

Exploring compiler behavior on applications from Miniapps up to large scale applications on modern processors

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ACKNOWLEDGEMENTS: ALTAIR, AWS, MEGWARE, ATOS/EVIDEN and CALMIP



Objectives



The first goal is to analyze and assess quantitatively, compiler and compiler options impact on performance.

The ultimate goal is to optimize application performance

- Identify strengths/weakness of various compilers options and compilers
- Leverage optimizations between compilers
- Study ISA impact
- Develop corresponding methodology and test on a real industrial strength application



TALK OVERVIEW



- Methodology (MAQAO/ONEVIEW/QaaS)
- Mini App results
- LAMMPS Results
- OpenRadioss results
- Conclusion





METHODOLOGY



Methodology (1)



Standard case: Compiler A with options OPT1 is slightly faster than compiler B with options OPT2.

Easy (superficial) conclusion: use Compiler A with options OPT1

Better (more complex) approach: analyze compiler behavior

ISSUE: Compiler A can outperform compiler B for Function FOO and the situation can be reversed for another Function BOO. There can be compensation between various functions.

Performance analysis has to go down at least to the function level and very often down to the loop level.

Due to the number of functions/loops involved, Analysis/assessment has to be automated.



Methodology (2)



Timing will be performed at three levels: whole app, function level, loop level

Goals require detailed analysis of compiler outputs: assembly code

Relying on MAQAO/ONE View capabilities

- To evaluate capabilities, weakness and strengths of various ASM codes using simplified simulators
- To perform matching between source code and different ASM variants: essential requisite to analyze advanced compiler strategies multiversioning



Analyzing Code Quality (1)



Focus on loops: innermost/in between/outermost

Evaluate ASM using CQA (Code Quality Analysis) included in MAQAO.

- Generic topics of interest
 - Port / Functional Units usage
 - Vectorization
 - Instruction set use
 - Vectorization Roadblocks
 - Data access
- Two types of analysis: Static at the ASM level and Dynamic requiring measurement

IMPORTANT: By looking directly at ASM, both compiler mistakes but also source code issues will be taken into account.

Analyzing Code Quality (2)



Classify performance issues into 5 main categories

- 1. Loop computation: issues related to the computation organization (FMA, SQRT/DIV, etc...)
- 2. **Control Flow:** issues relevant to control (branches, call,)
- 3. **Data access:** issues essentially related to memory operations (stride, indirect, spill/fill,)
- 4. **Vectorization roadblocks:** issues preventing vectorization (complex control flow, ...)
- 5. **Inefficient vectorization:** issues related to vectorization quality (vector length, masked, ...)

| Loop ID | Analysis | Penalty Score |
|--|---|------------------|
| ▼ Loop 29963 - engine_linuxa64_gf_ompi | Execution Time: 1 % - Vectorization Ratio: 21.05 % - Vector Length Use: 59.87 % | |
| ▼ Loop Computation Issues | | 6 |
| 0 | [SA] Less than 10% of the FP ADD/SUB/MUL arithmetic operations are performed using FMA - Reorganize arithmetic expressions to exhibit potential for FMA. This issue costs 4 points. | 4 |
| 0 | [SA] Presence of a large number of scalar integer instructions - Simplify loop structure, perform loop splitting or perform unroll and jam. This issue costs 2 points. | 2 |
| ▼ Control Flow Issues | | 2 |
| 0 | [SA] Several paths (2 paths) - Simplify control structure or force the compiler to use masked instructions. There are 2 issues (= paths) costing 1 point each. | 2 |
| ▼ Data Access Issues | | 12 |
| 0 | [SA] Presence of constant non unit stride data access - Use array restructuring, perform loop interchange or use gather instructions to lower a bit the cost. There are 2 issues (= data accesses) costing 2 point each. | 4 |
| 0 | [SA] Presence of indirect accesses - Use array restructuring or gather instructions to lower the cost. There are 2 issues (= indirect data accesses) costing 4 point each. | 8 |
| ► Vectorization Roadblocks | | 14 |



Global Characteristics: OneView typical output (1)



| Clabal Maratan | 0 |
|--------------------------------------|---------|
| Global Metrics | • |
| Total Time (s) | 7.51 E3 |
| Max (Thread Active Time) (s) | 7.42 E3 |
| Average Active Time (s) | 6.77 E3 |
| Activity Ratio (%) | 90.2 |
| Average number of active threads | 86.565 |
| Affinity Stability (%) | 100.0 |
| Time in analyzed loops (%) | 85.8 |
| Time in analyzed innermost loops (%) | 81.3 |
| Time in user code (%) | 87.7 |
| Compilation Options Score (%) | 74.9 |
| Array Access Efficiency (%) | 70.6 |

48 MPI Ranks + 2 OMP Threads/ranks

4 essential metrics:

- Average active time: Sum over all threads of their active time divided by thread count. IDEAL = total execution time
- 2. Activity ratio: Sum over all threads of their active time divided by the sum of their wall time. IDEAL: 100%
- 3. Average active number of threads: Sum over all threads of their active time divided by longest wall clock time: IDEAL = number of threads used
- **4. Affinity stability:** evaluates percentage of time spent without thread migration between physical cores: **IDEAL 100%**

Link to MAQAO report

OpenRadioss Taurus GFortran -O3 on G4



Global Characteristics: OneView typical output (2)



| Perfect Flow Complexity 1.05 | | | | | | | | | |
|--|---------------------|------|--|--|--|--|--|--|--|
| Perfect Flow Complexity | | 1.05 | | | | | | | |
| Perfect OpenMP + MPI + | Pthread | 1.05 | | | | | | | |
| Perfect OpenMP + MPI + Pthread + Perfect Load Distribution | | | | | | | | | |
| No Scalar Integer | Potential Speedup | 1.20 | | | | | | | |
| | Nb Loops to get 80% | 32 | | | | | | | |
| FP Vectorised | Potential Speedup | 1.11 | | | | | | | |
| rr vectoriseu | Nb Loops to get 80% | 24 | | | | | | | |
| Fully Vactorised | Potential Speedup | 1.28 | | | | | | | |
| Fully Vectorised | Nb Loops to get 80% | 41 | | | | | | | |
| FP Arithmetic Only | Potential Speedup | 1.56 | | | | | | | |
| FF Antillieuc Only | Nb Loops to get 80% | 41 | | | | | | | |

For each thread, we gather a full picture of their activity: time spent in various functions including time spent in various libraries: OpenMP, MPI and Pthreads.

From these measurements we extrapolate impact of time spent in OpenMP/MPI/Pthread libraries and load distribution.

Perfect OpenMP + MPI + Pthread: max (Original Thread time)/ max (Stripped Thread Time): Stripped ⇔ time spent in OpenMP/MPI/Pthread set to 0.

48 MPI Ranks + 2 OMP Threads/ranks

Perfect OpenMP + MPI + Pthread + Perfect Load Distribution: max (Original Thread time)/ average (Stripped Thread Time):

OpenRadioss Taurus GFortran –O3 on G4

A performance optimization goal is to have these 2 metrics under 1.1

https://datafront.exascale-computing.eu/public/OpenRadioss/TAURUS10M/G4_AWS/gnu/OpenRadioss_TAURUS10M-short_g4-aws_o2_m48_gnu_engine/



QaaS Characteristics (1)



QaaS is an Open Source collaborative project aiming at providing a software environment exploring (understanding/characterizing) applications/systems performance, the ultimate goal being application optimization.

QaaS (Quality as a Service) relies on the following features

- Automation: pushed as much as possible. Large amount of data automatically generated
- Systematic exploration of key parameters space:
 - hardware platforms (AMD, ARM (Ampere, Grace, G3/G4), INTEL, etc...)
 - Compilers and compiler settings
 - number of cores and core mapping, more generally runtime and run time settings
 - More generally: software stack parameters



QaaS Characteristics (2)



- Uniform exploration: to enable systematic comparison
- > Reliability: built in repetition mechanisms to ensure reliable results
- Detailed level of comparison: use of MAQAO/OneView to provide several profiling levels: whole application, functions, loops and key application characteristics.
- > Flexible search and formatting through results
- Two levels of optimizations:
 - automatic (compilers/compiler switches/transformations),
 - recommendations for "manual" optimizations.





MINIAPP RESULTS



Miniapps



For the miniapps used in our tests, a good description/reference is provided on the site: https://proxyapps.exascaleproject.org/app/.

