTRANT** flag causes some code (particularly the templates from the Standard C++ Library) to compile with thread synchronization disabled, which can result in programs silently getting wrong answers.

Workaround: Include the **-D_REENTRANT** flag on the compiler command line whenever you include the -xopenmp option (http://docs.sun.com/source/816-6727/relnotes.html#Documentation).

Between parallel regions the slave threads go to sleep. How they are woken up is controlled by the environment variable **SUNW_MP_THR_IDLE**. The possible values are:

```
$ export SUNW_MP_THR_IDLE=spin | sleep | ns | nms
```

The slave threads wait either actively (busy waiting, by default) 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 wait first actively and fall asleep ***n*** seconds or ***n*** milliseconds later. With fine-grained parallelization active waiting and with coarse-grained parallelization passive waiting is recommended. Idle waiting might be advantageous on an overloaded system.

Setting

```
$ export SUNW_MP_WARN=TRUE
```

enables additional warning messages of the OpenMP run time system.

Use the new Fortran compiler option

```
-XlistMP
```

to receive additional OpenMP related messages in the listing files (***.lst**)

5.2.2 KAP/Pro Toolset RWTH

The KAP/Pro Toolset from the Kuck & Assoc. Inc. (KAI) contains OpenMP compilers and tools.

The Guide compilers interpret OpenMP directives in Fortran, C and C++ programs and generate intermediate programs with calls to the pthread library.

By just replacing the compiler and linker calls to

```
$ guidef77 | guidef90 | guidec | guidec++
```

appropriate compiler drivers are used.

By adding the

```
-WGkeep
```

flag the intermediate programs are kept. By linking with the option

```
-WGstats
```

a statistics file is written during program execution, which can be nicely visualized with

```
$ guideview
```

A remarkable tool for the verification of the correctness of OpenMP programs is **Assure**. Replacing the compiler and linker calls by

```
$ assuref77|assuref90|assurec|assurec++ \
      -WGpname=project
```

the program is instrumented, such that during the program execution every memory access is traced in order to detect possible data races.

The results of this analysis can be displayed with the GUI

```
$ assureview -pname=project
```

or printed out in line mode by

```
$ assureview -txt -pname project
```

The instrumented program will take about 10 times more CPU time and 10 times more memory!

Recommendation: Never put an OpenMP code into production, before using Assure!

5.2.3 Automatic shared memory parallelization of loops

The Sun Fortran- and C-compilers are able to parallelize loops automatically.

Success or failure to do so depends on the compiler's ability to be able to prove it is safe to parallelize a (nested) loop. This is often application area specific (e.g. finite differences versus finite elements), language dependent (pointers may make the analysis hard) and coding style.

The respective option is

```
-xautopar
```

The `-autopar` option is an abbreviation for

```
-xautopar -depend -xO3
```

The combination of explicit parallelism by directives and automatic parallelism is accessible by the option

```
-xparallel
```

as an abbreviation for

```
-xautopar -xexplicitpar -depend -xO3
```

Not only OpenMP directives are interpreted, but also proprietary parallelization directives of Sun and Cray, which, since OpenMP becomes more and more a standard, should not be used anymore. Adding

```
-mp=openmp
```

limits the compiler to OpenMP directives, if for historical reasons also different directives should be still contained in the program.

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

supplies information about the parallelization.

If the number of loop iterations is unknown during compile time, then code is produced, which decides at run-time whether a parallel execution of the loop is more efficient or not (*alternate coding*).

Also with automatic parallelization, the number of the used threads can be specified by the environment variable **OMP_NUM_THREADS**.

5.4 Hybrid Parallelization

The combination of MPI and OpenMP and/or autoparallelization is called hybrid parallelization. Each MPI process is multi-threaded. It is important to link the thread-safe version of the MPI library:

```
$ mpf90 -openmp -fast -c program.f90
$ mpf90 -openmp -fast -o a.out program.o -lmpi_mt
$ export OMP_NUM_THREADS=n
$ mprun -np m a.out
```

KAI's guide preprocessors can be used as well:

```
$ guidef90 -Wgcompiler=mpf90 -openmp -fast -c \
program.f90
$ guidef90 -Wgcompiler=mpf90 -openmp -fast \
     -o a.out program.o -lmpi_mt
$ export OMP_NUM_THREADS=n
$ mprun -np m a.out
```

6 Debugging

If your program is causing problems, it might be good opportunity to lean back and think for a while.

