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Impact of different compilers and build types on Geant4 simulation execution time

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Motivation

- Currently**, Monte Carlo detector simulation at LHC** can occupy up to **40 %** of World Wide LHC computing grid's resources. This percentage is set to grow when LHC luminosity will be further increased.

- It is necessary to find a new approach for improving the execution time of simulations without sacrificing the quality of simulated data.

- The purpose of this preliminary study is to investigate how to **reduce the Geant4 simulation execution time**.

- This is achieved by running **standalone Geant4 simulations**, whose performance can then be evaluated independently from other libraries and control frameworks.

Method

Several factors can have an impact on the compilation process:

- **Static linking** is expected to lead to a **faster execution**, and will be compared here to the traditional dynamic linking.

- Compiler **optimization**. Machine code can be optimized by:
    1. avoiding redundancy (reuse instead of recompute data);
    2. reducing amount of code to fit as much as possible into CPU cache;
    3. preferring sequential code instead of many jumps, parallelizing as much as possible (e.g. loops), etc.

- Compiler **version**.

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Method

- As a benchmark, **standalone G4 simulation** with two different geometries (from A. Dotti [1]) has been used. **50 GeV pions** are used as source particles. The number of simulated primaries varies according to the detector geometry.

- Compiled G4 (version 10.5) both **statically** and **dynamically**.

- Three versions of the GCC compiler, namely **4.8.5, 6.2.0 and 8.2.0**, have been used for these investigations.

- A comparison between four GCC optimization levels (**Os, O1, O2 and O3**) have also been performed. The default level used by most build systems is -O2 and it will be used as reference.

- The computations were carried out on **a standalone machine at CERN IT** and on **a university cluster** in Lund.

- CPU and memory resources on both machines (standalone and cluster) were **exclusively allocated** to the simulations and not shared with any concurrent process other than the minimum OS tasks.