- > AMG
- Cloverleaf
- > CoMD
- > Hacc MK
- > MiniQMC
- Kripke



COMPILER AND COMPILER OPTIONS FOR G3 RUNS (64 cores)



| _ | | | | | | | | |
|------------|---|---------------------------------------|-----------------|---------------|------------------|--------------|--|--|
| orig | default | | | | | | | |
| gcc | default | | | | | | | |
| armclang 1 | O2 -mcpu=r | native -armpl | | | | | | |
| armclang 2 | O2 -mcpu=n | ative -fno-vect | torize -armpl | | | | | |
| armclang 3 | O3 -mcpu=n | ative -armpl | | | | | | |
| armclang 4 | O3 -mcpu=n | O3 -mcpu=native -fno-vectorize -armpl | | | | | | |
| armclang 5 | Ofast -mcpu= | native -armpl | | | | | | |
| armclang 6 | Ofast -mcpu= | native -fno-ve | ctorize -armpl | | | | | |
| gcc 1 | O2 -mcpu=na | tive -funroll-lo | ops -larmpl | | | | | |
| gcc 2 | O2 -mcpu= | native -fno-tr | ee-vectorize -f | no-openmp-si | md -funroll-lo | ops -larmpl | | |
| gcc 3 | O3 -mcpu=n | ative -funroll-l | oops -larmpl | | | | | |
| gcc 4 | O3 -mcpu= | native -fno-tr | ee-vectorize -f | no-openmp-si | md -funroll-lo | ops -larmpl | | |
| gcc 5 | Ofast -mcpu=native -funroll-loops -larmpl | | | | | | | |
| gcc 6 | Ofast -mcpu | u=native -fno-t | ree-vectorize | -fno-openmp-s | simd -funroll-lo | oops -larmpl | | |



PERFORMANCE OF MINIAPPS ON G3 (64 cores)



| | AMG | CLOVERLEAF | COMD | HACC mk | MINIQMC | KRIPKE |
|------------|------|------------|------|---------|---------|--------|
| orig | 1,01 | 1,01 | 1,10 | 4,40 | 1,00 | 1,02 |
| gcc | 1,00 | 1,00 | 1,00 | 1,00 | 1,01 | 2,13 |
| armclang 1 | 1,02 | 1,02 | 1,08 | 4,39 | 1,00 | 1,01 |
| armclang 2 | 1,01 | 1,02 | 1,07 | 9,01 | 1,01 | 1,00 |
| armclang 3 | 1,01 | 1,02 | 1,09 | 4,39 | 1,00 | 1,01 |
| armclang 4 | 1,01 | 1,01 | 1,09 | 9,01 | 1,00 | 1,01 |
| armclang 5 | 1,01 | 1,01 | 1,04 | 1,44 | 1,00 | 1,23 |
| armclang 6 | 1,01 | 1,01 | 1,04 | 2,50 | 1,02 | 1,00 |
| gcc 1 | 1,02 | 1,00 | 1,02 | 2,62 | 1,02 | 1,23 |
| gcc 2 | 1,03 | 1,00 | 1,02 | 2,62 | 1,02 | 1,23 |
| gcc 3 | 1,00 | 1,00 | 1,00 | 1,00 | 1,01 | 2,00 |
| gcc 4 | 1,00 | 1,00 | 1,00 | 2,62 | 1,01 | 1,23 |
| gcc 5 | 1,00 | 1,00 | 1,04 | 1,00 | 1,01 | 1,97 |
| gcc 6 | 1,00 | 1,00 | 1,02 | 2,62 | 1,01 | 1,23 |

BEST: TIMING RATIOS: current timing over best timing across all compilers and compiler options.

- Green cells corresponds to best or very close to best (< 1%)
- Yellow cells correspond to performance losses between 1% and 5%
- Red cells correspond to performance losses > 5%



A FEW CONCLUSIONS



| | AMG | CLOVERLEAF | COMD | HACC mk | MINIQMC | KRIPKE |
|------------|------|------------|------|---------|---------|--------------|
| orig | 1,01 | 1,01 | 1,10 | 4,40 | 1,00 | 1,02 |
| gcc | 1,00 | 1,00 | 1,00 | 1,00 | 1,01 | 2,13 |
| armclang 1 | 1,02 | 1,02 | 1,08 | 4,39 | 1,00 | 1,01 |
| armclang 2 | 1,01 | 1,02 | 1,07 | 9,01 | 1,01 | 1,00 |
| armclang 3 | 1,01 | 1,02 | 1,09 | 4,39 | 1,00 | 1,01 |
| armclang 4 | 1,01 | 1,01 | 1,09 | 9,01 | 1,00 | 1,01 |
| armclang 5 | 1,01 | 1,01 | 1,04 | 1,44 | 1,00 | 1,23 |
| armclang 6 | 1,01 | 1,01 | 1,04 | 2,50 | 1,02 | 1,00 |
| gcc 1 | 1,02 | 1,00 | 1,02 | 2,62 | 1,02 | 1,23 |
| gcc 2 | 1,03 | 1,00 | 1,02 | 2,62 | 1,02 | 1,2 3 |
| gcc 3 | 1,00 | 1,00 | 1,00 | 1,00 | 1,01 | 2,00 |
| gcc 4 | 1,00 | 1,00 | 1,00 | 2,62 | 1,01 | 1,23 |
| gcc 5 | 1,00 | 1,00 | 1,04 | 1,00 | 1,01 | 1,97 |
| gcc 6 | 1,00 | 1,00 | 1,02 | 2,62 | 1,01 | 1,23 |

For half of the miniapp (AMG, Cloverleaf, Min,iQMC) compiler and compiler options have limited impact.

For the other half, compiler (CoMD, HACC mk, Kripke) compiler and compiler options have a large impact

The original compiler options are not the best choice....

Neither GCC nor ARMCLANG are always winning.





LAMMPS RESULTS



LAMMPS CODE



Source: https://www.lammps.org/#gsc.tab=0

- LAMMPS is a classical molecular dynamics code with a focus on materials modeling. It's an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.
- LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale.
- LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. Many of its models have versions that provide accelerated performance on CPUs, GPUs, and Intel Xeon Phis. The code is designed to be easy to modify or extend with new functionality.



LAMMPS on Graviton 3 (64 cores) AWS: Armclang versus GCC



| | ARMCLANG 1 - O3 - mcpu=neoverse- v1 -armpl -ffast- math | | v1 | v1 -armpl -fno- | | | GCC2 -O3 - mcpu=neovers e-v1 -larmpl - msve-vector- bits=256 - funroll-loops - ffast-math | se-v1 -larmpl - msve-vector- bits=128 - | v1+nosve+no sve2 -larmpl - | se-v1 -larmpl - | se-v1 -larmpl - funroll-loops - ffast-math |
|----------------------------------|---|------------|------------|-----------------|------------|--------|---|---|-------------------------------|-----------------|--|
| Metric | ARMCLANG 1 | ARMCLANG 2 | ARMCLANG 4 | ARMCLANG 5 | ARMCLANG 6 | GCC 1 | GCC 2 | GCC 3 | GCC 4 | GCC 5 | GCC 6 |
| Total Time (s) | 420,57 | 422,54 | 423,42 | 430,12 | 421,46 | 434,58 | 433,02 | 433,38 | 434,74 | 432,86 | 440,65 |
| Best | 1,00 | 1,00 | 1,01 | 1,02 | 1,00 | 1,03 | 1,03 | 1,03 | 1,03 | 1,03 | 1,05 |
| Max (Thread Active Time) (s) | 418,66 | 420,65 | 421,57 | 428,29 | 419,53 | 432,68 | 431,32 | 431,52 | 432,7 | 431,22 | 438,59 |
| Average Active Time (s) | 418,43 | 420,29 | 421,23 | 427,84 | 419,19 | 432,35 | 430,79 | 431,13 | 432,43 | 430,67 | 438,33 |
| Activity Ratio (%) | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 |
| Average number of active threads | 63,67 | 63,66 | 63,67 | 63,66 | 63,66 | 63,67 | 63,67 | 63,67 | 63,66 | 63,68 | 63,66 |
| Affinity Stability (%) | 99,9 | 100 | 99,9 | 100 | 99,9 | 99,9 | 100 | 100 | 99,9 | 100 | 99,9 |

BEST: TIMING RATIOS: current timing over best timing across all compilers and compiler options.

- Green cells corresponds to best or very close to best (< 1%)
- Yellow cells correspond to performance losses: 1% < and < 3%
- Red cells correspond to performance losses > 3%



LAMMPS on Graviton 3 (64 cores) AWS: Armclang versus GCC



| | ARMCLANG 1 | ARMCLANG 2 | ARMCLANG 4 | ARMCLANG 5 | ARMCLANG 6 | GCC 1 | GCC 2 | GCC 3 | GCC 4 | GCC 5 | GCC 6 |
|---|------------|------------|------------|------------|------------|-------|-------|-------|-------|-------|-------|
| LAMMPS_NS::PairEAM::compute(int, int) | 1,00 | 1,00 | 1,01 | 1,02 | 1,00 | 1,03 | 1,04 | 1,04 | 1,04 | 1,03 | 1,05 |
| LAMMPS_NS::NPairBin<1, 1, 0, 0, 1>::build(LAMMPS_NS::NeighList* | 1,00 | 1,01 | 1,00 | 1,03 | 1,01 | 1,05 | 1,02 | 1,02 | 1,03 | 1,03 | 1,04 |
| LAMMPS_NS::FixNVE::initial_integrate(int) | 1,00 | 1,00 | 1,00 | 1,00 | 1,01 | 1,00 | 1,00 | 1,00 | 1,00 | 1,00 | 1,00 |
| LAMMPS_NS::FixNVE::final_integrate() | 1,00 | 1,00 | 1,00 | 1,00 | 1,00 | 1,01 | 1,00 | 1,01 | 1,00 | 1,00 | 1,00 |
| LAMMPS_NS::CommBrick::borders() | 1,02 | 1,00 | 1,01 | 1,01 | 1,01 | 1,01 | 1,00 | 1,01 | 1,03 | 1,00 | 1,01 |
| LAMMPS_NS::AtomVec::pack_comm(int, int*, double*, int, int*) | 1,04 | 1,05 | 1,04 | 1,04 | 1,03 | 1,01 | 1,03 | 1,02 | 1,01 | 1,06 | 1,00 |
| LAMMPS_NS::AtomVec::unpack_reverse(int, int*, double*) | 1,08 | 1,10 | 1,09 | 1,10 | 1,10 | 1,00 | 1,05 | 1,01 | 1,00 | 1,02 | 1,05 |
| LAMMPS_NS::Neighbor::check_distance() | 1,00 | 1,00 | 1,01 | 1,00 | 1,00 | 1,01 | 1,01 | 1,00 | 1,00 | 1,00 | 1,00 |

TIMING RATIOS: current timing over best timing across all compilers and compiler options.