Take a step back:

- What were the last changes that you made? (A source code revision system (RCS, CVS) might help.)
- Reduce the number of CPUs in a parallel program, try a serial program run if possible.
- Reduce the optimization level of your compilation.
- Chose 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 6.1).
- Try a dynamic analysis with appropriate compiler options (see chapter 6.2). In case of an OpenMP program, use Assure (see chapter 5.2.2).
- Use a debugger. Use the smallest case which shows the error (see chapter 6.3).

6.1 Static program analysis

First, an exact static analysis of the program is recommended for error detection. The Fortran compiler offers an **-Xlist** option which generates warning and error messages into additional listing files (file extension **.lst**). For OpenMP programs there is a new option **-XlistMP**. Furthermore the following tools can be used for static analysis:

`cc -v ..`	stricter semantic checks of C programs by the compiler
`lint`	more accurate syntax check of C programs
`ftnchek`	more accurate syntax check of Fortran77 programs
`foresys`	more accurate syntax check of Fortran77 and Fortran90 programs and more

Sometimes, program errors occur only after high optimization by the compiler. That can be a compiler error or a programming error. If the program runs correctly without compiler optimizations, the module causing the trouble can be found by systematic bisectioning.

6.2 Dynamic program analysis

The program can be further checked by translation with certain options:

-C	array bound check of **Fortran** programs
-Xlist	global program analysis, write detailed list to files with the ending **.lst**
-ftrap=%all	pursue of floating point errors, like division by zero, overflow, underflow. The error handling can be programmed also explicitly, see: **man ieee_handler**
-g	enrich the binary program with debugger information, for step-by-step debugging, turn off all optimizations)
-xcheck=stkovf	check stack overflow at runtime, new with version 7

A new extension to the **-xcheck** option flag enables special initialization of local variables. 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.

The sampling collector (see chapter 7.1) is now also able to detect memory leaks

```
$ collect -H
```

A core dump can be analyzed with the debugger, if the program was translated with **-g** :

```
$ dbx a.out core
$ totalview a.out core
```

If a program with optimization delivers other results than without, then the changed rounding error behavior can be responsible. There is a possibility to test this by optimizing the program “carefully”:

```
$ f90 ... –fsimple=0 -xnolibmopt...
```

Thus, the sequence of the floating point operations is not changed by the optimization, which can increase the run time.

6.3 Debuggers

At present four different debuggers are available. In all cases the program must be translated and linked with the option **–g** and without optimization (at least in the interesting program parts).

Don't 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 don't forget to purge core files afterwards!

6.3.1 dbx

dbx is a powerful line orientated debugger with a detailed online help.

It can as well be used to debug long running programs in batch mode. Collect the **dbx** commands in an input file and start your program under control of **dbx**:

```
$ cat  >> dbx.in < EOF
catch FPE
catch SIGSEGV
catch SIGBUS
run inputfile
where
dump
quit
EOF
$ dbx a.out < dbx.in
```

You may as well debug MPI-Programs this way:

```
$ mprun -np ntasks -o dbx a.out < dbx.in
```

It might be more comfortable only to run a few MPI processes through the debugger. This can be accomplished by starting a small shell script like the following:

```
#!/bin/ksh
# giving the corefile a useful name ...
coreadm -p core.%n.%f.p%p.j${MP_JOBID}.t$MP_RANK  $$;
# mechanism to restrict debugging to a subset of MPI
processes ...
if [[ $MP_RANK < 2  ]]
then
        dbx a.out < dbx.in > dbx.out.t$MP_RANK
        mpkill -9 $MP_JOBID
else
        debug.exe
fi
```

This script, using the same input file **dbx.in** for **dbx** like above, is than run with

```
$ mprun ... rundebug.ksh
```

This will leave some core files with meaningful names behind, which then can be analyzed with

```
dbx a.out core.machinename.a.out.pnnnn.jmmmm.tkk
```

6.3.2 Prism

prism is a graphic debugger for Sun MPI programs.