[1] https://gitlab.cern.ch/adotti/Geant4HepExpMTBenchmark

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Computing resources

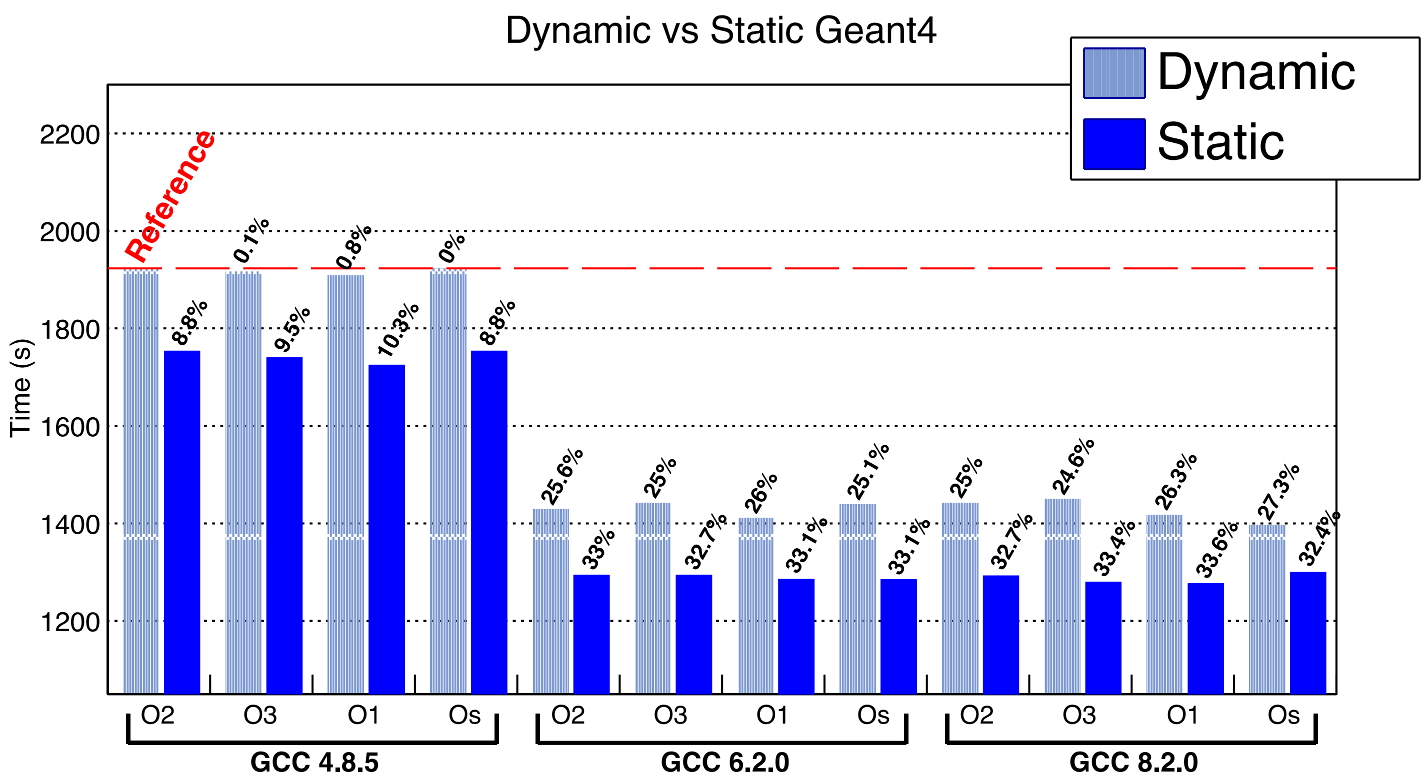
CERN standalone machine

- CPU: Intel Xeon E5-2630 v3 2.40GHz
- 16 cores / 32 threads
- 20 MB Cache (L1: 64 KB, L2: 256 KB, L3: 20 MB)
- 64 GB RAM
- Filesystem: XFS
- Operating System: CentOS 7

Compute node on Lund University cluster

- CPU: Intel Xeon E5-2650 v3 2.30GHz
- 10 cores / 20 threads
- 25 MB Cache (L1: 64 KB, L2: 256 KB, L3: 25 MB)
- 128 GB RAM
- Filesystem: IBM General Parallel File System (GPFS)
- Operating System: CentOS 7

Static vs dynamic performance with **full detector geometry**



- The computations were carried out **on CERN machine** considering 5000 initial events and using 4 threads. The computation was repeated 3 times for each configuration.
- The static approach, for all the GCC versions, reduces the execution time by more than **10%** in some cases.
- Regardless of the build approach, switching from GCC 4.8.5 to GCC 6.2.0 and GCC 8.2.0 results in an average of **30%** improvement in the execution time.
- A static build with GCC 8.2.0 leads to an improvement of almost **34%** with respect to the default configuration (GCC 4.8.5, dynamic, O2).
- The different GCC optimizations do not seem to have visible effects on the execution time.

