CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

Summer School 2016

Programming Environment
http://github.com/eth-cscs/SummerSchool2016/wiki - DAY1
18th July 2016

Summary

- Accessing CSCS
- Remote display
- Compiling my code
- Running my code
- Editing my code
- Transferring files from/to CSCS
- Debugging tools

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Accessing CSCS

Accessing CSCS: SSH

Secure shell: 2 steps

- Piz Daint is hidden: ela / daint10x / daint0x / `nidxxx`
- frontend first `Ela`: ssh -X courseNN@ela.cscs.ch
- then login node `Piz Daint`: ssh -X daint

ssh -X course51@ela.cscs.ch

```
 ================================================================
             IMPORTANT REMINDER FOR USERS of CSCS facilities
          help@cscs.ch - +41 91 610 82 10 - http://user.cscs.ch
 ================================================================

course51@ela1:~
```

ssh -X daint

```
course51@ela1:~  ssh -X daint
course51@daint101:~  xclock
```

Accessing CSCS: VNC (1/2)

Virtual Network Computing: 2 steps

- Start the VNC server on `Piz Daint`: vncserver
- Start the VNC client on your laptop: vncviewer ...

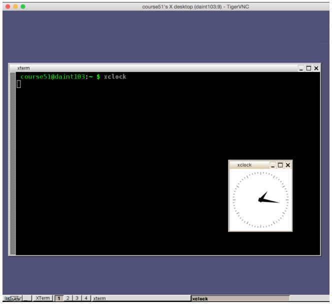
vnc server

```
 course51@daint103:~ $ vncpasswd
  Password: ******
  Verify:   ******
Would you like to enter a view-only password (y/n)? n

 course51@daint103:~ $ vncserver
 New 'X' desktop is daint103:9
```

vnc client

```
 jg@mylaptop:~ ssh -f \
        -l course51 \
        -L 5909:daint103.login.cscs.ch:5909 \
        -C ela.cscs.ch \
        sleep 60

 jg@mylaptop:~ vncviewer localhost:9
  TigerVNC Viewer 64-bit v1.4.0
  CConn:       connected to host localhost port 5909
```

Accessing CSCS: VNC (2/2)



```
course51@daint103:~ $ xclock
```

- More infos: https://github.com/eth-cscs/SummerSchool2016/wiki

Don't forget to kill the server when done

```
course51@daint103:~ vncserver -kill :9
```

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Compiling the code

Compiling the code: setup your PE

Cray Programming Environment

- 4 compilers available: `CCE`*, `GNU`, `INTEL`, `PGI`
- 4 predefined Programming Environment:
  - PrgEnv-`cray`, PrgEnv-`gnu`, PrgEnv-`intel`, PrgEnv-`pgi`
  - `echo $PE_ENV` to get the current PrgEnv
- 3 wrappers available: `ftn` (Fortran), `cc` (C), `CC` (C++)
  - You `must` use the wrappers to compile for the compute node,
  - The wrappers support serial, OpenMP, MPI and Cuda codes.
- The wrappers are based on the `module` command
  - dynamic modification of the `programming environment` via modulefiles,
  - the wrappers will detect the loaded `modulefiles`,
  - and will automatically add the needed flags and libraries.

