Uni.lu HPC School 2019

PS4b: Monitoring & Profiling II: Advanced Performance engineering



Uni.lu High Performance Computing (HPC) Team V. Plugaru, X. Besseron

University of Luxembourg (UL), Luxembourg 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:

ulhpc-tutorials.rtfd.io/en/latest/debugging/advanced/









2019













Summary

- Introduction
- 2 Debugging and profiling tools
- Conclusion







So we have some news...



































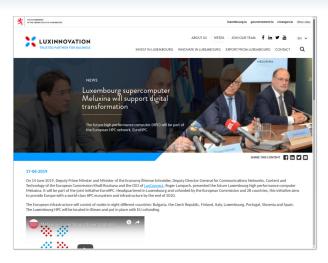














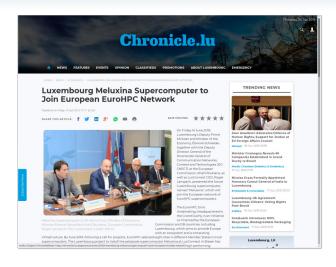




























HIGH PERFORMANCE COMPUTING IN LUXEMBOURG







MeluXina National Supercomputer

MeluXina - coming in 2020

- 10 PetaFlop supercomputer
- Modular architecture covering a wide variety of needs
- High performance network & storage for HPC, BigData & AI





MeluXina National Supercomputer

MeluXina - coming in 2020

- 10 PetaFlop supercomputer
- Modular architecture covering a wide variety of needs
- High performance network & storage for HPC, BigData & AI

What this means for you

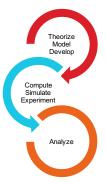
- Algorithms and applications must be run at scale
- Code development will play a large role
- Need to use different computing elements and memory hierarchy
 - → will play a critical role in your application performance







Main Objectives of this Session

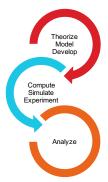


This session is meant to show you some of the various tools you have at your disposal on the UL HPC platform to:

understand and solve development & runtime problems understand and improve application performance



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 and solve development & runtime problems understand and improve application performance

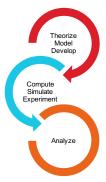
During the session we will (also):

- discuss what happens when an application runs out of memory and how to discover how much memory it actually requires.
- see debugging tools that help you understand why your code is crashing.
- see profiling tools that show the bottlenecks of your code - and how to improve it.





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 and solve development & runtime problems understand and improve application performance

During the session we will (also):

- discuss what happens when an application runs out of memory and how to discover how much memory it actually requires.
- see debugging tools that help you understand why your code is crashing.
- see profiling tools that show the bottlenecks of your code - and how to improve it.

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





Debugging and profiling tools

Summary

- Introduction
- 2 Debugging and profiling tools
- 3 Conclusion





Tools at your disposal (I)

Common tools used to understand problems

- Common tools at a glance:
 - \hookrightarrow **htop**: process/thread live CPU & memory utilization, affinity
 - \hookrightarrow strace: understand what system calls a process is making & where it gets 'stuck'
 - → gdb: general purpose debugger
 - → valgrind: memory debugging and profiling
- SLURM scheduler built-in tools and utilities:
 - → sstat: running job and jobstep statistics
 - → sacct: historic job and jobstep statistics
 - → seff: postmortem CPU/memory utilization and efficiency

Some times simple tools help you solve big issues.





Tools at your disposal (II)

HPC specific tools - Arm (prev. Allinea)

- Arm DDT (part of Arm Forge)
 - \hookrightarrow Visual debugger for C, C++, Fortran & **Python** // code
- Arm MAP (part of Arm Forge)
 - \hookrightarrow Visual profiler for C, C++, Fortran & **Python**
- Arm Performance Reports
 - → Application characterization tool





Tools at your disposal (II)

HPC specific tools - Arm (prev. Allinea)

- Arm DDT (part of Arm Forge)
 - \hookrightarrow Visual debugger for C, C++, Fortran & **Python** // code
- Arm MAP (part of Arm Forge)
 - \hookrightarrow Visual profiler for C, C++, Fortran & **Python**
- Arm Performance Reports
 - \hookrightarrow Application characterization tool