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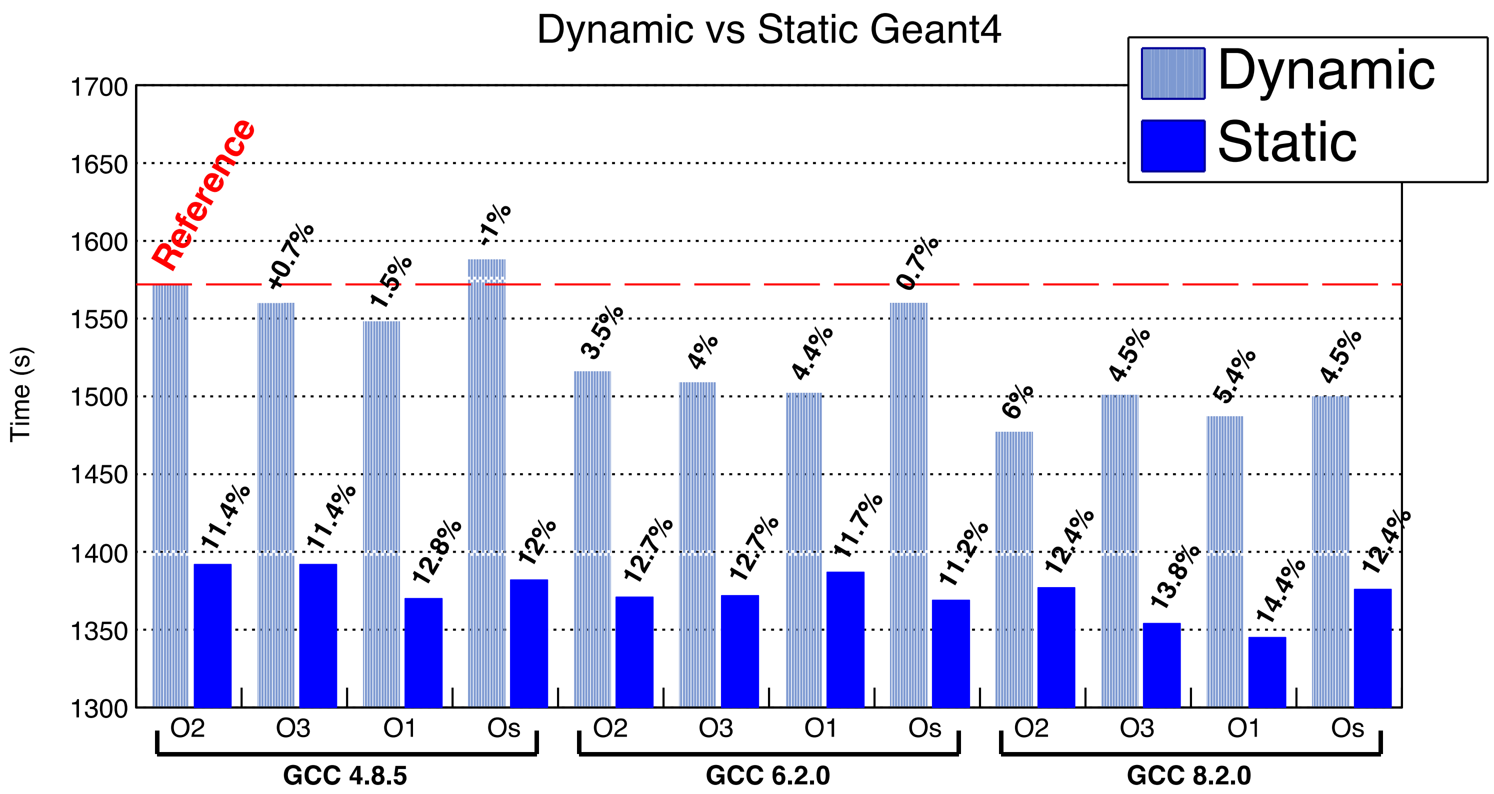