- Green cells corresponds to best or very close to best (< 1%)
- Yellow cells correspond to performance losses 1% < and < 5%
- Red cells correspond to performance losses > 5%



LAMMPS on Granite Rapids (256 cores) MEGWARE: ICX versus GCC



| | S | TANDARD LAN | IMPS PACKAG | GE | X86 | OPTIMIZED LA | AMMPS PACK | AGE |
|--------------------------------------|--------------|-------------|-------------|--------|--------------|--------------|------------|-------|
| Metric | orig_default | gcc_default | icx_2 | gcc_5 | orig_default | gcc_default | icx_2 | gcc_7 |
| Total Time (s) | 107,83 | 112,62 | 108,66 | 107,06 | 50,75 | 89,41 | 51,02 | 86,55 |
| BEST | 2,12 | 2,22 | 2,14 | 2,11 | 1,00 | 1,76 | 1,01 | 1,71 |
| Max (Thread Active Time) (s) | 92,39 | 99,71 | 93,2 | 95,12 | 34,68 | 77,39 | 34,91 | 75,07 |
| Average Active Time (s) | 91,71 | 99,38 | 92,5 | 95,04 | 34,05 | 76,94 | 34,19 | 74,69 |
| Activity Ratio (%) | 85,6 | 88,7 | 85,3 | 89,4 | 68 | 86,6 | 67,4 | 87 |
| Average number of active threads | 218 | 226 | 218 | 227 | 172 | 220 | 172 | 221 |
| Affinity Stability (%) | 87,5 | 89,3 | 87,1 | 90,2 | 71,8 | 87,4 | 71,2 | 87,8 |
| Time in analyzed loops (%) | 90,6 | 90,2 | 91 | 92,6 | 84,5 | 91 | 84,9 | 90,7 |
| Time in analyzed innermost loops (%) | 87,3 | 87,1 | 87,7 | 88,2 | 57 | 88,5 | 57,4 | 86,1 |
| Time in user code (%) | 90,9 | 90,5 | 91,3 | 92,9 | 88,8 | 91,2 | 89,1 | 92,7 |
| Compilation Options Score (%) | 100 | 50 | 100 | 100 | 100 | 50 | 100 | 87,5 |
| Array Access Efficiency (%) | 51,7 | 45,5 | 51,9 | 56,7 | 50,8 | 65,5 | 51,2 | 71,1 |

TIMING RATIOS: current timing over best timing across all compilers and compiler options.

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- Red cells correspond to performance losses > 5%



LAMMPS on Granite Rapids (256 cores) MEGWARE: ICX versus GCC



| | | S ⁻ | TANDARD LAN | IMPS PACKAG | GE | X86 | OPTIMIZED LA | AMMPS PACK | AGE |
|-------------------------|---------------------|----------------|-------------|-------------|--------|--------------|--------------|------------|-------|
| | Metric | orig_default | gcc_default | icx_2 | gcc_5 | orig_default | gcc_default | icx_2 | gcc_7 |
| To | otal Time (s) | 107,83 | 112,62 | 108,66 | 107,06 | 50,75 | 89,41 | 51,02 | 86,55 |
| | BEST | 2,12 | 2,22 | 2,14 | 2,11 | 1,00 | 1,76 | 1,01 | 1,71 |
| Pote | ential Speedups | | | | | | | | |
| Perfect Flow Complexity | | 3,06 | 3,5 | 3,08 | 3,59 | 1,01 | 1,01 | 1,01 | 1,97 |
| Perfect Oper | nMP/MPI/Pthread/TBB | 1,02 | 1,02 | 1,02 | 1,01 | 1,06 | 1,02 | 1,07 | 1,02 |
| - | nMP/MPI/Pthread/TBB | 1,1 | 1,1 | 1,1 | 1,07 | 1,11 | 1,09 | 1,11 | 1,07 |
| No Scalar | Potential Speedup | 1,3 | 1,21 | 1,3 | 1,3 | 1,06 | 1,06 | 1,06 | 1,07 |
| Integer | Nb Loops to get 80% | 3 | 3 | 3 | 3 | 7 | 6 | 7 | 6 |
| FP | Potential Speedup | 1,66 | 1,83 | 1,67 | 1,64 | 1,01 | 2,05 | 1,01 | 1,64 |
| Vectorised | Nb Loops to get 80% | 3 | 3 | 3 | 3 | 4 | 5 | 4 | 5 |
| Fully | Potential Speedup | 3,63 | 4,27 | 3,67 | 4,41 | 1,1 | 5,95 | 1,1 | 5,88 |
| Vectorised | Nb Loops to get 80% | 4 | 5 | 5 | 6 | 15 | 17 | 15 | 18 |
| Only FP | Potential Speedup | 1,5 | 1,28 | 1,5 | 1,41 | 2,41 | 1,11 | 2,42 | 1,2 |
| Arithmetic | Nb Loops to get 80% | 3 | 3 | 3 | 4 | 12 | 10 | 12 | 12 |

TIMING RATIOS: current timing over best timing across all compilers and compiler options.

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- Red cells correspond to performance losses > 5%





OpenRadioss RESULTS



Target code: OpenRadioss



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Altair[®] Radioss[®] & OpenRadioss[™] The Industry Standard Open Platform for Crash & Impact

OpenRadioss™ Open-Source Version

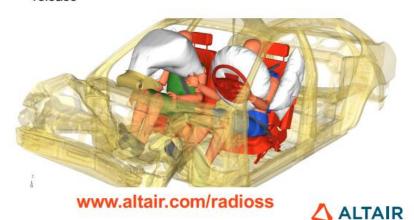
- Source code publicly accessible from: https://github.com/OpenRadioss
- Upstream version, with contributions from a fast-growing worldwide community
- Precompiled Linux & Windows executables to run latest builds with no license check
- Support from the community, via forum



www.openradioss.org

Altair® Radioss® Commercial Version

- Commercial releases with extensive QA, professional support, documentation and maintenance priority
- Available under Altair Units license
- Encrypted models for dummies & barriers
- Channels valuable community contributions into industrial release





Dataset and code parallelism



Realistic data sets have been used. Due to domain decomposition, data set size varies depending upon the number of MPI ranks used

 TAURUS (Public): 10 millions elements, reference 1.7 GB, after partitioning for 96 MPI ranks 17 GB

Code in Fortran combining MPI + OpenMP parallelism

- Excellent MPI scaling due to very good domain decomposition
- More limited OpenMP parallelism

OUR TWO REFERENCE TESTS: 96 MPI Ranks and 48 MPI Ranks + 2 OpenMP threads per rank



Experimental constraints



NUMERICAL ACCURACY

The code uses explicit method with very small time steps.

Accuracy and reproducibility is major concern. Therefore any code transformation which has an impact on numerical accuracy is prohibited. For example, fast math compiler flag and even the option enabling fused multiply add (FMA) is prohibited

EXECUTION TIME

Due to the nature of the code (mechanical crash), various code segments are used throughout the whole simulation => to be realistic (involving all key code segments) the run has to be long enough...

TAURUS on 96 cores Neoverse V2 takes over 2 hours!



Vectorization Taurus ACfl –O3 on G4



| Loop id | Source Location | Source Function | Level | Exclusive Coverage mpi_96_ranks_omp_1_thread (%) | Vectorization Ratio (%) | Vector Length Use (%) |
|------------|--|-----------------|-----------|---|----------------------------|-----------------------------|
| 40382 | engine_linuxa64_ompi_O3 - i7opt cd.F:202-243 [] | i7optcd | Innermost | 5.06 | 48.11 | 66.04 |
| 13300 | 0J.F:1205-1466 [] | czprojn | Innermost | 3.09 | 0 | 49.8 |
| 6105 | engine_linuxa64_ompi_O3 - assp ar4.F:165-173 | | Innermost | 2.73 | 45.45 | 72.73 |
| 44945 | engine_linuxa64_ompi_O3 - sigep s36c.F:269-269 | sigeps36c | Single | 2.55 | 97.83 | 98.91 |
| | engine_linuxa64_ompi_O3 - cupd tn3.F:653-692 | | Single | 2.36 | 25.96 | 62.5 |
| | e_crit.F:131-150 | | Outermost | 1.97 | 27.45 | 58.33 |
| | engine_linuxa64_ompi_O3 - depl a.F:95-104 | | Innermost | 1.63 | 42.11 | 71.05 |
| | t.F:157-159 | | Innermost | 1.54 | 88.89 | 100 |
| 52519 | engine_linuxa64_ompi_O3 - mula wc.F:2378-2384 | mulawc | Innermost | 1.53 | 59.02 | 79.1 |
| 6507 | engine_linuxa64_ompi_O3 - vites se.F:80-86 | vitesse | Innermost | 1.40 | 46.15 | 72.12 |
| 13455 | engine_linuxa64_ompi_O3 - czfin tn.F:355-443 | czfintn1 | Single | 1.36 | 92.36 | 96.84 |