If the help information browser does not start correctly, use

```
$ export PRISM_BROWSER_SCRIPT=yes
```

NEW The syntax for starting **prism** has changed in Sun HPC ClusterTools 5.0:

```
$ mprun <mprun_options> prism <prism_options>
```

The **<prism_options>** no longer include any options for controlling the number of processes, or process placement. Use the **<mprun_options>** for such control. Examples:

```
$ mprun -np 8 prism program
$ mprun -np 8 prism program jid
$ mprun -np 8 -Zt 2 prism program corefile
```

6.3.3 TotalView RWTH

The state-of-the-art debugger TotalView from Etnus (http://www.etnus.com/) can be used to debug serial and parallel Fortran, C and C++ programs. It is available on all major platforms.

NEW The latest version 6.3 of the **TotalView** debugger supports the latest Sun compilers as well as the latest version of the Sun HPC ClusterTools.

As an appendix a we include a TotalView Quick Reference Guide for the Sun Fire SMP cluster.

6.3.3.1 Invocation of TotalView for serial programs

```
$ . totalview.init
$ totalview program [corefile]
```

6.3.3.2 Debugging of Sun-MPI programs RWTH

```
$ . totalview.init
$ totalview mprun -a -np 2 -l "$(hostname) 2" \
    a.out
```

When the GUI appears, type g for go, or click Go in the TotalView window.

TotalView may display a dialog box:

Process mprun is a parallel job. Do you want to stop the job now?

Click **Yes** to open the TotalView debugger window with the Sun MPI source window and leave all processes in a traced state.

Outstanding non-blocking messages can be displayed with the **Tools > Message Queue Window** or the **Tools > Message Queue Graph**.

6.3.3.3 Debugging of 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 behaviour of the program is heavily influenced by debugging.

It is recommended to use the new Fortran compiler option

```
-XlistMP
```

to do a basic static program check. Furthermore the **Assure** tool is recommended for the verification of OpenMP programs (see chapter 5.2.2).

But interactive debugging is possible as well. By default the Sun compilers' OpenMP options require high optimisation (-xO3) which in turn prohibits debugging. Since Studio 8 it is possible to debug Fortran and C programs using OpenMP after compiling with a new suboption

```
$ f90 -openmp=noopt -g ...
$ cc -xopenmp=noopt -g ...   RWTH
```

As an alternative you can use KAI's guide precompiler, which can be combined with TotalView.

Example:

```
$ guidef90 –WG,-cmpo=i [-WGkeepcpp] –g –c *.f90
$ guidef90 –WG,-cmpo=i –g –o a.out *.o
$ export OMP_NUM_THREADS=2
$ . totalview.init
$ totalview a.out
```

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.

7 Programming 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.

7.1 Sampling Collector and Performance Analyzer

The Sampling Collector and the Performance Analyzer are a pair of tools that you use to collect and analyze performance data for your application.

The Collector 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 after the program has finished.

7.1.1 The Collector

At first you have to compile your program with the

```
-g
```

option. Link the program as usual and then start the executable under the control of the Sampling Collector

```
collect collect_options a.out
```

Every 10 milliseconds profile data will be gathered and written in the experiment file

```
test.1.er
```

The number will be automatically incremented on subsequent experiments. In fact the experiment file is an entire directory with a lot of information. One can manipulate these with the regular Unix 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

After

```
er_print test.1.er
```

you can generate a first ASCII report from the experiment with the command

```
functions
```

Further commands are explained after invoking **help** or through the man page of the er_print command.

By selecting the options of the collect command, many different kinds of performance data can be gathered:

-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, *counter1*,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	Follow descendant processes

Various hardware counters can be chosen for collecting. Typing the collect command without any parameters, will print out all the counters available for profiling. Some of the events can only be gathered in register 0 and some only in register 1. Favorite choices are given in the following table.

