Efficient HPC Development with Allinea Forge

DKRZ, Hamburg

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Agenda

- Debugging and profiling MPI applications at DKRZ
- Analysing memory issues
- Detecting deadlocks
- MPMD applications
- Best practices

About Allinea Tools

- Allinea Tools: leading toolkit for HPC application developers
  - Available on 65% of the top 100 HPC systems
  - Help maximise application efficiency with Performance Reports
  - Help the HPC community design the best applications with Forge
    - Available at DKRZ: 1024 tokens

- As of December 2016 Allinea is now part of ARM
  - Allinea objective: continue to be the trusted HPC Tools leader in tools across every platform

- This means:
  - The same team will continue to work with you, our customers and partners, and the wider HPC community
  - Being part of ARM gives us strength to deliver on our roadmap faster
  - We remain 100% committed to providing cross-platform tools for HPC
  - Our engineering roadmap is aligned with upcoming architectures from every vendor

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ARM HPC Tools

The mission:

Enable the software ecosystem for large-scale ARM systems.
Based in Manchester and Warwick, UK.

Research Compilers	ARM Performance Libraries	Userspace Performance Tools	Open Source HPC	Allinea Tools
New compiler technology to support and evaluate next-generation ARM architecture.	Commercially-supported BLAS, LAPACK and FFT routines optimized for ARM-compatible microarchitectures.	New commercial tools to deliver actionable performance improvement advice to software developers.	Identification of issues in ARM builds of open-source packages and the upstreaming of fixes.	Parallel debugger, profiler and performance analysis tools for HPC

www.developer.arm.com/hpc

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Debugging and Profiling MPI Applications

Print statement debugging

The first debugger: print statements

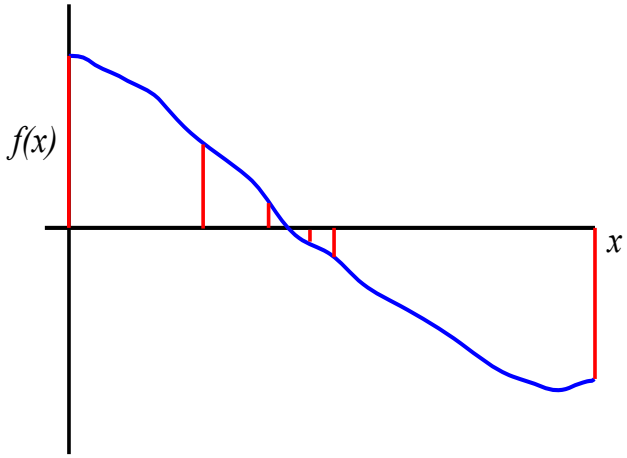
- Each process prints a message or value at defined locations
- Diagnose the problem from evidence and intuition

A long slow process

- Analogous to bisection root finding

Broken at modest scale

- Too much output – too many log files



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Typical types of bugs

- Steady and dependable, I'll be there for you.

BOHR BUG

- Oh, you are debugging? Let me hide for a sec!

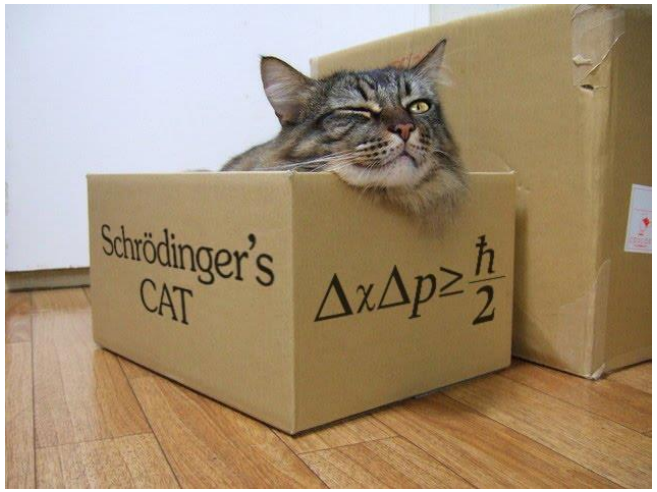
HEISEN BUG

- Chaos is my name and you shall fear me.

MANDEL BUG

- I am buggy ***AND*** not buggy. How about that?