Link to MAQAO report



Compiler flags: ACfl versus GFortran on AWS G4



Limited impact of Compiler Options

| Global metric | | GI | VU | | | Ad | :fL | |
|--------------------------------------|---------|---------|------------|-----------|---------|---------|------------|-----------|
| Global metric | O2 | O3 | O3 no SVE2 | O3 no SVE | O2 | O3 | O3 no SVE2 | O3 no SVE |
| Total Time (s) | 7.89 E3 | 7.51 E3 | 7.65 E3 | 7.41 E3 | 7.92 E3 | 7.91 E3 | 7.92 E3 | 8.26 E3 |
| Max (Thread Active Time) (s) | 7.71 E3 | 7.42 E3 | 7.47 E3 | 7.33 E3 | 7.89 E3 | 7.88 E3 | 7.88 E3 | 8.07 E3 |
| Average Active Time (s) | 7.02 E3 | 6.77 E3 | 6.78 E3 | 6.66 E3 | 7.77 E3 | 7.77 E3 | 7.77 E3 | 7.86 E3 |
| Activity Ratio (%) | 89.0 | 90.2 | 88.7 | 90.0 | 98.2 | 98.1 | 98.1 | 95.9 |
| Average number of active threads | 85.4 | 86.7 | 85.1 | 86.3 | 94.210 | 94.193 | 94.179 | 91.284 |
| Affinity Stability (%) | 99.2 | 100.0 | 99.1 | 100.0 | 100.0 | 100.0 | 100.0 | 98.5 |
| Time in analyzed loops (%) | 86.4 | 85.8 | 85.7 | 85.4 | 78.1 | 78.0 | 77.8 | 76.3 |
| Time in analyzed innermost loops (%) | 78.0 | 81.3 | 81.2 | 80.9 | 70.5 | 71.4 | 71.2 | 69.6 |
| Time in user code (%) | 88.1 | 87.7 | 87.6 | 87.4 | 80.9 | 80.8 | 80.6 | 79.2 |
| Compilation Options Score (%) | 62.5 | 74.9 | 74.9 | 74.9 | 99.5 | 99.5 | 99.5 | 99.5 |
| Array Access Efficiency (%) | 62.0 | 70.6 | 70.6 | 74.0 | 66.9 | 65.1 | 65.1 | 66.8 |

GFortran compiler flags: impact on AWS G4



Limited impact of Compiler Options

| Global metric | GNU | | | | AcfL | | | | |
|--------------------------------------|---------|---------|------------|-----------|---------|---------|------------|-----------|--|
| | O2 | O3 | O3 no SVE2 | O3 no SVE | O2 | O3 | O3 no SVE2 | O3 no SVE | |
| Total Time (s) | 7.89 E3 | 7.51 E3 | 7.65 E3 | 7.41 E3 | 7.92 E3 | 7.91 E3 | 7.92 E3 | 8.26 E3 | |
| Max (Thread Active Time) (s) | 7.71 E3 | 7.42 E3 | 7.47 E3 | 7.33 E3 | 7.89 E3 | 7.88 E3 | 7.88 E3 | 8.07 E3 | |
| Average Active Time (s) | 7.02 E3 | 6.77 E3 | 6.78 E3 | 6.66 E3 | 7.77 E3 | 7.77 E3 | 7.77 E3 | 7.86 E3 | |
| Activity Ratio (%) | 89.0 | 90.2 | 88.7 | 90.0 | 98.2 | 98.1 | 98.1 | 95.9 | |
| Average number of active threads | 85.4 | 86.7 | 85.1 | 86.3 | 94.210 | 94.193 | 94.179 | 91.284 | |
| Affinity Stability (%) | 99.2 | 100.0 | 99.1 | 100.0 | 100.0 | 100.0 | 100.0 | 98.5 | |
| Time in analyzed loops (%) | 86.4 | 85.8 | 85.7 | 85.4 | 78.1 | 78.0 | 77.8 | 76.3 | |
| Time in analyzed innermost loops (%) | 78.0 | 81.3 | 81.2 | 80.9 | 70.5 | 71.4 | 71.2 | 69.6 | |
| Time in user code (%) | 88.1 | 87.7 | 87.6 | 87.4 | 80.9 | 80.8 | 80.6 | 79.2 | |
| Compilation Options Score (%) | 62.5 | 74.9 | 74.9 | 74.9 | 99.5 | 99.5 | 99.5 | 99.5 | |
| Array Access Efficiency (%) | 62.0 | 70.6 | 70.6 | 74.0 | 66.9 | 65.1 | 65.1 | 66.8 | |

> FOR GFortran: O2 is worse (6%), O3 no-sve is the best



ACfl compiler flags: impact on AWS G4



Limited impact of Compiler Options?

| Global metric | GNU | | | | AcfL | | | |
|--------------------------------------|---------|---------|------------|-----------|---------|---------|------------|-----------|
| | O2 | O3 | O3 no SVE2 | O3 no SVE | O2 | O3 | O3 no SVE2 | O3 no SVE |
| Total Time (s) | 7.89 E3 | 7.51 E3 | 7.65 E3 | 7.41 E3 | 7.92 E3 | 7.91 E3 | 7.92 E3 | 8.26 E3 |
| Max (Thread Active Time) (s) | 7.71 E3 | 7.42 E3 | 7.47 E3 | 7.33 E3 | /.89 E3 | /.୪୪ ೬૩ | /.୪୪ ೬૩ | 8.07 E3 |
| Average Active Time (s) | 7.02 E3 | 6.77 E3 | 6.78 E3 | 6.66 E3 | 7.77 E3 | 7.77 E3 | 7.77 E3 | 7.86 E3 |
| Activity Ratio (%) | 89.0 | 90.2 | 88.7 | 90.0 | 98.2 | 98.1 | 98.1 | 95.9 |
| Average number of active threads | 85.4 | 86.7 | 85.1 | 86.3 | 94.210 | 94.193 | 94.179 | 91.284 |
| Affinity Stability (%) | 99.2 | 100.0 | 99.1 | 100.0 | 100.0 | 100.0 | 100.0 | 98.5 |
| Time in analyzed loops (%) | 86.4 | 85.8 | 85.7 | 85.4 | 78.1 | 78.0 | 77.8 | 76.3 |
| Time in analyzed innermost loops (%) | 78.0 | 81.3 | 81.2 | 80.9 | 70.5 | 71.4 | 71.2 | 69.6 |
| Time in user code (%) | 88.1 | 87.7 | 87.6 | 87.4 | 80.9 | 80.8 | 80.6 | 79.2 |
| Compilation Options Score (%) | 62.5 | 74.9 | 74.9 | 74.9 | 99.5 | 99.5 | 99.5 | 99.5 |
| Array Access Efficiency (%) | 62.0 | 70.6 | 70.6 | 74.0 | 66.9 | 65.1 | 65.1 | 66.8 |

For ACfl: O3 no-sve is the worst (5%), O2/O3/O3 no-sve are identical and the best



Compiler flags: ACfl versus GFortran on AWS G4



Limited impact of Compiler Options?

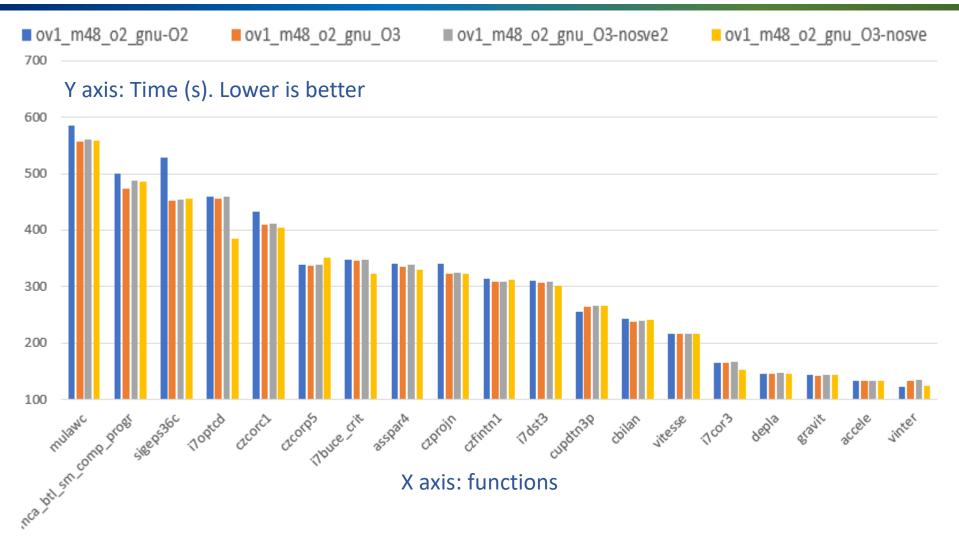
| Global metric | | GNU | | | | AcfL | | | | |
|--------------------------------------|---------|---------|------------|-----------|---------|---------|------------|-----------|--|--|
| | O2 | O3 | O3 no SVE2 | O3 no SVE | O2 | O3 | O3 no SVE2 | O3 no SVE | | |
| Total Time (s) | 7.89 E3 | 7.51 E3 | 7.65 E3 | 7.41 E3 | 7.92 E3 | 7.91 E3 | 7.92 E3 | 8.26 E3 | | |
| Max (Thread Active Time) (s) | 7.71 E3 | 7.42 E3 | 7.47 E3 | 7.33 E3 | 7.89 E3 | 7.88 E3 | 7.88 E3 | 8.07 E3 | | |
| Average Active Time (s) | 7.02 E3 | 6.77 E3 | 6.78 E3 | 6.66 E3 | 7.77 E3 | 7.77 E3 | 7.77 E3 | 7.86 E3 | | |
| Activity Ratio (%) | 89.0 | 90.2 | 88.7 | 90.0 | 98.2 | 98.1 | 98.1 | 95.9 | | |
| Average number of active threads | 85.4 | 86.7 | 85.1 | 86.3 | 94.210 | 94.193 | 94.179 | 91.284 | | |
| Affinity Stability (%) | 99.2 | 100.0 | 99.1 | 100.0 | 100.0 | 100.0 | 100.0 | 98.5 | | |
| Time in analyzed loops (%) | 86.4 | 85.8 | 85.7 | 85.4 | 78.1 | 78.0 | 77.8 | 76.3 | | |
| Time in analyzed innermost loops (%) | 78.0 | 81.3 | 81.2 | 80.9 | 70.5 | 71.4 | 71.2 | 69.6 | | |
| Time in user code (%) | 88.1 | 87.7 | 87.6 | 87.4 | 80.9 | 80.8 | 80.6 | 79.2 | | |
| Compilation Options Score (%) | 62.5 | 74.9 | 74.9 | 74.9 | 99.5 | 99.5 | 99.5 | 99.5 | | |
| Array Access Efficiency (%) | 62.0 | 70.6 | 70.6 | 74.0 | 66.9 | 65.1 | 65.1 | 66.8 | | |