Compiling the code: module list

module list

```
*course51@daint103:~ $ module list
 Currently Loaded Modulefiles:
  1) modules/3.2.10.3
  2) eswrap/1.1.0-1.020200.1231.0
  3) switch/1.0-1.0502.60522.1.961.ari
  4) craype-network-aries
* 5) cce/8.3.12
  6) craype/2.4.0
  7) totalview-support/1.1.4
  8) totalview/8.11.0
* 9) cray-libsci/13.0.4
 10) udreg/2.3.2-1.0502.10518.2.17.ari
 11) ugni/6.0-1.0502.10863.8.29.ari
 12) pmi/5.0.10-1.0000.11050.0.0.ari
 13) dmapp/7.0.1-1.0502.11080.8.76.ari
 14) gni-headers/4.0-1.0502.10859.7.8.ari
 15) xpmem/0.1-2.0502.64982.5.3.ari
 16) dvs/2.5_0.9.0-1.0502.2188.1.116.ari
 17) alps/5.2.4-2.0502.9822.32.1.ari
 18) rca/1.0.0-2.0502.60530.1.62.ari
 19) atp/1.8.2
*20) PrgEnv-cray/5.2.82
*21) craype-sandybridge
 22) slurm
*23) cray-mpich/7.2.2
 24) ddt/6.0
```

Compiling the code: module swap

module swap from CCE to GNU

```
 course51@daint103:~ module swap PrgEnv-cray PrgEnv-gnu
  Currently Loaded Modulefiles:
  4) craype-network-aries
 *5) gcc/4.8.2
  6) craype/2.4.0
  7) craype-sandybridge
  9) cray-mpich/7.2.2
 13) cray-libsci/13.0.4
*24) PrgEnv-gnu/5.2.82

 course51@daint103:~ ftn --version
GNU Fortran (GCC) 4.8.2 20131016 (Cray Inc.)
```

module swap from GNU to CCE

```
 course51@daint103:~ module swap PrgEnv-gnu PrgEnv-cray
  Currently Loaded Modulefiles:
  4) craype-network-aries
  5) craype-sandybridge
  7) cray-mpich/7.2.2
 *9) cce/8.3.12
 10) craype/2.4.0
 13) cray-libsci/13.0.4
*24) PrgEnv-cray/5.2.82

 course51@daint103:~ ftn -V
        Cray Fortran : Version 8.3.12
```

Compiling the code: module avail

module avail

```
  course51@daint103:~ module avail

# --- COMPILERS ---
PrgEnv-cray/5.2.82 PrgEnv-gnu/5.2.82
PrgEnv-intel/5.2.82 PrgEnv-pgi/5.2.82
cce/8.3.12 gcc/4.8.2 intel/15.0.1.133 pgi/15.3.0
cray-mpich/7.2.2 Python/3.5.1-CrayGNU-2016.03

# --- TOOLS ---
ddt/6.0
perftools/6.2.4
scalasca/1.4.2 scorep/1.4.2 vampir/9.0
visit/2.10 paraview/5.0

# --- LIBS ---
cray-libsci/13.0.4
cray-hdf5-parallel/1.8.14 cray-netcdf-hdf5parallel/4.3.3.1
cray-petsc-64/3.5.3.1 cray-tpsl-64/1.5.0 cray-trilinos/11.12.1.3
fftw/3.3.4.3

# --- GPU ---
craype-accel-nvidia35
cudatoolkit/6.5.14-1.0502.9836.8.1
cray-libsci_acc/3.1.1

# --- APPS ---
cp2k/2.6 espresso/5.1.2 gromacs/5.0.6
lammps/10Feb15 namd/2.9 nwchem/6.3r2 vasp/5.3
```

Compiling the code: module show/help

module avail cray-hdf5-parallel

```
  course51@daint103:~ module avail cray-hdf5

---------------------------- /opt/cray/modulefiles ---
cray-hdf5/1.8.11               cray-hdf5-parallel/1.8.11
cray-hdf5/1.8.12               cray-hdf5-parallel/1.8.12
cray-hdf5/1.8.13               cray-hdf5-parallel/1.8.13
cray-hdf5/1.8.14(default)      cray-hdf5-parallel/1.8.14(default)
cray-hdf5/1.8.16               cray-hdf5-parallel/1.8.16
cray-hdf5/1.8.9                cray-hdf5-parallel/1.8.9
```

module show cray-hdf5-parallel

```
module show cray-hdf5-parallel   # CCE
        setenv  HDF5_DIR /opt/cray/hdf5-parallel/1.8.14/CRAY/83

module swap PrgEnv-cray PrgEnv-gnu  # GNU
module show cray-hdf5-parallel      # GNU
        setenv  HDF5_DIR /opt/cray/hdf5-parallel/1.8.14/GNU/4.9
```

module help cray-hdf5-parallel

```
  course51@daint103:~ module help cray-hdf5-parallel
        # Module Specific Help for 'cray-hdf5-parallel/1.8.14'
        # Doc: http://www.hdfgroup.org/HDF5/doc/index.html
        # ...
```