-h cycles,on,insts,on	Cycle count, instruction count The quotient is the CPI rate (clocks per instruction) The optimum would be 0.25. The Mhz rate of the CPU multiplied with the instruction count divided by the cycle count gives the MIPS rate.
-h fpadd,on,fpmul,on	Floating point additions and multiplications The sum divided by the runtime in □s gives the Mflop/s rate
-h cycles,on,dtlbm,on	Cycle count, data translation look-aside buffer (DTLB) misses A high rate of DTLB misses indicates an unpleasant memory access pattern of the program. Large pages might help (Solaris 9)
-h cycles,on,ecstall, on	L2 cache stall cycles.
-h cycles,on,dcstall, on	L1 plus L2 cache stall cycles
-h ecref,on,ecm	L2 cache references and misses
-h dcr,on,dcrm,on	L1 cache read references and read misses
-h dcw,on,dcwm,on	L1 cache write references and write misses

7.1.2 The Performance Analyzer

For the standard case of just collecting clock profiling and printing out the most important information in text mode a simple shell script is available:

```
$ /usr/local_rwth/bin/sample a.out
$ more sample.out                                    RWTH
```

A program call tree with performance information can be displayed with the locally developed utility

```
$ /usr/local_rwth/bin/er_view                        RWTH
```

The full result of the analysis can be displayed graphically afterwards with the Performance Analyzer GUI, which has been redesigned in the latest version.

```
$ analyzer experimentfile.er
```

7.1.3 The Performance Tools Collector Library API

Sometimes it is convinient to group performance data in self defined samples, and to collect performance data only of a specific part of the program.

For this purpose the libcollector library can easily be used.

In the following example Fortran program, performance data only of the subroutines **work1** and **work2** is collected:

```
program test_collector
call collector_pause()
call preproc
call collector_resume()
call collector_sample("start")
call work1
call collector_sample("work1")
call work2
call collector_sample("work2")
call collector_terminate_expt()
call postproc
end program test_collector
```

The **libfcollector** library (C: **libcollector**) has to be linked. And if this program is started by

```
$ collect -S off a.out
```

performance data is only collected between the **collector_resume** and the **collector_terminate_expt** calls. No periodic sampling is done, but single samples are recorded whenever **collector_sample** is called. (The label is not currently used). When the experiment file is evaluated, the filter mechanism can be used to restrict the displayed data to the interesting program parts.

See the **libcollector** manual page for further information.

7.2 Frequency analysis with `tcov`

For error detection and tuning it might be helpful to know, how often each statement

is executed. For testing a program it is important that all program branches are passed (*test coverage*). For this purpose, the program must be compiled and linked with the option

```
-xprofile=tcov
```

In the following program execution the frequencies of all statements recorded. The values can be entered in modified program sources using the command

```
$ tcov -a -50 -x a.out.profile \
      [-p srcdir objdir] source_files...
```

Statements which have never been executed are marked by "#".

7.3 Run time analysis with gprof

With **gprof**, a run time profile on module level can be generated. The program must be translated and linked with the option **–pg** (Fortran) resp. **–xpg** (C). During the execution a file named **gmon.out** is generated, which 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 to use the Callers-Callees info in the Performance Analyzer to gather this kind of information. It is much more reliable.

7.4 Run time analysis of MPI programs

7.4.1 Sampling Collector and Performance Analyzer

With MPI programs, the Sampling Collector (see chapter 6.1) collects run time information for each MPI task, which can also be displayed for each task separately:

```
$ mprun -np n collect a.out
```

With a new option of the Sampling Collector MPI events can be traced as well

```
$ mprun -np n \
      collect -m on -g experiment_group.erg a.out
```

together with the ability to bundle experiment files written by all MPI processes to experiment groups and display them with the Analyzer

```
$ analyzer experiment_group
```

Running collect with a large number of MPI processes, the amount of experiment data might become overwhelming. Starting the MPI program with a little script will help:

```
$ mprun -np 4 run.ksh
```

with

```
#!/bin/ksh
# filename: run.ksh
if [[$MP_RANK < 2 ]]
then
     collect -m on -g test.erg a.out
else
     a.out
fi
```

Performance information will be collected only for the MPI processes with rank 0 and 1.

7.4.2 Prism

The runtime analysis feature of Prism is no longer support. The usage of the analyzer is recommended instead.