SCHRODIN BUG



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Debugging by discipline

Debugging a problem is much easier when you can :

- Make and undo changes fearlessly
  - Use a source control (CVS, …)
- Track what you've tried so far
  - Write logbooks
- Reproduce bugs with a single command
  - Create and use test script

```
$ mkdir logs
$ vim logs/segfault-at-4096-procs

When running lu.E.4096 with the trace-4410.dat set,
the job exited with: "An error occurred in MPI_Send
[li346-209:25319] on communicator MPI_COMM_WORLD
MPI_ERR_RANK: invalid rank".

To reproduce: mpiexec -n 4096 lu.W.4096 trace-4410.dat
on supermuc. Seems to happen every time.

* Tried reading core file with gdb, "File truncated"
* Set ulimit -c unlimited and ran again: ...
```

```
$ logs/segfault-at-4096-procs.sh
Sep 27 15:29: Queued as job.43214
Sep 27 18:01: Running...
Sep 27 19:29: FAIL
```


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Allinea DDT helps to understand

Who had a rogue behaviour ?

- Merges stacks from processes and threads

Where did it happen?

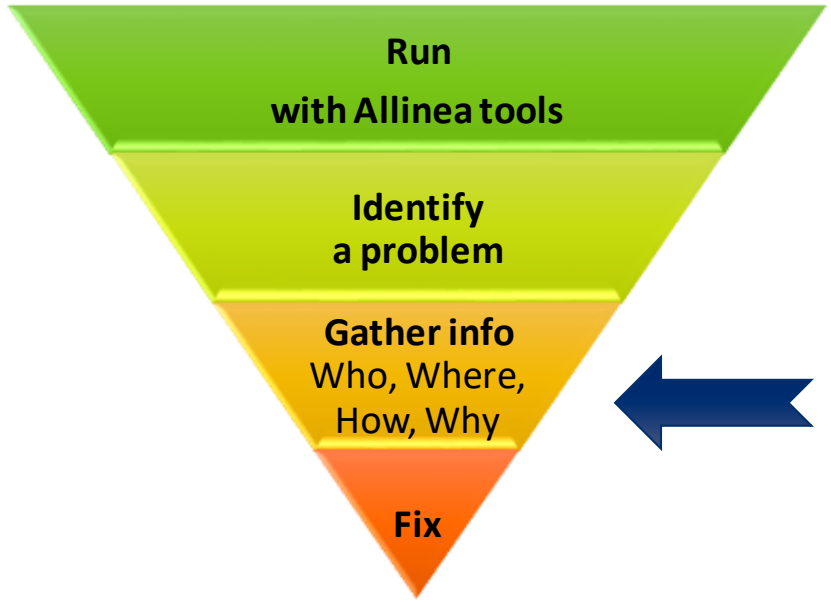
- Allinea DDT leaps to source automatically

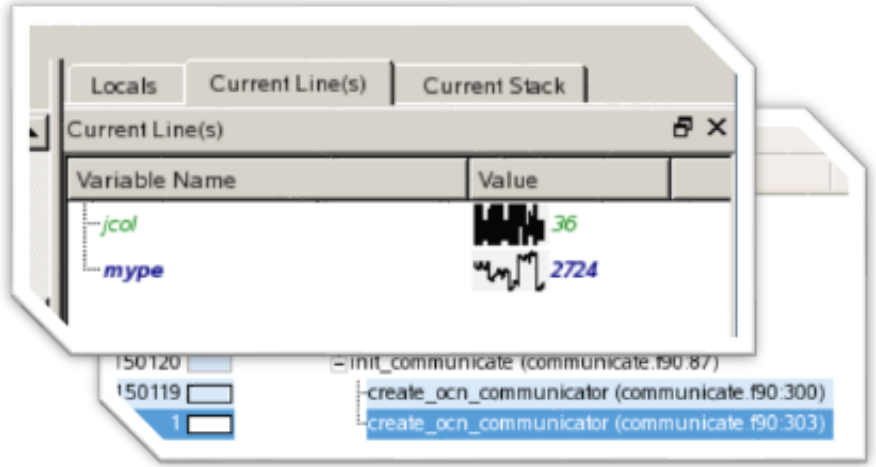
How did it happen?

- Detailed error message given to the user
- Some faults evident instantly from source

Why did it happen?

