UL HPC School 2017

PS4b: Debugging, profiling and performance analysis

UL High Performance Computing (HPC) Team

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http://hpc.uni.lu

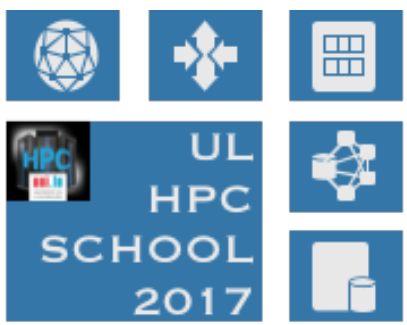
Latest versions available on Github:

UL HPC tutorials: https://github.com/ULHPC/tutorials

UL HPC School: http://hpc.uni.lu/hpc-school/

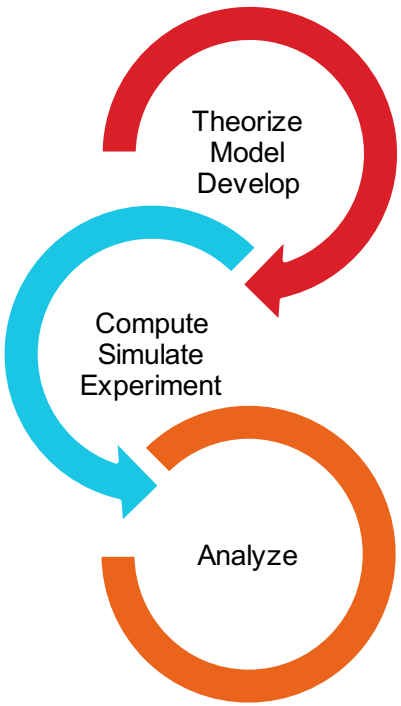
PS4b tutorial sources:

https://github.com/ULHPC/tutorials/tree/devel/advanced/debugging



Summary

Main Objectives of this Session



This session is meant to show you some of the various tools you have at your disposal on the UL HPC platform to

understand & solve problems

During the hands-on session you will:

- see what happens when an application runs **out of memory** and how to discover how much memory it actually requires.
- use **debugging tools** to understand **why your code is crashing**.
- use **profiling tools** to understand the (slow) **performance of your code** - and **how to improve** it.

Knowing what to do when you experience a problem is half the battle.

Summary

Tools at your disposal (I)

Common tools used to understand problems

- Do you know what time it is?
  ↪ **/usr/bin/time -v** is just magic sometimes
- Don't remember where you put things?
  ↪ **Valgrind** can help with your memory issues
- Is your application firing on all cylinders?
  ↪ with **htop** green means go! (red is bad)
- Got stuck?
  ↪ **strace** can tell you where you are and how you got there

Some times simple tools help you solve big issues.

Tools at your disposal (II)

HPC specific tools

- Allinea DDT (part of Allinea Forge)
  - ↪ Visual debugger for C, C++ and Fortran threaded and // code
- Allinea MAP (part of Allinea Forge)
  - ↪ Visual C/C++/Fortran profiler for high performance Linux code
- Allinea Performance Reports
  - ↪ Application characterization tool

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Allinea tools are licensed

Make sure enough tokens available to profile/debug your code in the requested configuration (#cores)!

- ↪ license check will be integrated in SLURM
- ↪ ... so your jobs will be able to wait for it to be available

Allinea DDT - highlights

DDT features

- **Parallel debugger**: threads, OpenMP, MPI support
- Controls processes and threads
  - ↪ step code, stop on var. changes, errors, breakpoints
- Deep **memory debugging**
  - ↪ find memory leaks, dangling pointers, beyond-bounds access
- C++ debugging – including STL
- Fortran – including F90/F95/F2008 features
- See vars/arrays **across multiple processes**
- Integrated editing, building and **VCS integration**
- Offline mode for **non-interactive debugging**
  - ↪ record application behavior and state