- For GFortran: O2 is worse (6%), O3 no-sve is the best
- For ACfl: O3 no-sve is the worst (5%), O2/03/O3 no-sve are identical and the best
- > ACfl is using active waiting counted as activity while GFortran is using passive waiting counted as inactivity
- > GFortran is better than ACfl: 6%
- For both compilers and options: a large amount of time is spent in loops



Compiler flags impact: GFortran on AWS G4





Every compiler option is losing sometimes, winning at other times



GFortran on AWS G4: Some detailed analyses



17optcd function

Difference comes from a loop conditionally setting arrays values to zero

- no-sve option produces a scalar version taking ~25s
- Without excluding option, SVE version is taking ~90s

Multiple factors: scalar version can use dedicated instructions/registers when comparing/setting with zero whereas SVE instruction set lack such feature and requires to have every store instruction under predication

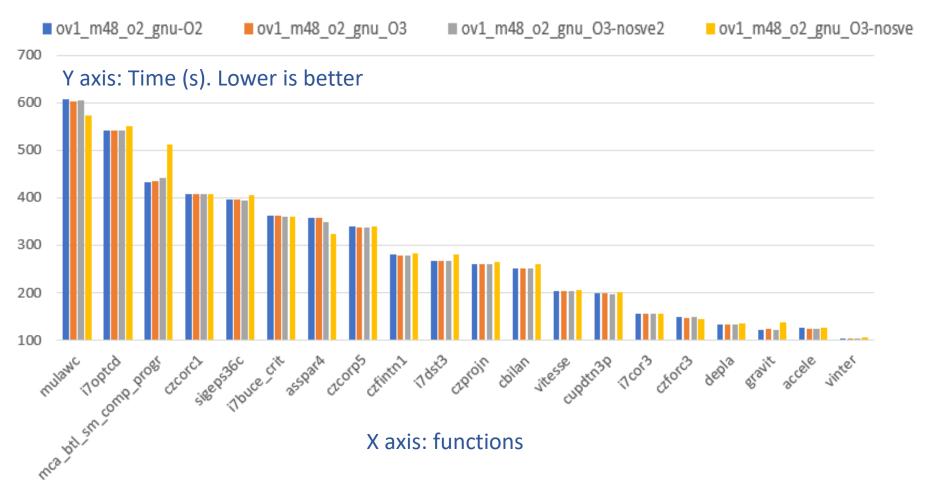
17bucecrit function

One of the loop is vectorized in NEON ONLY if SVE is disabled Bug/Cost model?



Compiler flags impact: ACfl on AWS G4



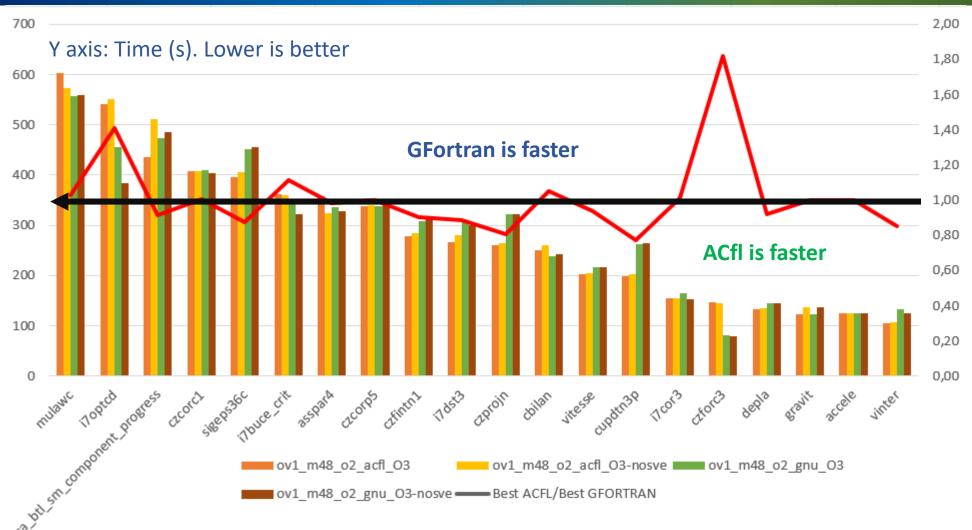


O3 no-sve is the compiler option with the largest impact (positive or negative!)



Best ACfl/best GFortran on AWS G4





Red Curve is Best ACfl time / Best GFortran time: greater than 1 means ACfl is slower, lower than 1 means GFortran is slower



Compiler Analysis of OpenRadiOss



- 1) Fine tuning compiler options: up to 5% performance gain
- 2) Fine tuning across compiler and compiler options: up to 10% performance gain

Future work



- > Analyze more compiler options: fastmath, funroll, etc....
- Automate backport from one compiler to the other: pragma insertion: if a compiler has been able to vectorize a loop, the information could be provided through pragmas to compilers which were unsuccessful in vectorizing the same loop.
- > Interact with compiler developers to refine/improve cost models
- > Interact with application developers to use this technology





CONCLUSIONS



Conclusions



- Non uniform behavior of compiler options across subroutines/loops: some options perform better with some subroutines
- Non uniform behavior between compilers across subroutines/loops: no silver bullet compiler....
- Non uniform means non negligible performance difference: these performance difference are worth exploring/exploiting

Above all of these are well known "generic facts"



Conclusions



- Non uniform behavior of compiler options across subroutines/loops: some options perform better with some subroutines
- Non uniform behavior between compilers across subroutines/loops: no silver bullet compiler....
- Non uniform means non negligible performance difference: these performance difference are worth exploring/exploiting

Above all of these are well known "generic facts" but MAQAO/QaaS allows to bring in:

- Quantitative estimation : essential for driving optimization
- Explanation of performance differences: this opens the door to backport optimization between compilers





Performance Optimisation and Productivity 3

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Backup Results



A FEW SPECIFIC MAQAO METRICS (1)



First, most of our dynamic measurements are based on sampling.

We distinguish and measure for every thread two types of wasted time

- Inactive time (obtained by comparing wall clock with active time = sum of collected samples)
- Time spent in OpenMP, MPI, Pthreads activity

With these measurements we generate 4 essential metrics:

- Average active time: Sum over all threads of their active time divided by thread count.
 IDEAL = total execution time
- Activity ratio: Sum over all threads of their active time divided by the sum of their wall time. IDEAL: 100%
- 3. Average active number of threads: Sum over all threads of their active time divided by longest wall clock time: IDEAL = number of threads used
- 4. Affinity stability: evaluates percentage of time spent without thread migration between physical cores: IDEAL 100%



A FEW SPECIFIC MAQAO METRICS (2)



For each thread, we gather a full picture of their activity: time spent in various functions including time spent in various libraries: OpenMP, MPI and Pthreads.

From these measurements we extrapolate impact of time spent in OpenMP/MPI/Pthread libraries and load distribution.

Perfect OpenMP + MPI + Pthread: max (Original Thread time)/ max (Stripped Thread Time): Stripped ⇔ time spent in OpenMP/MPI/Pthread set to 0.

Perfect OpenMP + MPI + Pthread + Perfect Load Distribution: max (Original Thread time)/ average (Stripped Thread Time):

A performance optimization goal is to have these 2 metrics under 1.1.