- Unique “Smart Highlighting”
- Sparklines comparing data across processes





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Allinea DDT cheat sheet

Prepare the code

- $ mpicc **-O0 -g** myapp.c –o myapp.exe

Load the environment module

- $ module load **allinea-forge**

Start Allinea DDT in interactive mode (in an interactive job session)

- $ **ddt** srun ./myapp.exe arg1 arg2

Or use the reverse connect mechanism (by submitting a batch job)

- On the login node:
  - $ ddt &
- (or use the remote client http://www.allinea.com/products/downloads/)
- Then, edit the job script to run the following command and submit:
  - **ddt --connect** mpirun -n 8 ./myapp.exe arg1 arg2

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Example 1

Copy the archive in your working directory

- $ cp /scratch/k/k203064/flebeau/allinea_workshop.tar.gz .
- $ tar xzvf allinea_workshop.tar.gz
- $ cd allinea_workshop

Load the environment

- $. env

And go to the first exercise

- $ cd 1_interactive_debugging/

Compile with:

- $ make

And submit the job

- $ sbatch job.sub

The initial application crashes

Recompile for debugging with:

- $ make DEBUG=1

Launch Allinea DDT on the login node, edit the job script to prefix the execution command with “ddt --connect” and debug the application

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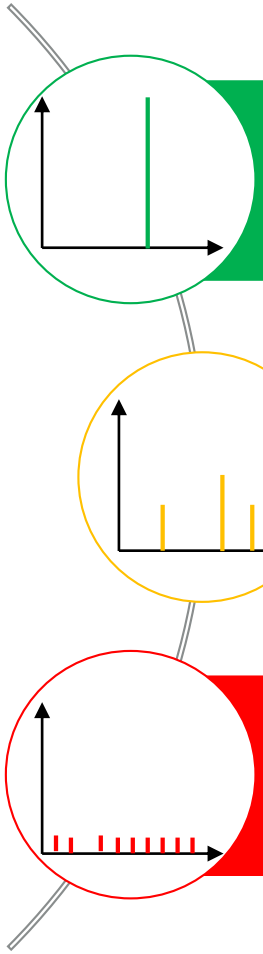
How to profile?

Different methods

- Tracing
  - Records and timestamps all operations
  - Intrusive
- Instrumenting
  - Add instructions in the source code to collect data
  - Intrusive
- Sampling
  - Automatically collect data
  - Not intrusive

Some types of profiles



Hotspot

- One function corresponds to more 80% of the runtime
- Large speed-up potential
- Best optimisation scenario

Spike

- The application spends most of the time in a few functions
- Speed-up potential depends on the aggregated time
- Variable optimisation time

Flat

- Runtime split evenly between numerous functions, each one with a very small runtime
- Little speed-up potential without algorithmic changes
- Worst optimisation scenario

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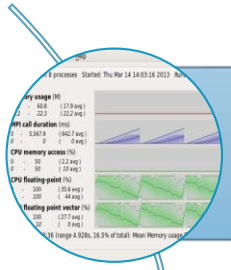
Allinea MAP: Performance made easy

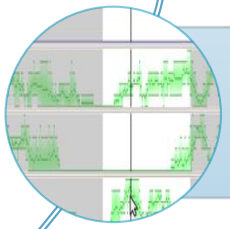


Low overhead measurement

- Accurate, non-intrusive application performance profiling
- Seamless – no recompilation or relinking required

Easy to use

- Source code viewer pinpoints bottleneck locations
- Zoom in to explore iterations, functions and loops



Deep

- Measures CPU, communication, I/O and memory to identify problem causes
- Identifies vectorization and cache performance

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Allinea MAP cheat sheet

Prepare the code

- $ mpicc –O3 **-g** myapp.c –o myapp.exe

Load the environment module

- $ module load **allinea-forge**

Edit the job script to run Allinea MAP in “profile” mode

- $ **map --profile** srun ./myapp.exe arg1 arg2

Open the results

- On the login node:
  - $ map myapp_Xp_Yn_YYYY-MM-DD_HH-MM.map
- (or load the corresponding file using the remote client http://www.allinea.com/products/downloads/)

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Example 2

Go to

- $ cd 2_profiling/

Compile with:

- $ make

Edit the job script to prefix the execution command with “map --profile” and submit the job