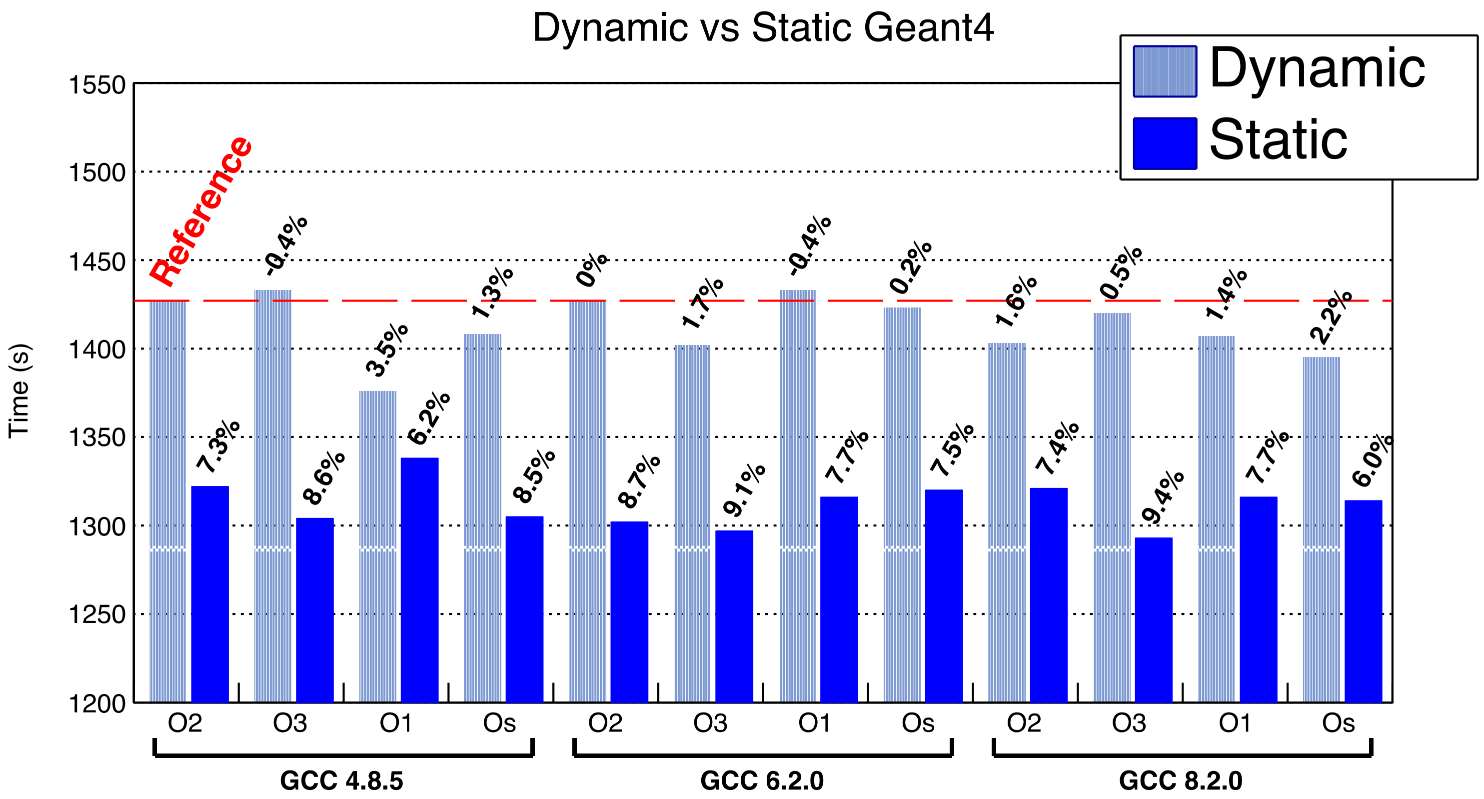
Static vs dynamic performance with **full detector geometry**