OpenMP Results





Backup Slides



G4 NEONM11 runs: 1 MPI Rank, 96 OpenMP threads, ACFL -O3 (1/3)

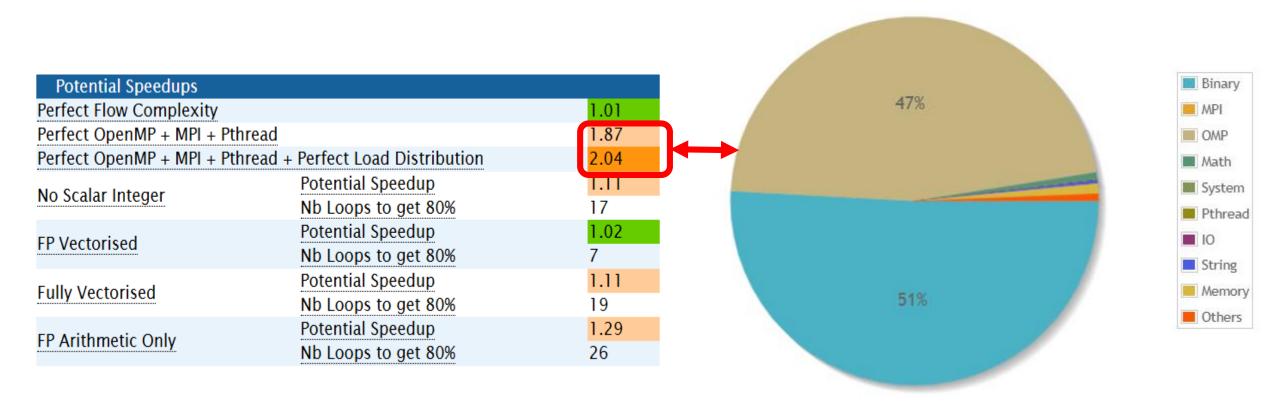


| Global Metrics | ? | Large gap indicates a large | |
|--------------------------------------|--------------------------------------|---|--|
| Total Time (s) | 3.90 E3 | amount of thread inactive time amount of thread inactive time | |
| Max (Thread Active Time) (s) | 2.82 E3 | amount of thread mactive time | |
| Average Active Time (s) | 2.59 E3 | | |
| Activity Ratio (%) | 66.4 | Low numbers: poor resource usage | |
| Average number of active threads | rage number of active threads 63.729 | | |
| Affinity Stability (%) | 100.0 | | |
| Time in analyzed loops (%) | 48.0 | | |
| Time in analyzed innermost loops (%) | 40.6 | | |
| Time in user code (%) | 50.9 | | |
| Compilation Options Score (%) | 100 | | |
| Array Access Efficiency (%) | 73.6 | | |

https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/OpenRadioss_NEON1M11-full_G4-aws_o96_m1_acfl-o3/index.html



G4 NEONM11 runs: 1 MPI Rank, 96 OpenMP threads, ACFL -O3 (2/3)





G4 NEONM11 runs: 1 MPI Rank, 96 OpenMP threads, ACFL - O3 (3/3)



| Name | Module | Coverage mpi 1_rank_omp_96_threads (% | Nb Threads 6) mpi_1_rank_omp_96_threads |
|---|--------------------------|--|--|
| aarch64_cas4_acq_rel | libomp.so | 14.96 | 96 |
| intkmp_dispatch_next_algorithm<int>(int, dispatch_priv ate_info_template<int>*, dispatch_shared_info_template<int> volatile*, int*, int*, int*, traits_t<int>::signed_t*, int, int)</int></int></int></int> | libomp.so | 14.21 | 96 |
| kmp_wait_4 | libomp.so | 7.74 | 96 |
| aarch64_ldadd4_acq_rel | libomp.so | 7.28 | 96 |
| ► asspar4 | engine_iinuxao 4_ompi | 6.63 | 96 |
| ► mulawc | engine_linuxa6 4_ompi | 6.56 | 96 |
| ► i7buce_crit | engine_linuxa6 4_ompi | 5.12 | 96 |
| ► m2cplr | engine_linuxa6 4_ompi | 3.95 | 96 |
| ► cupdt3p | engine_linuxa6 4 ompi | 3.26 | 96 |

MAIN ISSUES

- critical section (OMP CRITICAL) in i7buce_crit
- locks (OMP_SET_LOCK) mostly from i7optcd (lockon.inc:28)

https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/OpenRadioss_NEON1M11-full_G4-aws_o96_m1_acfl-o3/fcts_and_loops.html



MPI Results



G4 NEONM11 runs: 96 MPI Ranks, 1 OpenMP threads, ACFL – O3 (1/3)



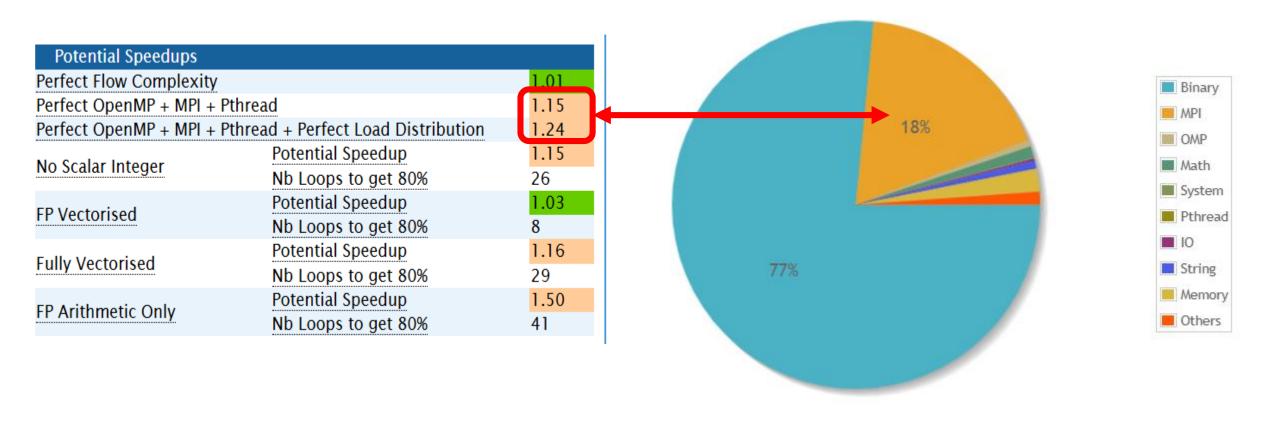
| Global Metrics | | |
|--------------------------------------|-------------------------------|------|
| Total Time (s) | 1.71 E3 Small gap indicates a | sma |
| Max (Thread Active Time) (s) | 1.63 E3 amount of thread inac | |
| Average Active Time (s) | 1.61.F3 | |
| Activity Ratio (%) | 93.7 High numbers: good re | esou |
| Average number of active threads | 90.878 usage | |
| Affinity Stability (%) | 98.9 | |
| Time in analyzed loops (%) | 71.3 | |
| Time in analyzed innermost loops (%) | 63.7 | |
| Time in user code (%) | 76.5 | |
| Compilation Options Score (%) | 100 | |
| Array Access Efficiency (%) | 73.4 | |

https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/OpenRadioss_NEON1M11-full_G4aws_o1_m96_acfl-o3/



G4 NEONM11 runs: 96 MPI Ranks, 1 OpenMP threads, ACFL – O3 (2/3)





https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/OpenRadioss_NEON1M11-full_G4-aws_o1_m96_acfl-o3/



G4 NEONM11 runs: 96 MPI Ranks, 1 OpenMP threads, ACFL – O3 (3/3)



| Name | Module | Coverage mpi_96_ranks_omp_1_thread (%) | Nb Threads mpi_96_ranks_omp_1_thread |
|---|---------------------------|--|---|
| mca_btl_sm_component_progress | libopen-pal. so.80.0.5 | 13.09 | 96 |
| ► mulawc | engine_linu xa64_ompi | 10.79 | 96 |
| ► asspar4 | engine_linu xa64_ompi | 7.57 | 96 |
| ► m2cplr | engine_linu xa64_ompi | 6.62 | 96 |
| ► cupdt3p | engine_linu xa64_ompi | 5.41 | 96 |
| ► chvis3 | engine_linu xa64_ompi | 4.65 | 96 |

https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/OpenRadioss_NEON1M11-full_G4-aws_o1_m96_acflo3/fcts_and_loops.html



AMPERE SKYCAB runs: 80/160/3220/640 MPI Ranks, 1 OpenMP threads, ACFL – O3 (1/2)



| Global Metrics | | | | | | | | | |
|--------------------------------------|---------|---------|---------|---------|--|--|--|--|--|
| Metric | r0 | r1 | r2 | r3 | | | | | |
| Total Time (s) | 3.76 E3 | 1.93 E3 | 1.04 E3 | 585.62 | | | | | |
| Max (Thread Active Time) (s) | 3.74 E3 | 1.92 E3 | 1.02 E3 | 575.77 | | | | | |
| Average Active Time (s) | 3./3 E3 | 1.91 E3 | 1.02 E3 | 569.99 | | | | | |
| Activity Ratio (%) | 99.3 | 99.0 | 98.0 | 97.3 | | | | | |
| Average number of active threads | 79.451 | 158.408 | 313.725 | 622.917 | | | | | |
| Affinity Stability (%) | 0.89 | 0.97 | 1.39 | 1.14 | | | | | |
| Time in analyzed loops (%) | 82.4 | 78.6 | 74.5 | 68.7 | | | | | |
| Time in analyzed innermost loops (%) | 79.4 | 75.6 | 71.4 | 65.1 | | | | | |
| Time in user code (%) | 86.9 | 83.0 | 78.8 | 72.9 | | | | | |
| Compilation Options Score (%) | 0 | 0 | 0 | 0 | | | | | |
| Array Access Efficiency (%) | 69.9 | 70.6 | 68.4 | 71.1 | | | | | |