7.4.3 Vampir and VampirTrace *RWTH*

Vampir/Vampirtrace is an MPI performance analysis toolset sold by the company Pallas. After linking the **VampirTrace** library to the MPI program, a trace file is written during the program execution, which then can be displayed with the **Vampir** graphical user interface.

Example in C:

```
$ . vampir.init
$ mpcc -o a.out  ... *.c \
     -L/usr/local_rwth/lib -lVT -lmpi -lnsl
$ mprun -np 4 a.out
$ vampir a.out.bvt
```

Example in Fortran:

```
$ . vampir.init
$ mpf90 -o a.out  ... *.f90 -R/usr/local_rwth/lib \
     -L/usr/local_rwth/lib -lVT -lmpi -lnsl
$ mprun -np 4 a.out
$ vampir UNKNOWN.bvt
```

The functioning Vampirtrace library can be highly parametrized with a configuration file. The name of this file has to be specified by the environment variable **VT_CONFIG**.

7.4.4 Jumpshot and the MPE Library

The Multi-Processing Environment (MPE) attempts to provide programmers with a complete suite of performance analysis tools for their MPI programs based on post processing approach. These tools include a set of profiling libraries, a set of utility programs, and a set of graphical visualization tools.

The most useful and widely used profiling libraries in MPE are the logging libraries. Various logfile formats are supported, the most powerful one is SLOG. As the

default format is the CLOG, the programmer must set an environment variable to overwrite the default format:

```
$ export MPE_LOG_FORMAT=SLOG
```

After linking the libraries liblmpe.a (MPE logging interface) and libmpe.a (MPE graphics, logging, and other extensions) and, in the case of a Fortran program, the additional wrapper library libmpe_f2cmpi.a, the (binary) logfiles will be generated during runtime. Visualize these logfiles with the jumpshot (version 3) utility.

```
$ mpcc -c foo.c
$ mpcc -o foo foo.o \
     -L/usr/local_rwth/lib -llmpe -lmpe -lmpi
$ export MPE_LOG_FORMAT=SLOG
$ mprun -np 4 foo
$ jumpshot foo.slog
```

Example in Fortran:

```
$ mpf90 -c foo.f90
$ mpf90 -o foo foo.o -L/usr/local_rwth/lib \
     -lmpe_f2cmpi -llmpe -lmpe -lmpi
$ export MPE_LOG_FORMAT=SLOG
$ mprun -np 4 foo
$ jumpshot Unknown.slog
```

NOTE: The trace file produced at the end of a Fortran program run is always called **`Unknown.bvp.`**

8 Application software

8.1 Application software and program libraries RWTH

You will find the list of available application software and program libraries at http://www.rz.rwth-aachen.de/sw/

8.2 The Sun Performance Library

The Sun Performance Library is a part of the Sun One Studio Compiler Collection environment and contains highly optimized and parallelized versions of the well known standard libraries LAPACK version 3.0, BLAS, FFTPACK version 4 and VFFTPACK Verson 2.1 from the field of linear algebra, Fast Fourier transforms and solution of sparse linear systems of equations (Sparse Solver, SuperLU) (see http://www.netlib.org). Please link your program with the options:

-xarch=vplus8b -xlic_lib=sunperf	32 bit addressing
-xarch=v9b -xlic_lib=sunperf	64 bit addressing

The performance of programs using the BLAS1-library can be improved by the new Fortran compiler option

```
-xknown_lib=blas
```

The corresponding routines will be inlined if possible.

The latest Performance Library contains new parallelized sparse BLAS routines for matrix-matrix multiplication and a sparse triangular solver. Linpack routines are no longer provided, it is stronly recommended to use the corresponding LAPACK routines.

Many of the contained routines have been parallelized using the shared memory programming model. Compare the execution times! Example:

```
$ f90 -dalign -mt -xlic_lib=sunperf ...
$ ptime a.out
$ ( export OMP_NUM_THREADS=4; ptime a.out )
```

The number of Threads used by the parallel Performance Library can be determined by the following call:

```
call USE_THREADS(n)
```

8.3 The Sun S3L library

The S3L-Library offers to MPI programs access to distributed arrays similar to the array descriptors, as they are used in the public domain packages ScaLAPACK and PETSc. The S3L-Library offers many functions from the fields linear algebra, Fourier transforms, etc. and further auxiliary functions (toolkit). Numerous kernel routines correspond to the ScaLAPACK interfaces.