- $ sbatch job.sub

Analyse the profiling results

- $ map *.map

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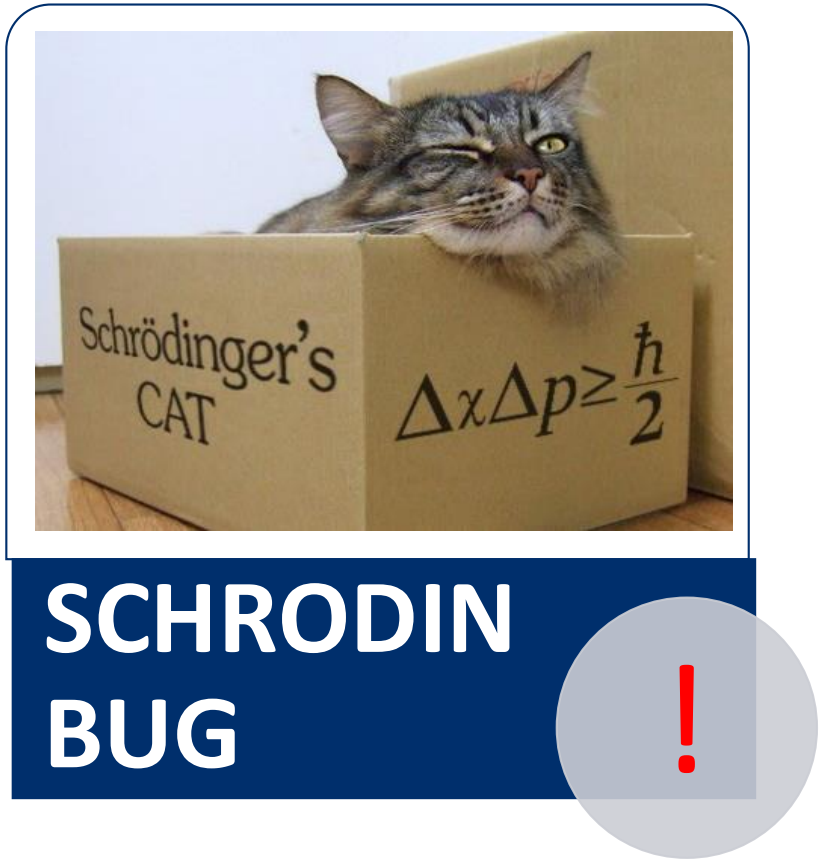
Analysing Memory Issues

It works… Well, most of the time



A strange behaviour where the application “sometimes” crashes is a typical sign of a memory bug

Allinea DDT is able to force the crash to happen

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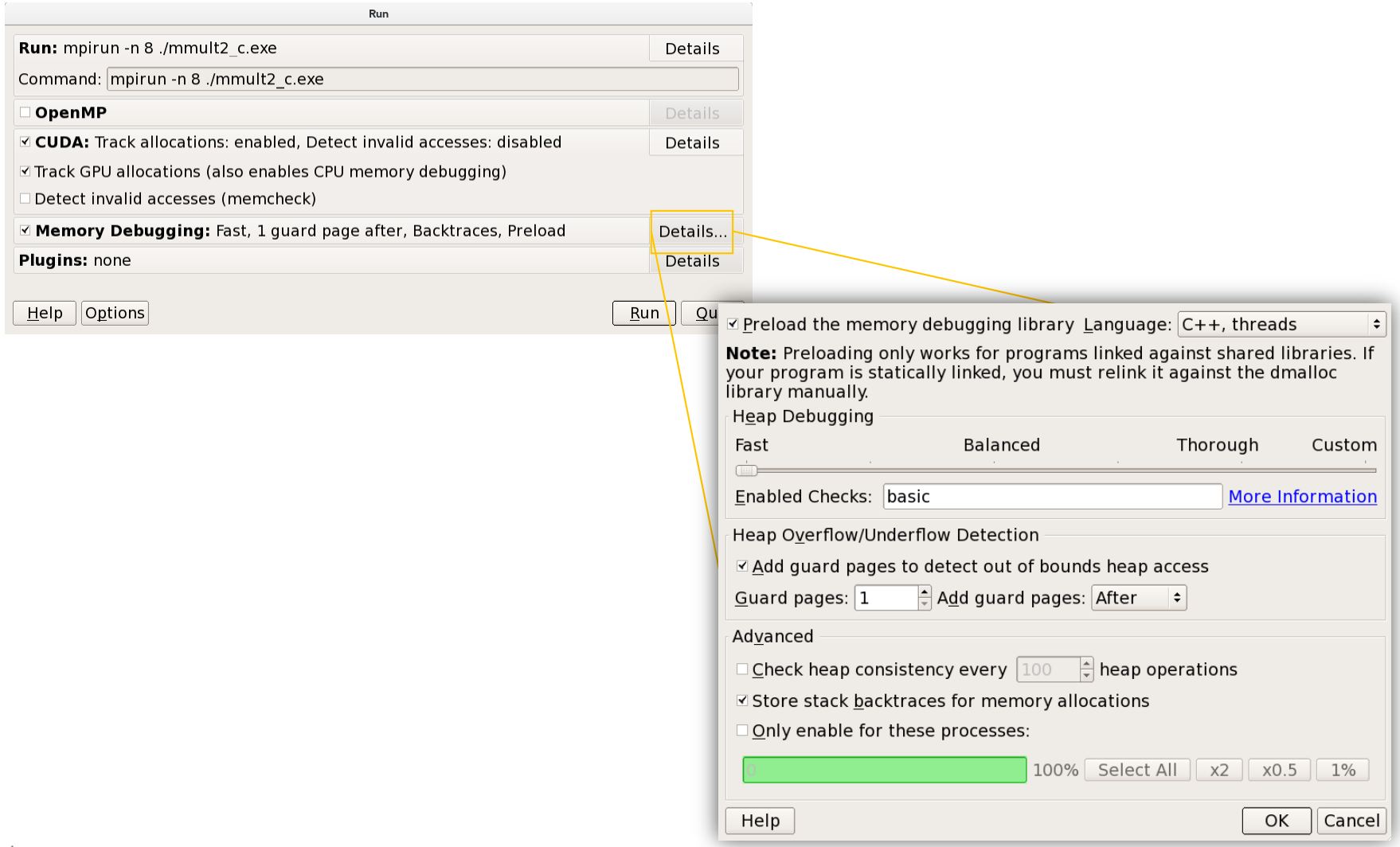
Memory debugging menu in Allinea DDT