Compiling the code: module load/rm

module load cray-hdf5-parallel

```
course51@daint103:~ module load cray-hdf5-parallel
course51@daint103:~ module list
course51@daint103:~ which h5dump
      # /opt/cray/hdf5/1.8.14/bin/h5dump
```

module rm cray-hdf5-parallel

```
course51@daint103:~ module rm cray-hdf5-parallel
course51@daint103:~ which h5dump
      # not set
```

Compiling the code: mini-app

Get the src

```
course51@daint103:~ git clone \
        https://github.com/eth-cscs/SummerSchool2016.git \
        SummerSchool2016.git
        # Cloning into 'SummerSchool2016.git'...
```

Compile the Fortran version

```
course51@daint103:~ cd SummerSchool2016.git/miniapp/serial/fortran/
course51@daint103:~ make clean
        # rm -f main *.o *.i *.mod output.*

course51@daint103:~ make
        # ftn -O3 -fopenmp  -c stats.f90 -o stats.o
        # ftn -O3 -fopenmp  -c data.f90 -o data.o
        # ftn -O3 -fopenmp  -c operators.f90 -o operators.o
        # ftn -O3 -fopenmp  -c linalg.f90 -o linalg.o
        # ftn -O3 -fopenmp *.o main.f90  -o main
```

Compile the C++ version

```
course51@daint103:~ cd SummerSchool2016.git/miniapp/serial/cxx/
course51@daint103:~ make clean; make
        # CC -O3 -fopenmp  -c stats.cpp -o stats.o
        # CC -O3 -fopenmp  -c data.cpp -o data.o
        # CC -O3 -fopenmp  -c operators.cpp -o operators.o
        # CC -O3 -fopenmp  -c linalg.cpp -o linalg.o
        # CC -O3 -fopenmp *.o main.cpp -o main
```

Running the code

Running the code: interactive session (1)

salloc

- The job submission system used at CSCS is `Native SLURM`.
- salloc allows to connect to the compute node (man salloc)
- salloc `--res=summerschool`: our reservation for the course
- salloc `-N`: number of compute nodes (8 cores max per node)
- salloc `-t`: duration of the session in minutes (default is 1h)
- `http://user.cscs.ch/getting_started/running_jobs/`

salloc

```
course51@daint102:~ salloc --res=summerschool -t120 -N2
       salloc: Pending job allocation 1145157
       salloc: job 1145157 queued and waiting for resources
       salloc: job 1145157 has been allocated resources
       salloc: Granted job allocation 1145157
course51@daint102:~ echo "Hourra :-) !"
```

Running the code: interactive session (2)

Other useful Slurm commands

- `squeue` -u $USER : what is the status of my salloc session ?
- `scontrol` show job `JOBID`: more details about my session ?
- `scancel` `JOBID`: cancel my session

squeue/scontrol/scancel

```
 course51@daint102:~ squeue -u course51
        JOBID    USER     ACCOUNT   ST      REASON  NODES    PRIORITY
        1145201  course51 courses   PD        None      2       15044

course51@daint102:~ scontrol show job 1145201
   JobId=1145201 Name=bash
   UserId=course51(22854) GroupId=courses(30340)
   Priority=15044 Nice=0 Account=courses QOS=normal
   JobState=RUNNING Reason=None Dependency=(null)
   ...
   NodeList=nid000[68-69]
   BatchHost=daint03
   NumNodes=2 NumCPUs=16 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   Socks/Node=* NtasksPerN:B:S:C=0:0:*:1 CoreSpec=0
   MinCPUsNode=1 MinMemoryCPU=2G MinTmpDiskNode=0
   WorkDir=/users/course51

 course51@daint102:~ scancel 1145201
```