The Toolkit functions are useful for working with parallel arrays and processor grids, as well as for parallel input or output. S3L arrays can be transformed into ScaLAPACK descriptors.

8.4 Nag Numerical Libraries RWTH

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 but a few.
They are available in three flavours:

1) The serial NAG Mark 19 FORTRAN-Library (32 bit addressing mode)

```
f90 -xarch=v8plusb -dalign ... \
-L/usr/local_rwth/lib -lnag19  \ -
xlic_lib=sunperf -lF77
```

2) The shared memory version, which includes 231 routines that benefit from shared memory parallelization (32- and 64-bit addressing modes) and has the identical programming interface as the serial version

```
f90 -dalign -xarch=v8plusb ...     \
 -L/usr/local_rwth/lib -lnagsmp32 \ -
xlic_lib=sunperf -lF77
```

```
f90 -dalign ... -xarch=v9b        \
-L/usr/local_rwth/lib -lnagsmp64 \ -
xlic_lib=sunperf -lF77
```

3) and the NAG Parallel Library Release 3.0, which contains 183 routines that have been specifically developed for use on distributed memory systems (32 bit addressing mode) using the MPI library.

```
mpf90 -dalign -xarch=v8plusb ... \
 -L/usr/local_rwth/lib -lnagmpi -ls31
```

9 Further information

9.1 Sun products

9.1.1 On Sun's web site

- Sun Product Documentation (Overview) (http://docs.sun.com)
- Sun ONE Studio 8 Compiler Collection (Overview) (http://docs.sun.com/coll/771.3?q=Forte+8)
  - Sun ONE Studio 8: Fortran User's Guide (http://docs.sun.com/db/doc/817-0930?q=Forte+8)
  - Sun ONE Studio 8: C User's Guide (http://docs.sun.com/db/doc/817-0924?q=Forte+8)
  - Sun ONE Studio 8: C++ User's Guide (http://docs.sun.com/db/doc/817-0926?q=Forte+8)
  - Sun ONE Studio 8: Fortran Programming Guide (http://docs.sun.com/db/doc/817-0929?q=Forte+8)
  - Sun ONE Studio 8: Fortran Library Reference (http://docs.sun.com/db/doc/817-0928?q=Forte+8)
  - Sun ONE Studio 8: OpenMP API User's Guide (http://docs.sun.com/db/doc/817-0933?q=Forte+8)
- Prism 7.0 Software User's Guide (http://docs.sun.com/db/doc/817-0088-10?q=Prism)
- Prism 7.0 Software Reference Manual (http://docs.sun.com/db/doc/817-0089-10?q=Prism)
- Sun HPC ClusterTools 5 Software Documentation (Overview) (http://docs.sun.com/coll/HPCCT5?q=Sun+MPI)
  - Sun HPC ClusterTools 5 Software User's Guide (http://docs.sun.com/db/doc/817-0084-10?q=Sun+MPI)
  - Sun MPI 6.0 Software Programming and Reference Guide (http://docs.sun.com/db/doc/817-0085-10?q=Sun+MPI)
  - Sun HPC ClusterTools 5 Software Performance Guide (http://docs.sun.com/db/doc/817-0090-10?q=Sun+MPI)
- Sun S3L 4.0 Software Programming Guide (http://docs.sun.com/db/doc/817-0086-10?q=Sun+S3L)
- Sun S3L 4.0 Software Reference Manual (http://docs.sun.com/db/doc/817-0087-10?q=Sun+S3L)

9.1.2 On local file systems

- Forte Developer: Documentation (Forte, C, C++, dbx, OpenMP, tcov) (/opt/SUNWspro/docs/index.html)
- HPC ClusterTools 5 Documentation (MPI, Prism, S3L) (/opt/SUNWhpc/doc/index.html)