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Heap debugging options available

basic

- Detect invalid pointers passed to memory functions (e.g. malloc, free, ALLOCATE, DEALLOCATE,...)

check-fence

- Check the end of an allocation has not been overwritten when it is freed.

free-protect

- Protect freed memory (using hardware memory protection) so subsequent read/writes cause a fatal error.

Added goodiness

- Memory usage, statistics, etc.

free-blank

- Overwrite the bytes of freed memory with a known value.

alloc-blank

- Initialise the bytes of new allocations with a known value.

check-heap

- Check for heap corruption (e.g. due to writes to invalid memory addresses).

realloc-copy

- Always copy data to a new pointer when re-allocating a memory allocation (e.g. due to realloc)

check-blank

- Check to see if space that was blanked when a pointer was allocated/freed has been overwritten.

check-funcs

- Check the arguments of addition functions (mostly string operations) for invalid pointers.

See user-guide:

Chapter 12.3.2

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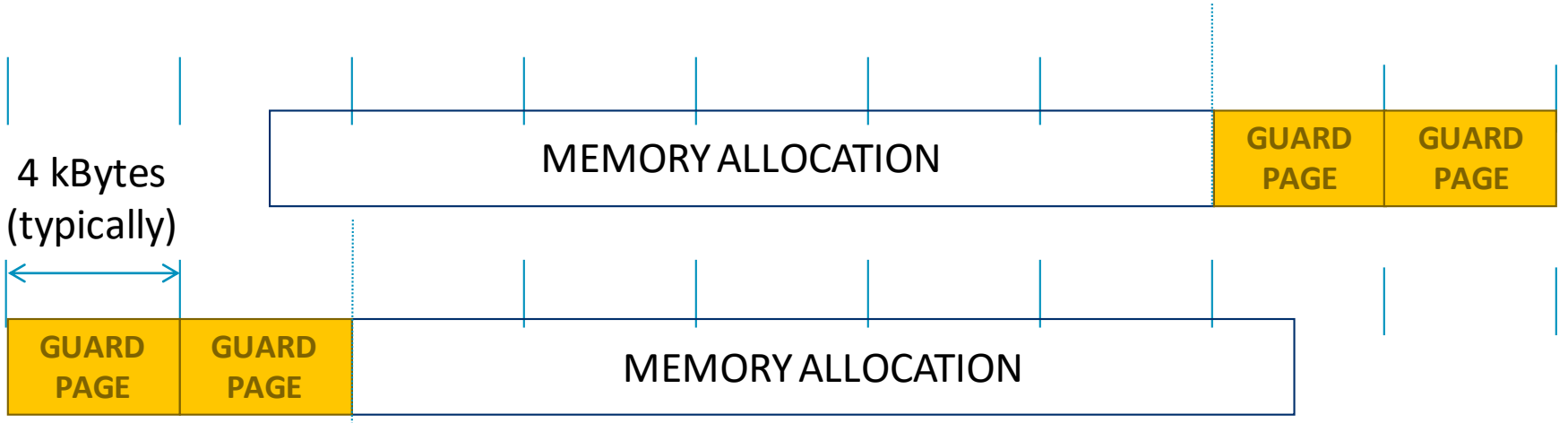
Guard pages (aka “Electric Fences”)