Full details at `allinea.com/products/ddt/features`

Allinea DDT - on ULHPC

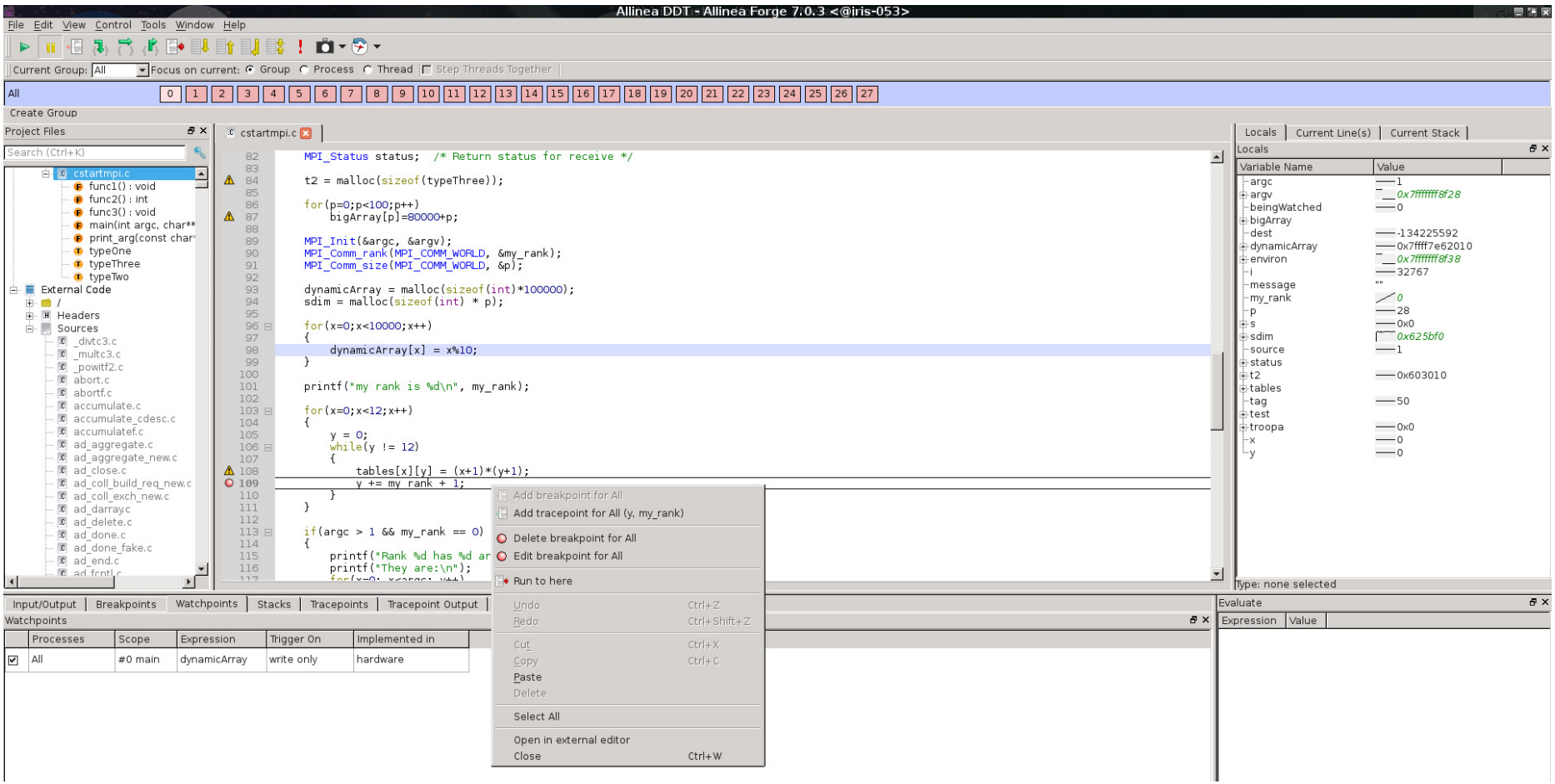
Modules

- On iris: `module load tools/AllineaForge`
- On gaia/chaos: `module load Allinea/Forge`
  - ↪ we'll synchronize the software set to match iris soon

Debugging with DDT

1. Load toolchain, e.g.
   - ↪ iris: `module load toolchain/intel`
   - ↪ gaia/chaos: `module load toolchain/ictce`
2. Compile your code, e.g. `mpiicc $code.c -o $app`
3. Run your code through DDT
   - ↪ iris: `ddt srun ./$app`
   - ↪ gaia/chaos: `ddt mpirun -hostfile $OAR_NODEFILE ./$app`

Allinea DDT - interface



Allinea MAP - highlights

MAP features

- Meant to show developers **where&why code is losing perf.**
- **Parallel profiler**, especially made for MPI applications
- Effortless profiling
  - ↪ no code modifications needed, may not even need to recompile
- Clear **view of bottlenecks**
  - ↪ in I/O, compute, thread or multi-process activity
- Deep insight in **CPU instructions affecting perf.**
  - ↪ vectorization and memory bandwidth
- **Memory usage over time** – see changes in memory footprint
- Integrated editing and building as for DDT