Arm tools are licensed

- license check integrated in SLURM: scontrol show license
- ask for licenses at job submission with e.g. srun -L forge:16





Tools at your disposal (III)

HPC specific tools - Intel

- Intel Advisor
 - → Vectorization + threading advisor: check blockers and opport.
- Intel Inspector
 - → Memory and thread debugger: check leaks/corrupt., data races
- Intel Trace Analyzer and Collector
 - → MPI communications profiler and analyzer: evaluate patterns
- Intel VTune Amplifier
 - \hookrightarrow Performance profiler: CPU/FPU data, mem. + storage accesses





Tools at your disposal (III)

HPC specific tools - Intel

- Intel Advisor
 - \hookrightarrow Vectorization + threading advisor: check blockers and opport.
- Intel Inspector
 - → Memory and thread debugger: check leaks/corrupt., data races
- Intel Trace Analyzer and Collector
 - → MPI communications profiler and analyzer: evaluate patterns
- Intel VTune Amplifier
 - $\hookrightarrow \ \, \mathsf{Performance} \,\, \mathsf{profiler} \colon \, \mathsf{CPU}/\mathsf{FPU} \,\, \mathsf{data}, \,\, \mathsf{mem}. \,\, + \, \mathsf{storage} \,\, \mathsf{accesses}$

Intel tools are licensed

All come as part of Intel Parallel Studio XE - Cluster edition!





Tools at your disposal (IV)

HPC specific tools - Scalasca & friends

- Scalasca
 - \hookrightarrow Study behavior of // apps. & identify optimization opport.
- Score-P
 - → Instrumentation tool for profiling, event tracing, online analysis.
- Extra-P
 - → Automatic performance modeling tool for // apps.





Tools at your disposal (IV)

HPC specific tools - Scalasca & friends

- Scalasca
 - → Study behavior of // apps. & identify optimization opport.
- Score-P
 - → Instrumentation tool for profiling, event tracing, online analysis.
- Extra-P
 - → Automatic performance modeling tool for // apps.

Free and Open Source!

See other awesome tools at http://www.vi-hps.org/tools





Arm DDT - highlights

DDT features

- Parallel debugger: threads, OpenMP, MPI support
- Controls processes and threads
- Deep memory debugging
 - $\,\hookrightarrow\,$ find memory leaks, dangling pointers, beyond-bounds access
- C++ debugging including STL
- Fortran including F90/F95/F2008 features
- Python scripts ran under CPython interpreter, mpi4py
- See vars/arrays across multiple processes
- Integrated editing, building and VCS integration
- Offline mode for non-interactive debugging
 - → record application behavior and state





Arm DDT - on ULHPC

Modules

- On Iris: module load tools/ArmForge
- Caution! May behave differently between
 - \hookrightarrow Debian+OAR (Gaia, Chaos) and CentOS+SLURM (Iris)

Debugging with DDT

- ① Load toolchain, e.g. (for Intel C/C++/Fortran, MPI, MKL):
 → module load toolchain/intel
- Compile your code, e.g. mpiicc \$code.c -o \$app
- Run your code through DDT (GUI version)
 - \hookrightarrow iris: ddt srun ./\$app
 - → gaia/chaos: ddt mpirun -hostfile \$OAR_NODEFILE ./\$app
- Run DDT in batch mode (no GUI, just report):
 - → ddt --offline -o report.html --mem-debug=thorough
 ./\$app



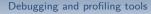


Debugging and profiling tools

Arm DDT - interface









Arm MAP - highlights

MAP features

- Meant to show developers where&why code is losing perf.
- Parallel profiler, especially made for MPI applications
- Recent Python support, incl. mpi4py, OpenMP, threading
- Effortless profiling
 - \hookrightarrow no code modifications needed, may not even need to recompile
- Clear view of bottlenecks
 - \hookrightarrow in I/O, compute, thread or multi-process activity
- Deep insight in CPU instructions affecting perf.
 - $\,\hookrightarrow\,$ vectorization and memory bandwidth
- Memory usage over time see changes in memory footprint
- Integrated editing and building as for DDT