A powerful feature…:

- Forbids read/write on guard pages throughout the whole execution

(because it overrides C Standard Memory Management library)

… to be used carefully:

- Kernel limitation: up to 32k guard pages max (“mprotect fails” error)
- Beware the additional memory usage cost

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Example 3

Go to

- $ cd 3_mem_dbg/

Compile with:

- $ make
- /!\ Don't forget to compile with "-O0 -g"

Edit the job script to prefix the execution command with "ddt --connect", launch ddt on the login node and submit the job

- $ ddt &
- $ sbatch job.sub

In the "Run" window, select "Fast" memory debugging first

Submit the job again and enable "Guard pages"

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Detecting Deadlocks

My application has been running for a while now…

A strange behaviour where the application runs for “longer than expected” is a typical sign of a deadlock.

The application is hanging in the queue: alive and dead…

Allinea DDT is able to attach to the running processes and observe what is happening.

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Example 4

Go to

- $ cd 4_deadlock/

Compile with:

- $ make
- Start Allinea DDT

Run the job with 10 processes: it works.

- $ srun --account=kg0166 --partition=compute -N 1 -n 10 ./cpi.exe

Run it again with 8 processes: it hangs!

- $ srun --account=kg0166 --partition=compute -N 1 -n 8 ./cpi.exe

In Allinea DDT's GUI, select "Attach" from the main menu.

Allinea DDT should be able to detect the application automatically. Select it and debug it!

MPMD Applications

Example 5: How to run Forge on MPMD applications

Same logic, just prefix the execution command with the command:

- $ cd 5_mpmd/
- $ **ddt --connect** mpirun -n 8 myapp1.exe : -n 16 myapp2.exe
- $ **map --profile** srun –multi-prog cmd.srun
  - With cmd.srun:

    0-7 ./myapp1.exe

    8-23 ./myapp2.exe

Since 7.1, the ranks to profile can be specified:

- $ map **--select-ranks=0-7** --profile srun cmd.srun

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Allinea DDT in manual launch

For complex launch mechanisms, for example if SLURM actually launches wrapper scripts, it is possible to launch the debugger in manual launch.

To do so:

- Launch the GUI on the login node and select “Manual Launch” from the Allinea DDT GUI
- Specify the number of processes and click on “Listen”
- The debugger now awaits for the processes to connect
  - Click on “Help” on the window to know how to connect the processes
    - By prefixing the processes to debug in the wrapper script with the following for example:
      - ddt-client --ddtsessionfile /home/flebeau/.allinea/session/toutatis-1 PROGRAM
  - Submit the job and see the processes attaching in the debugger

Increase Productivity with Automation

ESiWACE Project partner

Centre of Excellence in Simulation of Weather and Climate in Europe

A main goal of ESiWACE is to substantially improve efficiency and productivity of numerical weather and climate simulation on high-performance computing platforms by supporting the end-to-end workflow of global Earth system modelling in HPC environment.

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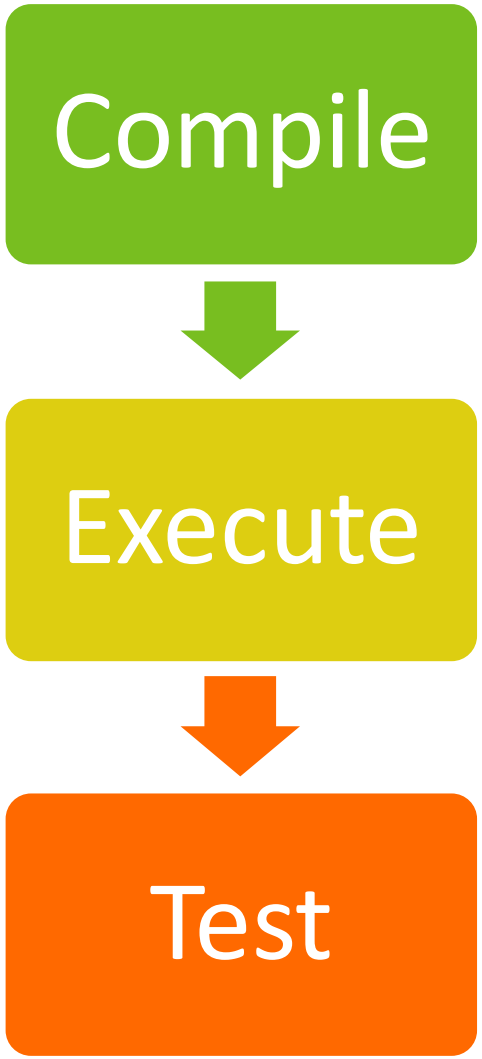
Automation script example

```
#!/bin/bash –l
# Job submission file name
jobfile=test_jacobi_mpi_omp_gnu.sub
# Load environment
module load compiler/gnu mpi/openmpi_gnu
module load allinea/perf-report
# Compile
make clean && make

# Job submission file configuration
cat << EOF > $jobfile
#!/bin/bash –l
#SBATCH --job-name=‘test_jacobi_mpi_omp_gnu‘
#SBATCH --time=00:05:00
#SBATCH --ntasks=128
#SBATCH –ntasks-per-node=2
export OMP_NUM_THREADS=16
srun ./jacobi_omp_mpi_gnu.exe
EOF

# Submit
sbatch $jobfile

# Check results
[…]
```