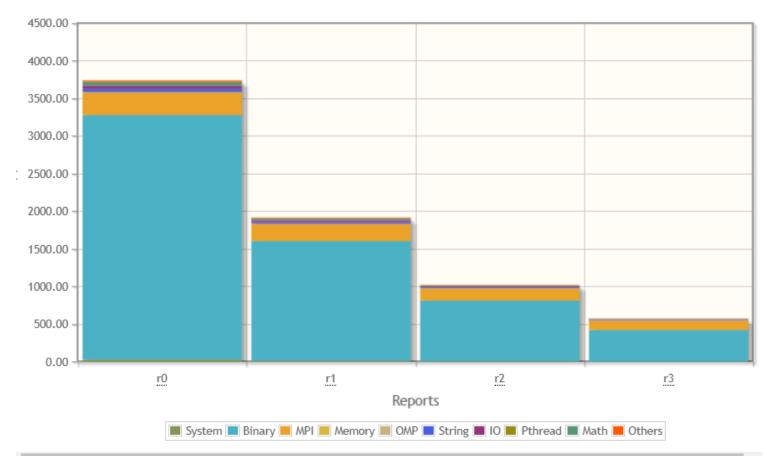
r0: 1 node (80 cores), r1: 2 nodes (160 cores), r2 (320 cores), r3 (640 cores)

https://datafront.exascale-computing.eu/public/OpenRadioss/compare/OpenRadioss_SkyCAB_turpan_o3_o1_m80-640_acfl_compare/



AMPERE Skycab runs: 80/160/320/640MPI Ranks, 1 OpenMP threads, ACFL - O3 (2/2)





r0:1 node (80 cores),

r1: 2 nodes (160 cores),

r2:4 nodes (320 cores),

r3:8 nodes (640 cores)

https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/OpenRadioss_NEON1M11-full_G4-aws_o1_m96_acfl-o3/fcts_and_loops.html

G4 NEONM11 runs: hybrid, ACFL – O3 (1/2)



| Global Metrics | | | | | | | | | |
|--------------------------------------|------------|------------|------------|------------|------------|------------|------------|------------|--|
| Metric | r0 | <u>r1</u> | r2 | r3 | r4 | r5 | r6 | <u>r7</u> | |
| Total Time (s) | 1.71 E3 | 1.75 E3 | 1.78 E3 | 2.01 E3 | 2.07 E3 | 2.48 E3 | 2.86 E3 | 3.90 E3 | |
| Max (Thread Active Time) (s) | 1.63 E3 | 1.61 E3 | 1.55 E3 | 1.66 E3 | 1.68 E3 | 1.89 E3 | 2.12 E3 | 2.82 E3 | |
| Average Active Time (s) | 1.61 E3 | 1.45 E3 | 1.37 E3 | 1.37 E3 | 1.40 E3 | 1.50 E3 | 1.73 E3 | 2.59 E3 | |
| Activity Ratio (%) | 93.7 | 82.6 | 77.5 | 68.2 | 67.6 | 60.5 | 60.7 | 66.4 | |
| Average number of active threads | 90.878 | 79.247 | 74.324 | 65.388 | 64.901 | 58.014 | 58.206 | 63.729 | |
| Affinity Stability (%) | 98.9 | 99.9 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | |
| Time in analyzed loops (%) | 71.3 | 79.1 | 83.1 | 83.3 | 82.5 | 78.5 | 68.0 | 48.0 | |
| Time in analyzed innermost loops (%) | 63.7 | 70.4 | 73.5 | 71.9 | 71.0 | 66.6 | 57.9 | 40.6 | |
| Time in user code (%) | 76.5 | 84.7 | 88.7 | 88.6 | 87.7 | 83.3 | 72.2 | 50.9 | |
| Compilation Options Score (%) | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | |
| Array Access Efficiency (%) | 73.4 | 74.2 | 74.3 | 75.1 | 74.9 | 75.1 | 74.9 | 73.6 | |

- r0: ov1_n1m_m96-o1_o3_acfl
- rl: ov1_n1m_m48-o2_o3_acfl
- r2: ov1_n1m_m24-o4_o3_acfl
- r3: ov1_n1m_m12-o8_o3_acfl
- r4: ov1_n1m_m8-o12_o3_acfl
- r5: ov1_n1m_m4-o24_o3_acfl
- r6: ov1_n1m_m2-o48_o3_acfl
- r7: ov1_n1m_m1-o96_o3_acfl

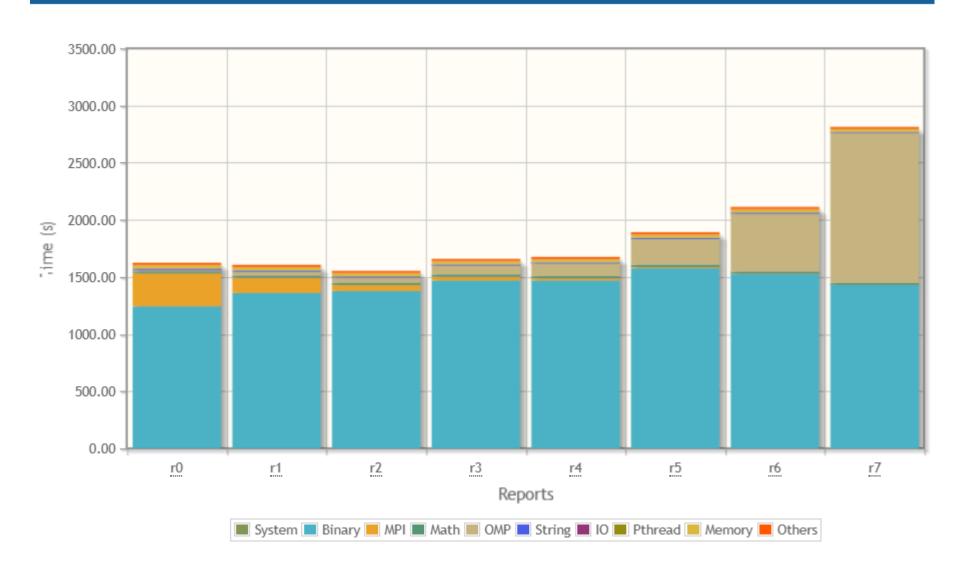
https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/OpenRadioss_NEON1M11-full_G4-aws_cr_o1-96_m96-1_acfl-o3/



G4 NEONM11 runs: hybrid, ACFL – O3 (2/2)



Time



- r0: ov1_n1m_m96-o1_o3_acfl
- r1: ov1_n1m_m48-o2_o3_acfl
- r2: ov1_n1m_m24-o4_o3_acfl
- r3: ov1_n1m_m12-o8_o3_acfl
- r4: ov1_n1m_m8-o12_o3_acfl
- r5: ov1_n1m_m4-o24_o3_acfl
- r6: ov1_n1m_m2-o48_o3_acfl
- r7: ov1_n1m_m1-o96_o3_acfl



G4 NEONM11 runs: hybrid, 8 MPI ranks, 12 OMP threads ACFL – O3 (1/2)



| Global Metrics | • |
|--------------------------------------|---------|
| Total Time (s) | 2.08 E3 |
| Max (Thread Active Time) (s) | 1.67 E3 |
| Average Active Time (s) | 1.40 E3 |
| Activity Ratio (%) | 67.2 |
| Average number of active threads | 64.434 |
| Affinity Stability (%) | 100.0 |
| Time in analyzed loops (%) | 82.5 |
| Time in analyzed innermost loops (%) | 70.9 |
| Time in user code (%) | 87.7 |
| Compilation Options Score (%) | 100 |
| Array Access Efficiency (%) | 75.2 |

https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/EO_OpenRadioss_NEON1M11-full_G4-aws_o12_m8_acfl-o3/index.html

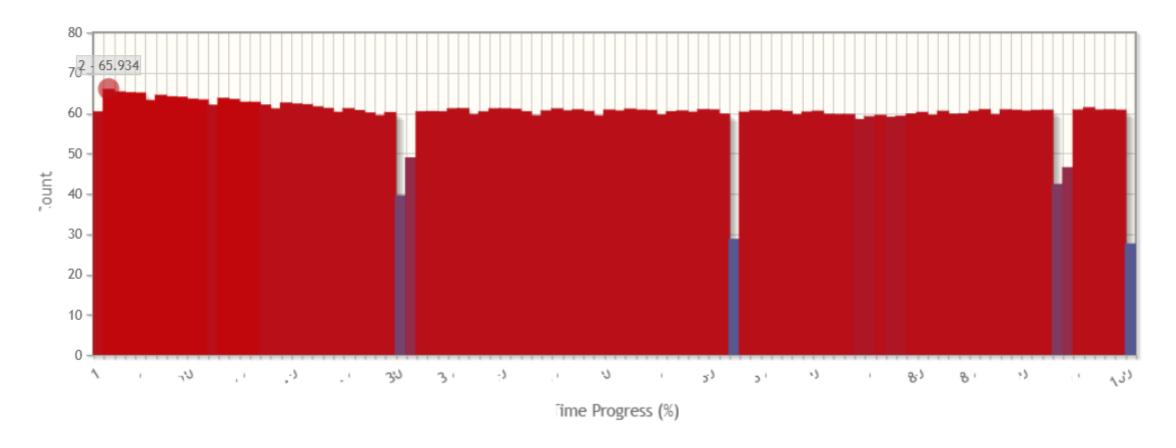


G4 NEONM11 runs: hybrid, 8 MPI ranks, 12 OMP threads ACFL – O3 (2/2)