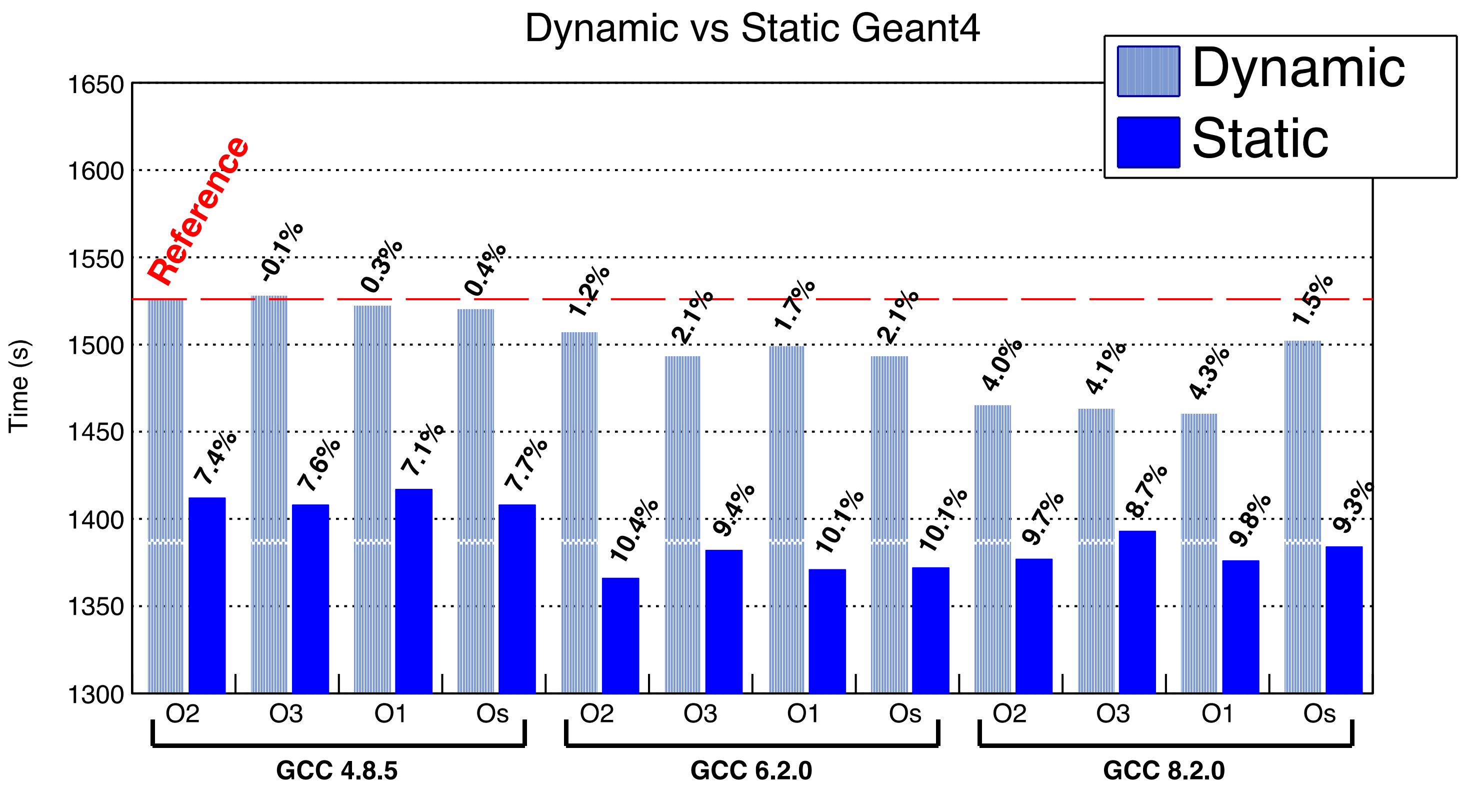
- The computations were performed on the **university cluster** considering 5000 initial events and using 4 threads. The computation was repeated 5 times for each configuration.
- The static approach allows a performance gain: it reduces the execution time by more than **10%** in some cases.
- The impact of different compilers is not relevant as in the previous case.