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Automate profiling

```
map --profile --output jacobi_omp_mpi_gnu_perf.map \
                      --stop-after=300
                      srun ./jacobi_omp_mpi_gnu.exe
map --export=jacobi_omp_gnu_perf.json jacobi_omp_gnu_perf.map
```

--output specifies the name of the output

- *.map file

--stop-after=X enables to stop sampling after X seconds after the program starts

--start-after=Y enables to start sampling after Y seconds after the program starts

--export=FILE exports a specified *.map file in JSON file

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Automate debugging

```
ddt --offline -o jacobi_omp_mpi_gnu_debug.txt \
                          --trace-at _jacobi.F90:83,residual \
                          srun ./jacobi_omp_mpi_gnu.exe
```

--offline enable non-interactive debugging

-o specifies the name and output of the non-interactive debugging session

- Html
- Txt

Automate debugging

#	Time	Tracepoint	Processes	Values
1	21:18.172	jacobi_mpi_omp_gnu.exe (_jacobi.f90:83)	0-127	residual: 2.57

```
fail=0
# --- check DDT tracepoint (residual)
f=jacobi_omp_mpi_gnu_debug.txt
resid=`grep ^tracepoint $f | awk -Fresidual:  '{print $2}' |tail -1 |cut -c2-5`
if [ "$resid" != "2.57" ] ; then
        ((fail++))
       echo "Test has failed resid=$resid“
else
        echo “Test has succeeded”
```


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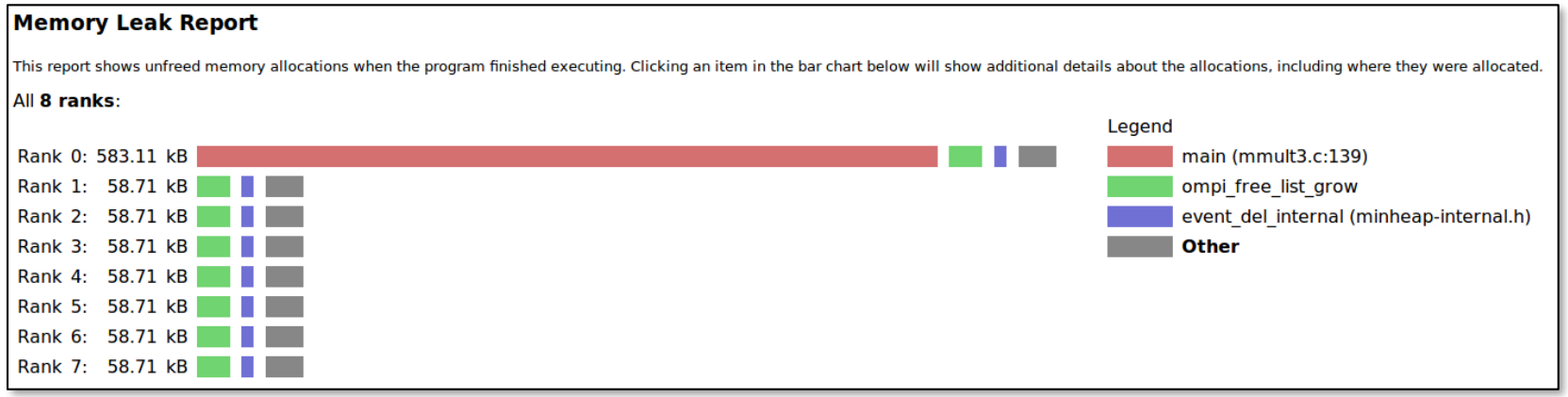
Automate debugging