Average Active Threads Count





https://datafront.exascale-computing.eu/public/OpenRadioss/NEON1M11/G4_AWS/acfl/EO_OpenRadioss_NEON1M11-full_G4-aws_o12_m8_acfl-o3/index.html



G4 TAURUS runs: hybrid, ACFL – O3 (1/2)



| Global Metrics | | | | • |
|---|---------|---------|---------|---------|
| Metric | r0 | r1 | r2 | r3 |
| Total Time (s) | 7.96 E3 | 7.96 E3 | 8.27 E3 | 8.84 E3 |
| Max (Thread Active Time) (s) | 7.93 E3 | 7.91 E3 | 8.22 E3 | 8.73 E3 |
| Average Active Time (s) | 7.83 E3 | 7.79 E3 | 8.04 E3 | 8.44 E3 |
| Activity Ratio (%) | 98.5 | 98.0 | 97.2 | 95.6 |
| Average number of active threads | 95.506 | 93.990 | 93.282 | 91.635 |
| Affinity Stability (%) | 0.42 | 0.12 | 0.07 | 0.06 |
| Time in analyzed loops (%) | 76.3 | 77.6 | 75.9 | 72.5 |
| Time in analyzed innermost loops (%) | 69.6 | 71.1 | 69.7 | 66.4 |
| Time in user code (%) | 79.2 | 80.4 | 78.6 | 75.0 |
| Compilation Options Score (%) | 99.5 | 99.5 | 99.5 | 99.5 |
| Array Access Efficiency (%) | 65.3 | 65.2 | 65.0 | 64.8 |

- r0: mpi_96_omp_1_thread
- r1: mpi_48_omp_2_threads
- r2: mpi_24_omp_4_threads
- r3: mpi_12_omp_8_threads

https://datafront.exascale-computing.eu/public/OpenRadioss/TAURUS10M/G4_AWS/acfl/OpenRadioss_TAURUS10M-short_g4-aws_o1-8_m12-96_acfl_engine/



G4 TAURUS runs: hybrid, ACFL – O3 (2/2)





- r0: mpi_96_omp_1_thread
- r1: mpi_48_omp_2_threads
- r2: mpi_24_omp_4_threads
- r3: mpi_12_omp_8_threads



GLOBAL CHARACTERISTICS TAURUS ACFL -O3 ON G4 (2)



| Loop id | Source Location | Source Function | Level | Exclusive Coverage mpi_48_ranks_omp_2_threads (%) | Vectorization Ratio (%) | Vector Length Use (%) |
|------------|---|-----------------|-----------|--|----------------------------|-----------------------------|
| 12/36 | proj.F:1205-1462 [] | czprojn | Single | 4.32 | 4.82 | 52.33 |
| 6583 | engine_linuxa64_gf_ompi - ass par4.F:172-172 | asspar4 | Innermost | 3.88 | 100 | 100 |
| 11257 | engine_linuxa64_gf_ompi - cu pdtn3.F:637-690 [] | cupdtn3p | Innermost | 3.50 | 40.68 | 70.34 |
| | engine_linuxa64_gf_ompi - i7o ptcd.F:200-233 [] | | Innermost | 2.64 | 0 | 45.54 |
| 30830 | engine_linuxa64_gf_ompi - i7b uce_crit.F:133-147 | i7buce_crit | Innermost | 2.01 | 6.25 | 52.6 |
| 6602 | pia.F:95-103 | depla | Innermost | 1.96 | 50 | 75 |
| | VIT.F:157-159 | - | Innermost | 1.91 | 0 | 46.83 |
| 6883 | engine_linuxa64_gf_ompi - vit esse.F:80-85 | vitesse | Innermost | 1.63 | 41.67 | 75 |
| 23947 | engine_linuxa64_gf_ompi - i7c or3.F:127-176 | i7cor3 | Innermost | 1.61 | 12.04 | 52.19 |
| | engine_linuxa64_gf_ompi - czf intn.F:355-445 | | Innermost | 1.54 | 100 | 100 |
| 30835 | engine_linuxa64_gf_ompi - i7b uce_crit.F:155-169 | i7buce_crit | Innermost | 1.44 | 6.52 | 39.67 |
| 30856 | engine_linuxa64_gf_ompi - i7o ptcd.F:200-238 | i7optcd | InBetween | 1.37 | 0 | 48.03 |
| | engine_linuxa64_gf_ompi - cbi lan.F:111-152 | cbilan | Single | 1.33 | 18.03 | 59.02 |
| 6887 | engine_linuxa64_gf_ompi - vit | vitassa | Innermost | 1 29 | 41.67 | 75 |

https://datafront.exascale-computing.eu/public/OpenRadioss/TAURUS10M/G4_AWS/gnu/OpenRadioss_TAURUS10M-short_g4-aws_o2_m48_gnu_engine/



LAMMPS on Graviton 3 (64 cores) AWS: Armclang versus GCC



| | | mcpu=neoverse- v1 -armpl -ffast- | ARMCLANG 2 - 03 - mcpu=neoverse- v1 -armpl -msve- vector-bits=256 - ffast-math | v1 +nosve+nosve2 - armpl -ffast- | v1 -armpl -fno- | mcpu=neover se-v1 -armpl - | GCC1 -O3 - mcpu=neovers e-v1 -larmpl - funroll-loops - ffast-math | | se-v1 -larmpl - msve-vector- bits=128 - | se- v1+nosve+no sve2 -larmpl - | se-v1 -larmpl - | se-v1 -larmpl - funroll-loops - ffast-math |
|-------------------------------|---------------------|-------------------------------------|---|--|-----------------|-------------------------------|---|--------|---|--------------------------------------|-----------------|--|
| Me | etric | ARMCLANG 1 | ARMCLANG 2 | ARMCLANG 4 | ARMCLANG 5 | ARMCLANG 6 | GCC 1 | GCC 2 | GCC 3 | GCC 4 | GCC 5 | GCC 6 |
| Total 1 | Time (s) | 420,57 | 422,54 | 423,42 | 430,12 | 421,46 | 434,58 | 433,02 | 433,38 | 434,74 | 432,86 | 440,65 |
| В | est | 1,00 | 1,00 | 1,01 | 1,02 | 1,00 | 1,03 | 1,03 | 1,03 | 1,03 | 1,03 | 1,05 |
| Max (Thread A | Active Time) (s) | 418,66 | 420,65 | 421,57 | 428,29 | 419,53 | 432,68 | 431,32 | 431,52 | 432,7 | 431,22 | 438,59 |
| Average Ac | tive Time (s) | 418,43 | 420,29 | 421,23 | 427,84 | 419,19 | 432,35 | 430,79 | 431,13 | 432,43 | 430,67 | 438,33 |
| Activity | Ratio (%) | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 | 99,5 |
| Average number | r of active threads | 63,67 | 63,66 | 63,67 | 63,66 | 63,66 | 63,67 | 63,67 | 63,67 | 63,66 | 63,68 | 63,66 |
| Affinity S | tability (%) | 99,9 | 100 | 99,9 | 100 | 99,9 | 99,9 | 100 | 100 | 99,9 | 100 | 99,9 |
| Time in analy | yzed loops (%) | 97,8 | 97,9 | 97,7 | 97,7 | 97,9 | 97,7 | 97,9 | 97,8 | 97,8 | 97,7 | 97,8 |
| ime in analyzed i | nnermost loops (% | 65,7 | 65,6 | 65,3 | 94,5 | 65,8 | 84,2 | 84,6 | 84,6 | 84,5 | 84,4 | 85,3 |
| Time in us | er code (%) | 98,1 | 98,2 | 97,9 | 98,1 | 98,2 | 98 | 98,1 | 98 | 98 | 98 | 98 |
| Compilation Options Score (%) | | 100 | 100 | 100 | 100 | 87,5 | 100 | 100 | 100 | 100 | 100 | 87,5 |
| Array Access | Efficiency (%) | 62,5 | 62,6 | 63 | 44,5 | 61,5 | 44,3 | 44,3 | 44,3 | 44,3 | 44,3 | 44,5 |
| | | | | | | | | | | | | |

BEST: TIMING RATIOS: current timing over best timing across all compilers and compiler options.

- Green cells corresponds to best or very close to best (< 1%)
- Yellow cells correspond to performance losses < 3%
- Red cells correspond to performance losses > 3%



Hardware/Software platforms



| Model Name | Frequency (GHz) | Number of cores/socket | | L1D (KB) | L1I (KB) | L2 (KB) | L3 (MB) | L3/Core (MB) |
|--|--------------------|------------------------|---|-------------|-------------|------------|------------|-----------------|
| Neoverse N1 Ampere ALTRA Q80-30 (CALMIP) | 3 | 80 | 1 | 64 | 64 | 1024 | 32 | 0,40 |
| Neoverse V1 G3E (AWS) | 2,6 | 64 | 1 | 64 | 64 | 1024 | 32 | 0,50 |
| Neoverse V2 G4 (AWS) | 2,8 | 96 | 1 | 64 | 64 | 2048 | 36 | 0,38 |

Neoverse N1: Arm C/C++/Fortran Compiler version 22.1 (build number 12) (based on LLVM 13.0.1)

Neoverse V1/V2: ACfL 24.10, GNU Fortran2008 13.2.0

Compiler options: O2, O3, O3 + no-sve, O3 + no-sve2

TALK FOCUS: AWS Graviton 4 Results