9.2 Third party products

- TotalView
  (http://www.etnus.com)
- KAP Pro/Toolset
  (http://support.rz.rwth-aachen.de/Manuals/KAI/KAP_Pro_Reference.pdf,
  http://developer.intel.com/software/products/kappro/)
- Vampir and VampirTrace
  (http://support.rz.rwth-aachen.de/Manuals/Vampir/Vampir-userguide.pdf,
  http://support.rz.rwth-aachen.de/Manuals/Vampir/Vampirtrace-userguide.pdf,
  http://www.pallas.com)
- KCC
  (http://support.rz.rwth-aachen.de/Manuals/KAI/KCC_docs/index.html,
  http://developer.intel.com/software/products/kcc/)
- Foresys
  (http://www.simulog.fr)

9.3 Public domain software

- mpich – Eine portierbare Implementierung von MPI
  (http://www-unix.mcs.anl.gov/mpi/mpich)
- PCL Performance Counter Library
  (http://www.fz-juelich.de/zam/PCL)

9.4 Problems and inquiries

- Helpdesk of the computer center (web interface)
  (http://www.rz.rwth-aachen.de/computing/support/)

10 Miscellaneous

10.1 Other Useful commands

/opt/SUNWspro/bin/dmake	Parallel make (compare gmake)
/usr/bin/csplit	Splits C programs
/opt/SUNWspro/bin/fsplit	Splits Fortran programs
/usr/ccs/bin/nm	Prints the name list of object programs
/usr/bin/ldd	Prints the dynamic dependencies of executable programs
/opt/SUNWspro/bin/lint	More accurate syntax examination of C programs
/opt/SUNWspro/bin/cflow	Prints the call hierarchy of a C program
/opt/SUNWspro/bin/cxref	Cross reference list of a C program
/opt/SUNWspro/bin/ctrace	Tracing of a C program
/opt/SUNWspro/bin/dumpstabs	Analysis of an object program
/usr/bin/showrev	Prints the software status of the machine
/usr/bin/ptime **/usr/bin/pstack** **/usr/bin/ptree** **/usr/bin/pmap**	Analysis of the /proc directory
/usr/sbin/sysdef	system parameters
/usr/sbin/prtconf	system configuration
/usr/platform/SUNW,Sun-Fire/sbin/prtdiag	diagnostic messages
/usr/sbin/psrinfo	processor information
/usr/bin/pkginfo	installed software packages
/opt/SUNWspro/bin/fpversion	processor information
/usr/dt/bin/sdtprocess	process list (compare top)
/usr/bin/sar	system activity report
/usr/bin/truss	log system calls
/usr/bin/sotruss	log of shared library calls
ld.so.1	Run time linker for dynamic objects
/usr/bin/vmstat	status of the virtual memory organization
/usr/bin/iostat	I/O statistics
/usr/bin/busstat	system bus performance counters
/usr/bin/prstat	Report active process statistics
gettimeofday **#include <sys/time.h>**	Portable real time counter

11 Appendix: Debugging with TotalView on the Sun Fire SMP-Cluster - Quick Reference Guide

This quick reference guide describes how to debug serial and parallel (OpenMP and MPI) programs written in C, C++ or Fortran90 using the TotalView debbuger from Etnus Inc. on the RWTH Sun Fire SMP-Cluster in a very condensed form. Here is a list of the current software versions: Solaris 8 and 9, TotalView 6.3, Sun ONE Studio 8 compilers, Sun HPC ClusterTools 5.0, KAP/Pro Toolset 4.0.

For further information see www.etnus.com or
www.rz.rwth-aachen.de/computing/hpc/prog/debug/totalview.

11.1 Debugging serial programs

11.1.1 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 (□) button, if available.
- **You can change all values, which are highlighted**.
- If at any time the source pane of the process window shows disassembled machine code, then the program is stopped in some internal routine. Select the first user routine in the **Stack Trace Pane** in order to see, where this internal routine has been evoked.

11.1.2 Compiling and Linking

Before debugging, **compile** your program with the **–g** option and without any optimisation. You do not need to use the **–g** option on your link command.

11.1.3 Starting TotalView

You can debug your program

- by either starting totalview with your program as a parameter
  totalview *a.out* [**-a** *options*]
- or by starting your program first and than attaching totalview to it. In this case start
  totalview
  which first opens its **root window**. Select your program after pushing **Unattached**.
- You can also analyse the core dump after your program crashed by
  totalview *a.out core*

Startup Parameters (runtime arguments, environment variables, standard IO) can be set in the **Process > Start Parameters** ... menu.