Running the code: interactive session (3)

srun [options] myexecutable

- To run an application on the compute nodes, use the srun command.
- Adapt the command to your needs:
  - `-n`: Total number of MPI tasks
  - `--ntasks-per-node`: Number of MPI tasks per compute node (8 max per node)
  - `-c`: Number of OpenMP threads per task

Running the miniapp (serial version)

```
 course51@daint102:~ srun -n 1 ./main 256 256 200 0.01
==========================================================
                       Welcome to mini-stencil!
 version :: Fortran90 serial
 mesh    ::  256 * 256     dx = 3.9215688593685627E-3
 time    ::  200 time steps from 0 ..  1.0000000000000002E-2
==========================================================
---------------------------------------------------------
      simulation took  5.2622885461896658  seconds
      13761  conjugate gradient iterations
      2615.0219394495398  CG interations per second
      1328  nonlinear newton iterations
------------------------------------------- Goodbye!
```

Editing the code

Editing the code

Many text editors are available

- `vim` filename (X version: gvim)
- `emacs` -nw filename (X version: emacs)
- X only:
  - `gedit`
  - /apps/pilatus/nedit/5.5/Linux-x86/bin/`nedit`

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Moving data from/to CSCS

Moving data: scp

SCP

- Getting a file: scp USER@FROM:remotefile localfile
- Sending a file: scp localfile USER@TO:remotefile
- Add the `-rp` flag to scp to copy an entire directory

Getting 1 (or more) file from CSCS

```
jg@mylaptop:
scp course51@ela.cscs.ch:~/SummerSchool2016.git/miniapp/*.pdf .
  # miniapp.pdf              30%   576KB 140.9KB/s   00:09 ETA
  # miniapp.pdf              52%   992KB 128.1KB/s   00:06 ETA
  # miniapp.pdf              85%  1600KB 116.1KB/s   00:02 ETA
  # miniapp.pdf             100%  1875KB 104.2KB/s   00:18

jg@mylaptop: evince miniapp.pdf &
```

Sending 1 (or more) file to CSCS

```
jg@mylaptop: scp      mycode.c        course51@ela.cscs.ch:~
```

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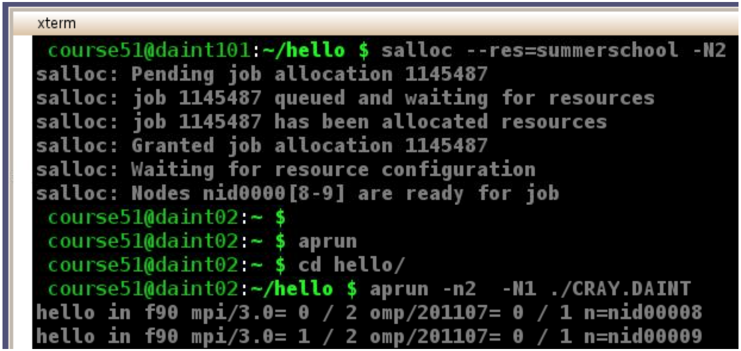
Debugging tools

Why a debugger ?