Full details at `allinea.com/products/map/features`

Allinea MAP - on ULHPC

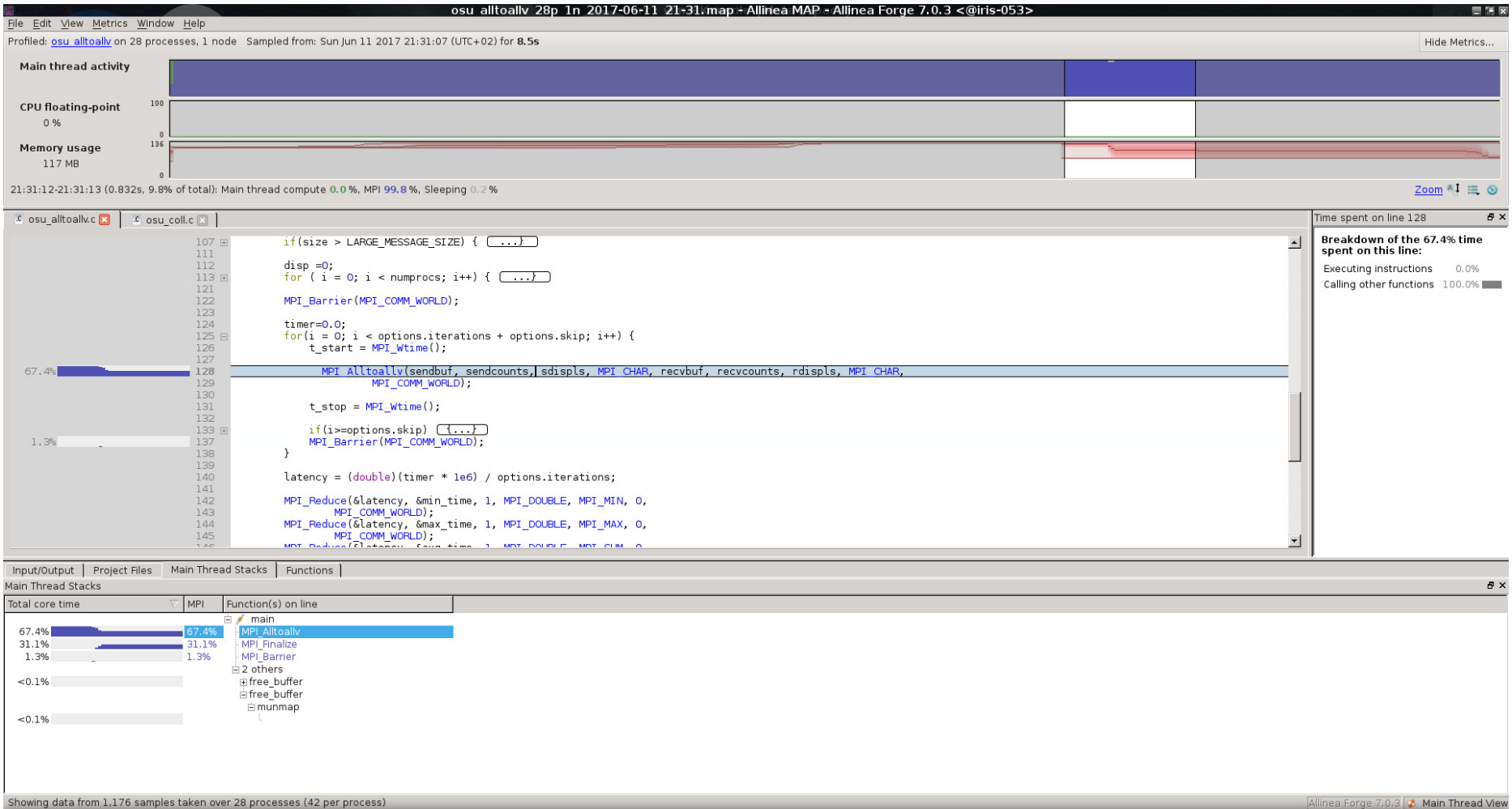
Modules

- On iris: `module load tools/AllineaForge`
- On gaia/chaos: `module load Allinea/Forge`

Profiling with MAP

1. Load toolchain that built your app., e.g.
   - ↪ iris: `module load toolchain/intel`
   - ↪ gaia/chaos: `module load toolchain/ictce`
2. Run your code through MAP
   - ↪ iris: `map srun ./$app`
   - ↪ gaia/chaos: `map mpirun -hostfile $OAR_NODEFILE ./$app`