After starting your program TotalView open 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 stack routine selected
- the **Threads Pane**, showing the threads of the current process.
- the **Action Points Pane**, listing all breakpoints, action points and evaluation points.

11.1.4 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 it's name in the **`Stack Trace Pane`** first.
- Select **`Action Points > At Location`** and input the function's name.

11.1.5 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 though 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 **`Group > Restart`**.

11.1.6 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 lets 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 using the **`Window > Dive Anew`** command or by selection of **`Dive Anew`** after clicking on the left mouse button.

11.1.7 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:

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**

- A **watchpoint** monitors a variable's value. 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 the select the **Tools > Watchpoint** command.
- You can save / reload your actions points by selecting **Action Point > Save All** resp. **Load All**.

11.2 Debugging parallel programs

11.2.1 Some general hints for parallel debugging

- 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?
- Get familiar with using TotalView by debugging a serial toy program first.

11.2.2 Debugging MPI programs

11.2.2.1 Starting TotalView

- You can start debugging your MPI program by
  totalview mprun –a ... -W –np *nprocs a.out* [*options*]
  The root window will at first display the **mprun** process itself, in which you might not be interested at all.
  Add **/opt/SUNWhpc/lib** and **/usr/platform** to the file path prefix list of dynamic libraries in the **File > Preferences > Dynamic Libraries** menu and select select **Stop the group** in the **File > Preferences > Parallel** menu.
  After clicking on the **Go** button in the **process window**, mprun is started and all the ***nprocs*** MPI user processes are started by **mprun**. They are automatically acquired by totalview and displayed in the **root window**.
  The **process window** will display your MPI root process.
- You can as well attach to a running MPI program. Find out the process id of the **mprun** command first with the **mpps –b** command and then start **totalview.** After selecting **File > New Program,** type **mprun** in the **Executable** field and its **PID** in the **Process ID** field. If TotalView is running on a different node than **mprun**, enter the host name in the **Remote Host** field as well.

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 Anew**

11.2.2.2 Setting a breakpoint

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 initialisation phase. Displaying and laminating the rank id after an initial call of MPI_Comm_rank reveils, if the MPI startup went well.

11.2.2.3 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 pulldown menu of the toolbar.

11.2.2.4 Printing a variable

You can examine the value of variables of all MPI processes by selecting **`View > Laminate`** in a variable window.
Laminated scalar variables or one-dimensional arrays or array slices can be graphically visualized. The rank id is interpreted as an additional dimension.

11.2.2.5 Message Queues

You can look into outstanding non-blocking message passing operations with the **`Tools > Message Queue Window`** or the **`Tools > Message Queue Graph`**

11.2.3 Debugging OpenMP programs

11.2.3.1 Some general hints for debugging OpenMP programs

In the case you are using Fortran, does the serial program compiled with **f95 –stackvar –xO3 …** (Sun) run correctly? Check the compiler's messages in the ***.lst** files after adding the **–XlistMP** option!
Typical OpenMP coding errors cause data races which can be detected with the **Assure** tool from KAI/Intel. It is very unlikely that you will detect a data race in a debugging session.

11.2.3.2 Compiling

The Sun compilers' **`–xopenmp`** and **`–xautopar`** compiler switches automatically evoke high optimisation (**`-xO3`**). Since Studio 8 you can use the **`–xopenmp=noopt -g`** switches for C and Fortran (but not for C++). As an alternative you can use the Guide OpenMP-compilers of KAI's KAP/Pro Toolset in combination with TotalView:
Compile your code with

```
guidef90|guidec|guidec++ -WG,-cmpo=i [-WGkeepcpp] -g …
```

11.2.3.3 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.

11.2.3.4 Setting a breakpoint

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.

11.2.3.5 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 pulldown menu of the toolbar.

11.2.3.6 Printing a variable

You can examine the value of variables of all threads by selecting **`View > Laminate`** in a variable window.
Laminated scalar variables or one-dimensional arrays or array slices can be graphically visualized. The thread id is interpreted as an additional dimension.