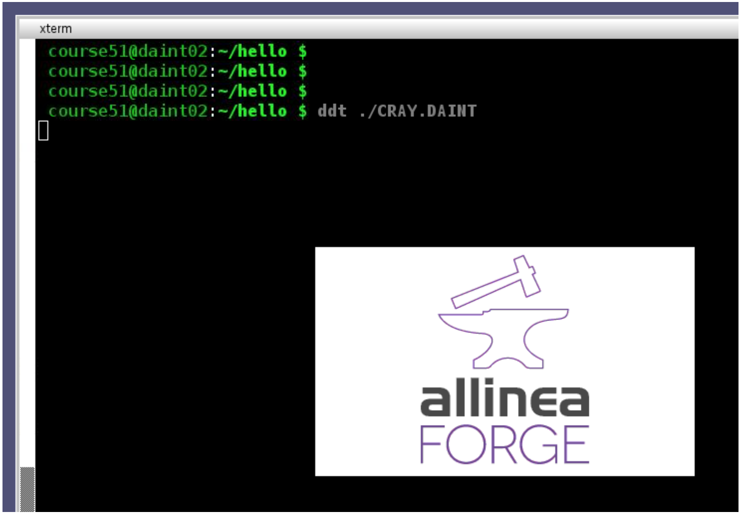
- Complexity can be so great that it appears chaotic :
  - `Many threads`, no synchronisation between them
  - Use printf or the command line debugger (cuda-gdb) within accelerator regions ?
  - Not optimal from a user perspective
- Key debugging features must include:
  - `Line by line` execution of functions & kernels (cpu & gpu)
  - `Pause execution` on the host & device (breakpoints)
  - `Inspect data` on the host & device (variables and arrays)
  - `Navigate` between MPI tasks, OpenMP & CUDA threads
  - `Detect memory` errors on the host & device
  - `Allinea DDT` (Distributed Debugging Tool)
    - Designed for debugging multi-threaded (`OpenMP`), multi-process (`MPI`), and accelerated (`Cuda, OpenACC`) codes
    - written with (`Fortran, C, C++`)
    - DDT is supported on all CSCS systems (including whole `PizDaint`)

DDT: a simple hello world example



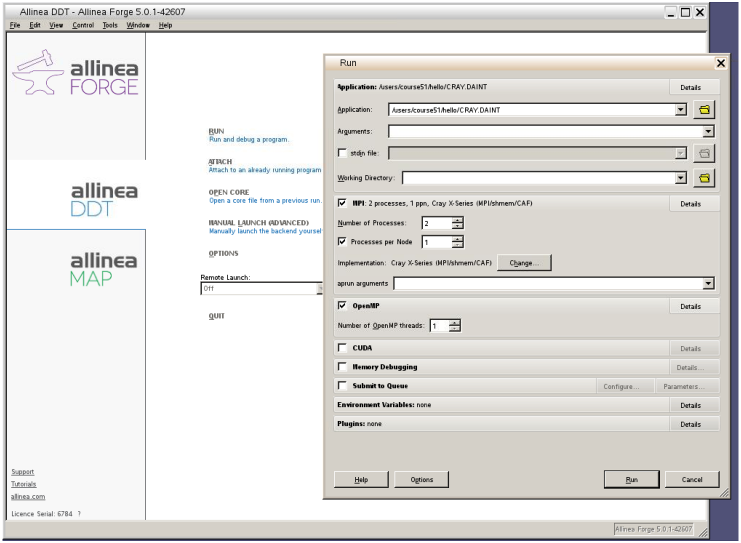
```
 course51@daint101:~/hello $ salloc --res=summerschool -N2
salloc: Pending job allocation 1145487
salloc: job 1145487 queued and waiting for resources
salloc: job 1145487 has been allocated resources
salloc: Granted job allocation 1145487
salloc: Waiting for resource configuration
salloc: Nodes nid0000[8-9] are ready for job
 course51@daint02:~ $
 course51@daint02:~ $ aprun
 course51@daint02:~ $ cd hello/
 course51@daint02:~/hello $ aprun -n2  -N1 ./CRAY.DAINT
hello in f90 mpi/3.0= 0 / 2 omp/201107= 0 / 1 n=nid00008
hello in f90 mpi/3.0= 1 / 2 omp/201107= 0 / 1 n=nid00009
```