Allinea MAP - interface



Allinea Perf. Reports - highlights

Performance Reports features

- Meant to answer **How well do your apps. exploit your hw.?**
- Easy to use, on unmodified applications
  - ↪ outputs HTML, text, CSV, JSON reports
- One-glance view if application is:
  - ↪ **well-optimized** for the underlying hardware
  - ↪ running **optimally at** the given **scale**
  - ↪ **affected by** I/O, networking or threading **bottlenecks**
- Easy to integrate with continuous testing
  - ↪ programatically improve performance by continuous profiling
- **Energy metric** integrated
  - ↪ using RAPL (CPU) for now on iris
  - ↪ IPMI-based monitoring may be added later

Full details at `allinea.com/products/allinea-performance-reports`

Allinea Perf. Reports - on ULHPC

Modules

- On iris: `module load tools/AllineaReports`
- On gaia/chaos: `module load Allinea/Reports`

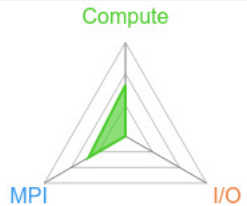
Using Performance Reports

1. Load toolchain that you run your app. with, e.g.
   - ↪ iris: `module load toolchain/intel`
   - ↪ gaia/chaos: `module load toolchain/ictce`
2. Run your application through Perf. Reports
   - ↪ iris: `perf-report srun ./$app`
   - ↪ gaia/chaos: `perf-report mpirun -hostfile $OAR_NODEFILE ./$app`

Allinea Perf. Reports - output (I)

allinea PERFORMANCE REPORTS

Command:	srun gmx_mpi mdrun -s bench_rnase_cubic.tpr -nsteps 10000
Resources:	1 node (28 physical, 28 logical cores per node)
Memory:	126 GiB per node
Tasks:	28 processes, OMP_NUM_THREADS was 0
Machine:	iris-053
Start time:	Sun Jun 11 2017 20:13:59 (UTC+02)
Total time:	19 seconds
Full path:	/mnt/irisgpfs/apps/resif/data/production/v0.1-20170602/default/software/bio/GROMACS/2016.3-intel-2017a-hybrid/bin



Summary: gmx_mpi is Compute-bound in this configuration

Compute	54.6%	Time spent running application code. High values are usually good. This is **average**; check the CPU performance section for advice
MPI	45.4%	Time spent in MPI calls. High values are usually bad. This is **average**; check the MPI breakdown for advice on reducing it
I/O	0.0%	Time spent in filesystem I/O. High values are usually bad. This is **negligible**; there's no need to investigate I/O performance

This application run was Compute-bound. A breakdown of this time and advice for investigating further is in the CPU section below.

CPU

A breakdown of the 54.6% CPU time:

Single-core code	5.5%
OpenMP regions	94.5%
Scalar numeric ops	5.2%
Vector numeric ops	44.2%
Memory accesses	50.6%

The per-core performance is memory-bound. Use a profiler to identify time-consuming loops and check their cache performance.

MPI

A breakdown of the 45.4% MPI time:

Time in collective calls	33.5%
Time in point-to-point calls	66.5%
Effective process collective rate	426 MB/s
Effective process point-to-point rate	419 MB/s

Most of the time is spent in point-to-point calls with an average transfer rate. Using larger messages and overlapping communication and computation may increase the effective transfer rate.

Allinea Perf. Reports - output (II)

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I/O

A breakdown of the 0.0% I/O time:

Time in reads	0.0%
Time in writes	0.0%
Effective process read rate	0.00 bytes/s
Effective process write rate	0.00 bytes/s

No time is spent in I/O operations. There's nothing to optimize here!

OpenMP

A breakdown of the 94.5% time in OpenMP regions:

Computation	99.5%
Synchronization	0.5%
Physical core utilization	100.0%
System load	101.9%

OpenMP thread performance looks good. Check the CPU breakdown for advice on improving code efficiency.

Memory

Per-process memory usage may also affect scaling:

Mean process memory usage	75.6 MiB
Peak process memory usage	86.6 MiB
Peak node memory usage	11.0%

The peak node memory usage is very low. Running with fewer MPI processes and more data on each process may be more efficient.

Energy

A breakdown of how the 0.899 Wh was used:

CPU	100.0%
System	not supported %
Mean node power	not supported W
Peak node power	not supported W

The whole system energy has been calculated using the CPU energy usage.

System power metrics: No Allinea IPMI Energy Agent config file found in (null). Did you start the Allinea IPMI Energy Agent?

Summary

Now it's up to you

Easy right?

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Well not exactly.

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Debugging always takes effort and real applications are never trivial.

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Well not exactly.
Debugging always takes effort and real applications are never trivial.

But we do guarantee it'll be /easier/ with these tools.

Conclusion and Practical Session start

We've discussed

- A couple of small utilities that can be of big help
- The Allinea tools available for you on UL HPC

And now..

Short DEMO time!

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Your Turn!

Questions?

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