Static vs dynamic performance with **Inner Detector geometry**



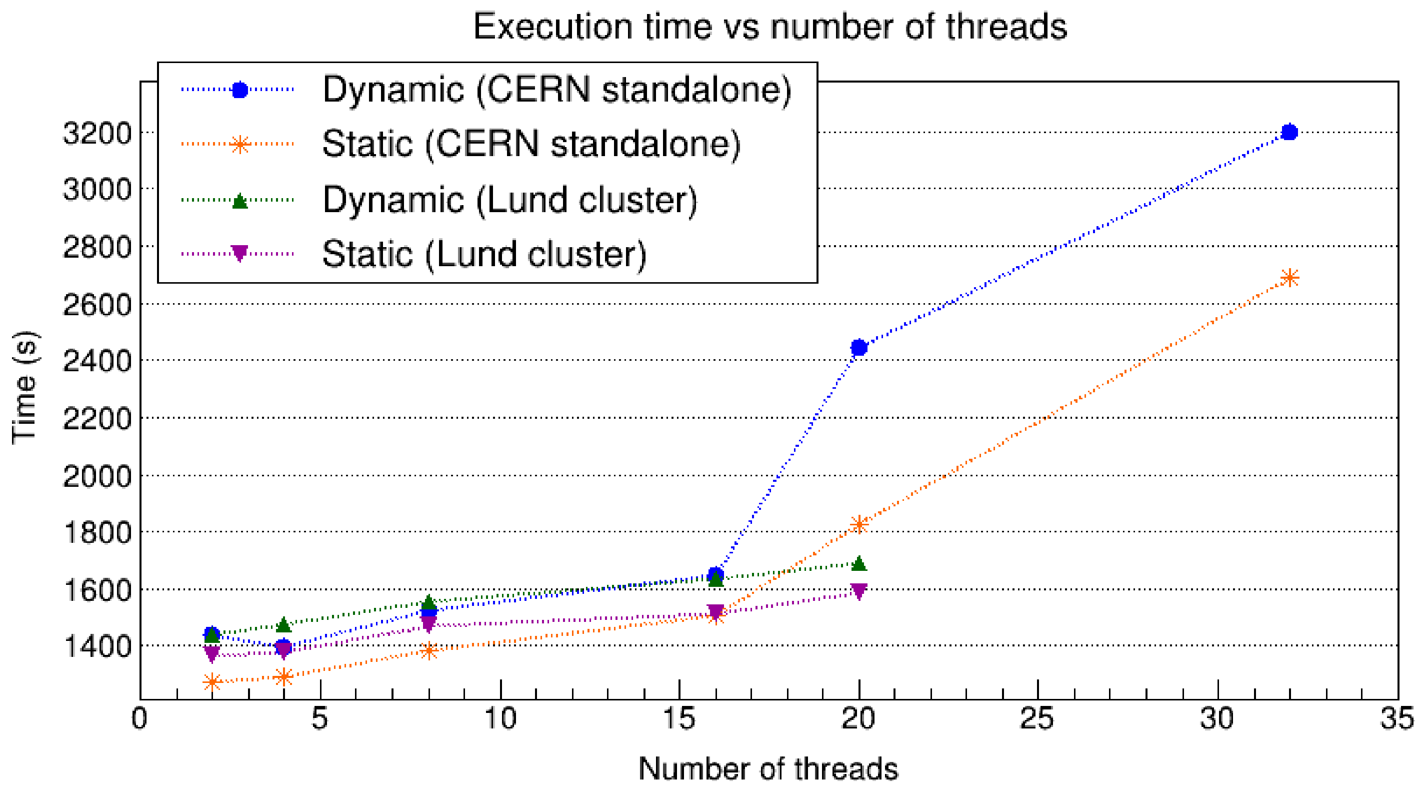
- The computations were carried out **on CERN machine** considering 50000 initial events and using 4 threads. The computation was repeated 3 times for each configuration.
- The static approach, for all the GCC versions, reduces the execution time by more than **9%** in some cases.
- The impact of different compilers is not relevant as in the full geometry case.
- The different GCC optimizations do not seem to have visible effects on the execution time.