DDT: launching the debugger



```
course51@daint02:~/hello $
course51@daint02:~/hello $
course51@daint02:~/hello $
course51@daint02:~/hello $ ddt ./CRAY.DAINT
```

DDT: setting up the job


Allinea DDT - Allinea Forge 5.0.1-42607

Run

Application: /users/course51/hello/CRAY.DAINT

Application: /users/course51/hello/CRAY.DAINT

Arguments:

☐ stdin file:

Working Directory:

☑ **MPI:** 2 processes, 1 ppn, Cray X-Series (MPI/shmem/CAF)

Number of Processes: 2

☑ Processes per Node 1

Implementation: Cray X-Series (MPI/shmem/CAF)

aprun arguments

☑ **OpenMP**

Number of OpenMP threads: 1

☐ **CUDA**

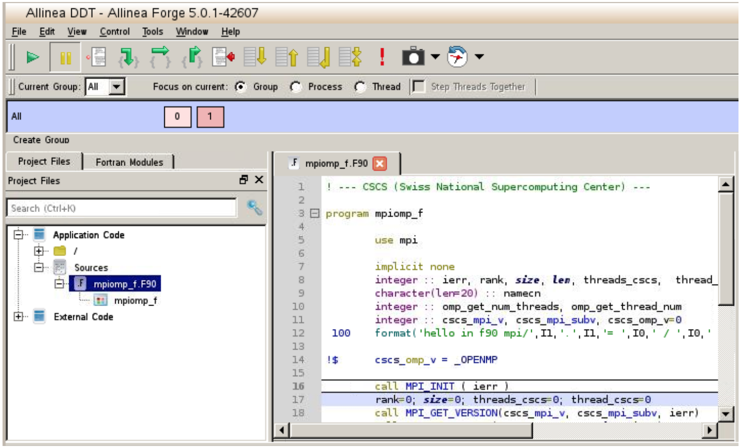
☐ **Memory Debugging**

☐ **Submit to Queue**

Environment Variables: none

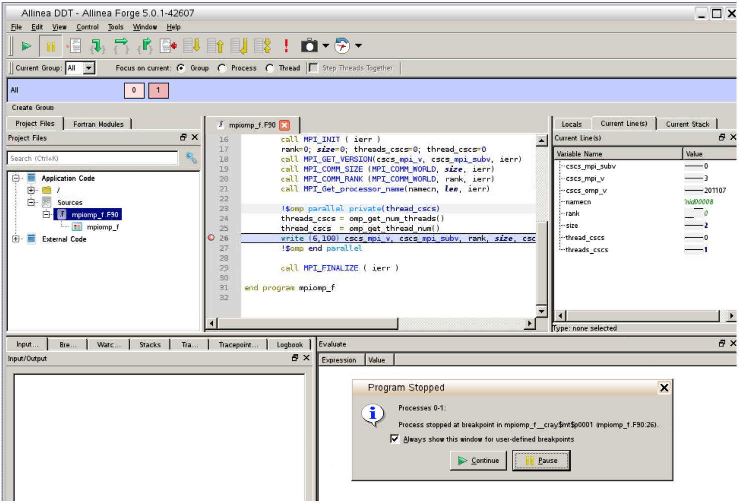
Plugins: none

DDT: starting the job



```
! --- CSCS (Swiss National Supercomputing Center) ---

program mpiomp_f

        use mpi

        implicit none
        integer :: ierr, rank, size, len, threads_cscs,  thread_
        character(len=20) :: namecn
        integer :: omp_get_num_threads, omp_get_thread_num
        integer :: cscs_mpi_v, cscs_mpi_subv, cscs_omp_v=0
 100    format('hello in f90 mpi/',I1,'.',I1,'= ',I0,' / ',I0,'

!$      cscs_omp_v = _OPENMP

        call MPI_INIT ( ierr )
        rank=0; size=0; threads_cscs=0; thread_cscs=0
        call MPI_GET_VERSION(cscs_mpi_v, cscs_mpi_subv, ierr)
```