Other available options:

- --trace-changes: set a tracepoint on the variable introduced by the latest commit (git, svn, mercurial)
- --break-at: set a breakpoint
- --mem-debug: check for memory defects and leaks
- --check-bounds: check for out of bounds array accesses



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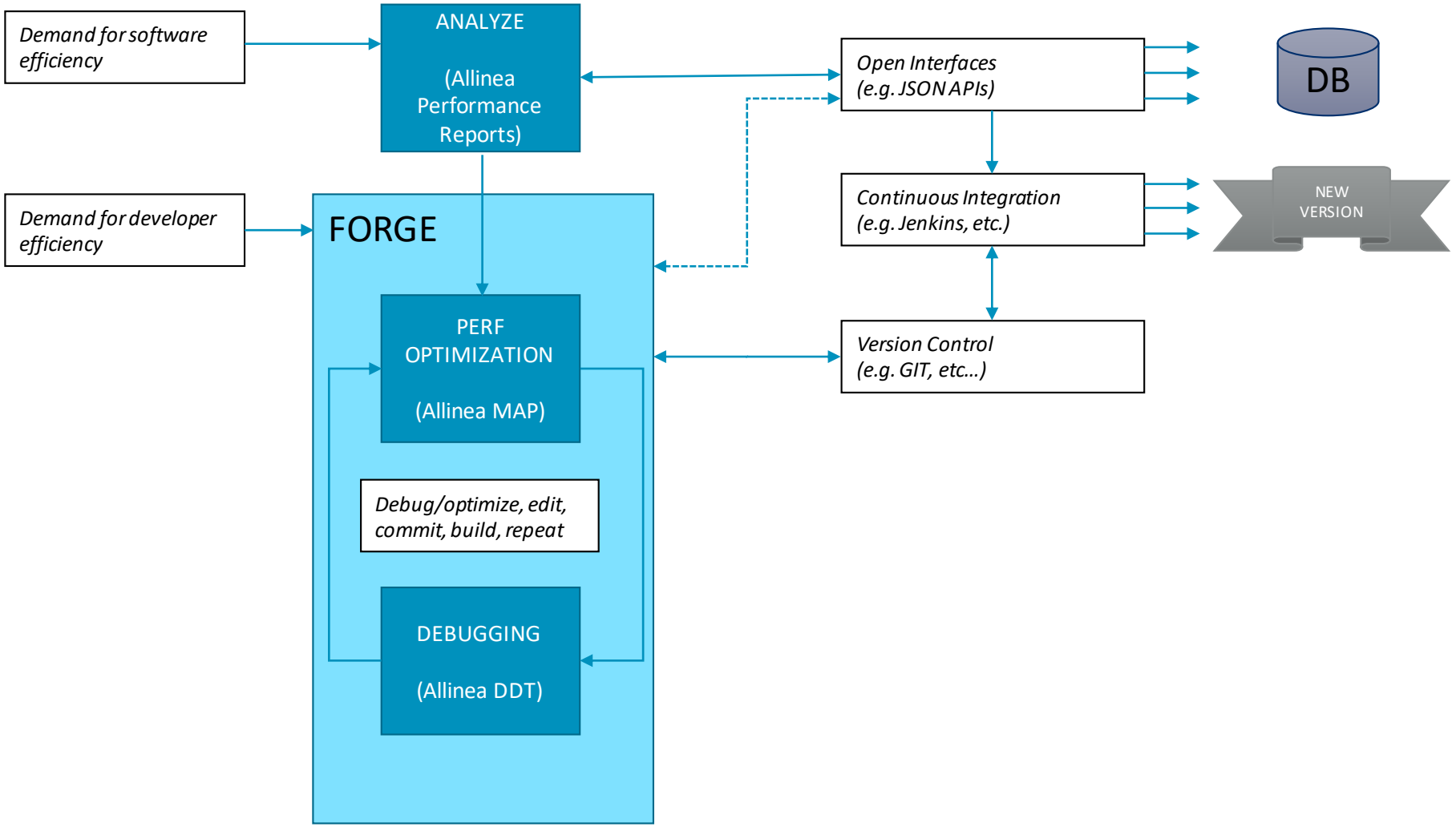
Development process workflow



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Thank You!
Danke!
Merci!
谢谢!
ありがとう!
Gracias!
Kiitos!