Arm MAP - on ULHPC

Modules

- On Iris: module load tools/ArmForge
- Caution! May behave differently between:
 - → Debian+OAR (Gaia, Chaos) and CentOS+SLURM (Iris)

Profiling with MAP

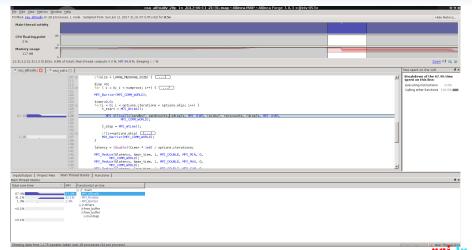
- 1 Load toolchain that built your app., e.g.
 - → module load toolchain/intel
- Run your code through MAP (attached, GUI version)
 - → iris: map srun ./\$app
 - → gaia/chaos: map mpirun -hostfile \$OAR_NODEFILE ./\$app
- Run MAP in batch mode (no GUI, create .map file):





Debugging and profiling tools

Arm MAP - interface





Arm Perf. Reports - highlights

Performance Reports features

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





Arm Perf. Reports - on ULHPC

Modules

- On Iris: module load tools/ArmReports
- Caution! May behave differently between:
 - → Debian+OAR (Gaia, Chaos) and CentOS+SLURM (Iris)
 - \hookrightarrow Gaia: can collect GPU metrics
 - $\hookrightarrow\,$ Iris: can collect GPU & energy metrics

Using Performance Reports

- 1 Load toolchain that you run your app. with, e.g.
 - → module load toolchain/intel
- 2 Run your application through Perf. Reports
 - → iris: perf-report srun ./\$app
- 3 Analysis by default in .html and .txt indicating also run config.





Arm Perf. Reports - output (I)



srun gmx mpi mdrun -s bench rnase cubic.tpr -nsteps 10000

1 node (28 physical, 28 logical cores per node) 126 GiB per node

28 processes, OMP_NUM_THREADS was 0 iris-053

Sun Jun 11 2017 20:13:59 (UTC+02) 19 seconds

/mnt/irisgpfs/apps/resif/data/production/v0.1-20170602/ default/software/bio/GROMACS/2016.3-intel-2017a-hybrid/



Summary: gmx mpi is Compute-bound in this configuration



Time spent running application code. High values are usually good. This is average; check the CPU performance section for advice Time spent in MPI calls. High values are usually bad. This is average; check the MPI breakdown for advice on reducing it 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

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

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

Effective process point-to-point rate 419 MB/s

computation may increase the effective transfer rate.

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

UNIVERSITÉ DU LUXEMBOURG

Uni.lu HPC School 2019/ PS4b



Arm Perf. Reports - output (II)

CPU

A breakdown of the 54.6% CPU time:

Single-core code 5.5% |

OpenMP regions 94.5% |

Scalar 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.

I/C

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!

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.

MPI

A breakdown of the 45.4% MPI time:
Time in collective calls
Time in point-to-point calls
66.5%
Effective process collective rate
426 MBis
Effective process point-to-point rate
419 MBis
Most of the time is spent in point-to-point calls with an average tr

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.

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.

Energy

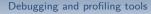
A breakdown of how the 0.899 Wh was used:

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?







Intel Advisor - highlights

Advisor features

- Vectorization Optimization and Thread Prototyping
- Analyze vectorization opportunities
 - → for code compiled either with Intel and GNU compilers
 - \hookrightarrow SIMD, AVX* (incl. AVX-512) instructions
- Multiple data collection possibilities
 - \hookrightarrow loop iteration statistics
 - → data dependencies
 - \hookrightarrow memory access patterns
- Suitability report predict max. speed-up
 - \hookrightarrow based on app. modeling



Intel Advisor - on ULHPC

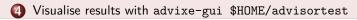
Modules

On iris/gaia/chaos: module load perf/Advisor

Using Intel Advisor

- Load toolchain: module load toolchain/intel
- Compile your code, e.g. mpiicc \$code.c -o \$app
- 3 Collect data e.g. on gaia:

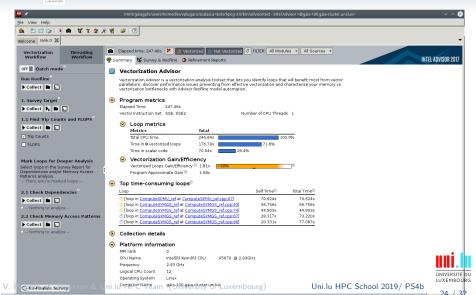
mpirun -n 1 -gtool "advixe-cl -collect survey \
-project-dir ./advisortest:0" ./\$app







Intel Advisor - interface





Scalasca & friends - highlights

Scalasca features

- Scalable performance analysis toolset
 - \hookrightarrow for large scale // applications on 100.000s of cores
- Support for C/C++/Fortran code with MPI, OpenMP, hybrid
- 3 stage workflow: instrument, measure, analyze
 - \hookrightarrow at compile time, run time and resp. postmortem
- Score-P for instrumentation + measurement, Cube for vis.
 - $\,\hookrightarrow\,$ Score-P can also be used with Periscope, Vampir and Tau
- Facilities for measurement optimization to min. overhead
 - \hookrightarrow by selective recording, runtime filtering

Full details at http://www.scalasca.org/about/about.html





Scalasca - on ULHPC

Modules

On iris/gaia/chaos:

module load perf/Scalasca perf/Score-P

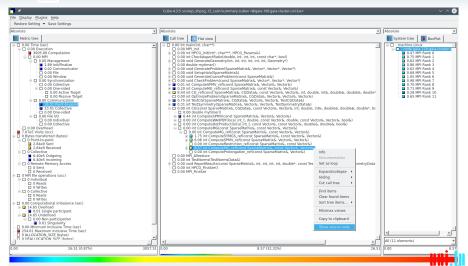
Using Scalasca

- 1 Load toolchain: module load toolchain/foss
- Compile your code, e.g. scorep mpicc \$code.c -o \$app
 - Collect data e.g. on gaia: scan -s mpirun -n 12 ./\$app
- Visualise results with square scorep_\$app_12_sum
 - \hookrightarrow or generate text report: square -s scorep_\$app_12_sum
 - → ... and print it: cat scorep_\$app_12_sum/scorep.score





Scalasca visualisation with Cube-P



Selected *int ComputeMG_ref(const SparseMatrix&, const Vector&, Vector&)*



Conclusion

Summary

- Introduction
- 2 Debugging and profiling tools
- 3 Conclusion





Conclusion

Now it's up to you

Easy right?





Conclusion

Now it's up to you

Easy right?

Well not exactly.







Now it's up to you

Easy right?

Well not exactly.

Debugging always takes effort and real applications are never trivial.







Now it's up to you

Easy right?

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
- HPC oriented tools available for you on UL HPC

And now...

Short DEMO time!





Conclusion and Practical Session start

We've discussed

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

And now...

Short DEMO time!

Your Turn!





Hands-on start

We will first start with running HPCG (unmodified) as per:

ulhpc-tutorials.rtfd.io/en/latest/advanced/HPCG/

- ... your tasks:
 - 1 perform a timed first run using unmodified HPCG v3.0 (MPI only)
 - √ use sacct -j \$JOBID -1 to get details
 - \checkmark single node, use \ge 80 80 for input params (hpcg.dat)
 - run HPCG (timed) through Allinea Perf. Report
 - \checkmark use perf-report for diff. // configurations: 1 vs 2 nodes all cores
 - instrument and measure HPCG execution with Scalasca
 - ✓ check MPI comm. measurements, especially collective operations
- Reservations for the workshop on Iris:
 - → regular nodes (batch partition): --reservation=hpcschool
 - → accel. nodes (gpu partition): --reservation=hpcschool-gpu





Questions?

http://hpc.uni.lu

High Performance Computing @ uni.lu

Prof. Pascal Bouvry Dr. Sebastien Varrette Valentin Plugaru Sarah Peter Hyacinthe Cartiaux Clement Parisot Dr. Fréderic Pinel Dr. Emmanuel Kieffer

University of Luxembourg, Belval Campus Maison du Nombre, 4th floor 2, avenue de l'Université L-4365 Esch-sur-Alzette mail: hpc@uni.lu