DDT: setting a breakpoint



mpiomp_f.F90

```fortran
        call MPI_INIT ( ierr )
        rank=0; size=0; threads_cscs=0; thread_cscs=0
        call MPI_GET_VERSION(cscs_mpi_v, cscs_mpi_subv, ierr)
        call MPI_COMM_SIZE (MPI_COMM_WORLD, size, ierr)
        call MPI_COMM_RANK (MPI_COMM_WORLD, rank, ierr)
        call MPI_Get_processor_name(namecn, len, ierr)

        !$omp parallel private(thread_cscs)
        threads_cscs = omp_get_num_threads()
        thread_cscs  = omp_get_thread_num()
        write (6,100) cscs_mpi_v, cscs_mpi_subv, rank, size, csc
        !$omp end parallel

        call MPI_FINALIZE ( ierr )

end program mpiomp_f
```

Current Line(s)

Variable Name	Value
cscs_mpi_subv	0
cscs_mpi_v	3
cscs_omp_v	201107
namecn	'nid00008
rank	0
size	2
thread_cscs	0
threads_cscs	1

Program Stopped

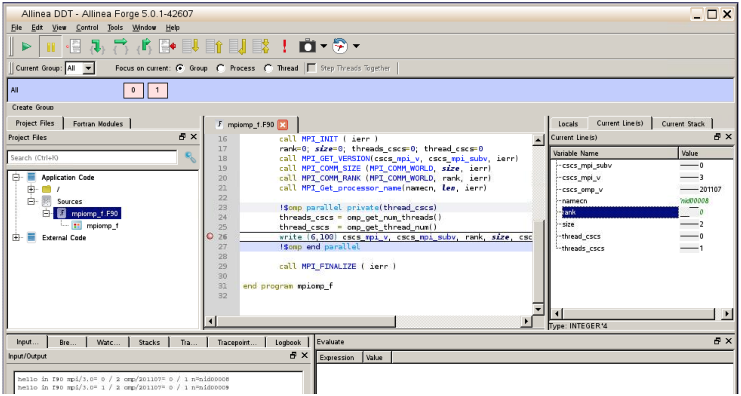
Processes 0-1:

Process stopped at breakpoint in mpiomp_f__cray$mt$p0001 (mpiomp_f.F90:26).

[✓] Always show this window for user-defined breakpoints

Continue Pause

DDT: inspecting data



Current Group: All   Focus on current: [✓ Group] Process Thread   Step Threads Together

```
        call MPI_INIT ( ierr )
        rank=0; size=0; threads_cscs=0; thread_cscs=0
        call MPI_GET_VERSION(cscs_mpi_v, cscs_mpi_subv, ierr)
        call MPI_COMM_SIZE (MPI_COMM_WORLD, size, ierr)
        call MPI_COMM_RANK (MPI_COMM_WORLD, rank, ierr)
        call MPI_Get_processor_name(namecn, len, ierr)

        !$omp parallel private(thread_cscs)
        threads_cscs = omp_get_num_threads()
        thread_cscs  = omp_get_thread_num()
        write (6,100) cscs_mpi_v, cscs_mpi_subv, rank, size, csc
        !$omp end parallel

        call MPI_FINALIZE ( ierr )

end program mpiomp_f
```

Current Line(s)

Variable Name	Value
cscs_mpi_subv	0
cscs_mpi_v	3
cscs_omp_v	201107
namecn	'nid00008
rank	0
size	2
thread_cscs	0
threads_cscs	1

Type: INTEGER*4

```
hello in f90 mpi/3.0= 0 / 2 omp/201107= 0 / 1 n=nid00008
hello in f90 mpi/3.0= 1 / 2 omp/201107= 0 / 1 n=nid00009
```