Static vs dynamic performance with **Inner Detector geometry**



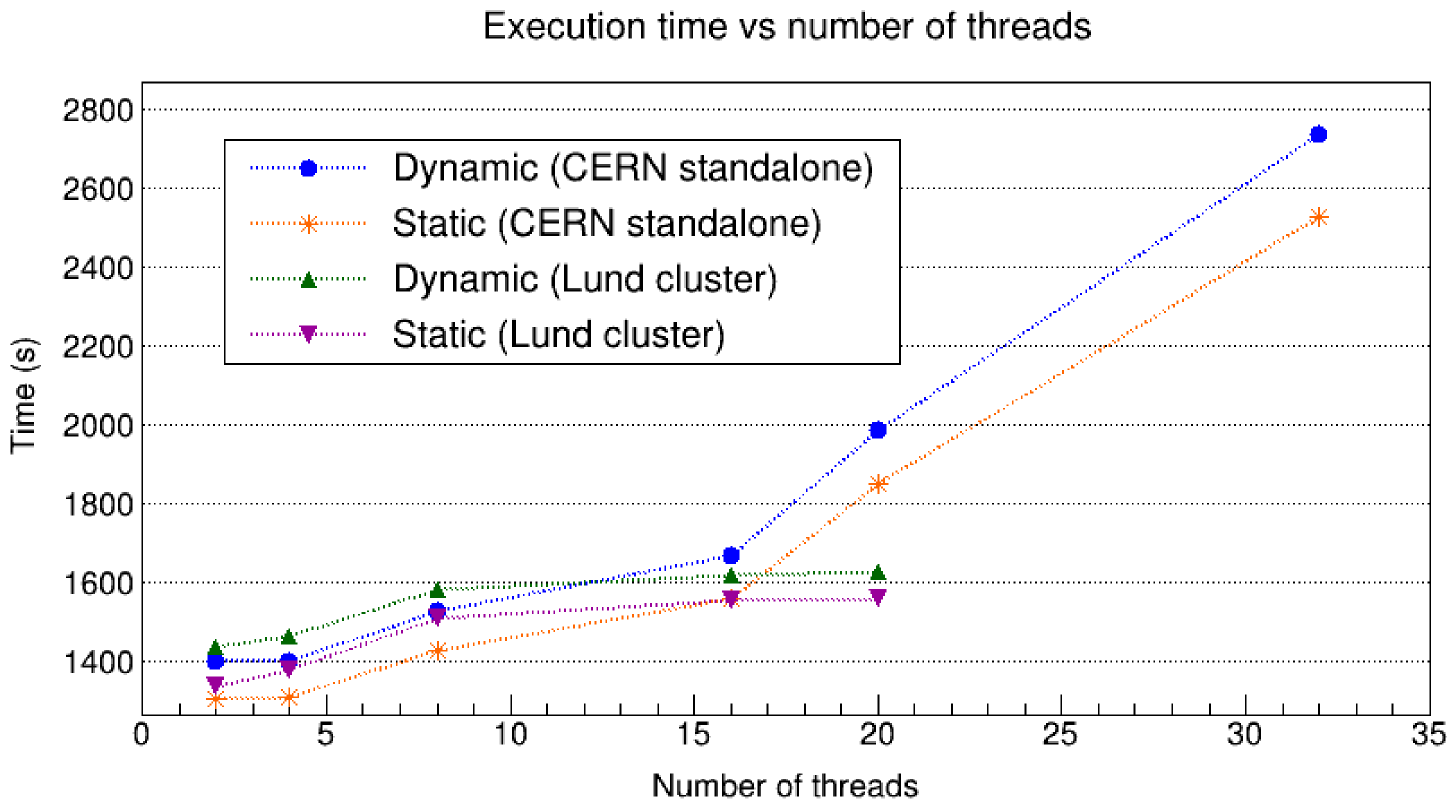
- The computations were performed on **the university cluster** considering 50000 initial events and using 4 threads. The computation was repeated 5 times for each configuration.
- The static approach allows a performance gain: it reduces the execution time by more than **10 %** in some cases.

Full detector geometry: execution time vs number of threads



- The number of events per thread has been set to 1250 events for each configuration. GCC 8.2.0 has been used.
- The improvement between static and dynamic linking is confirmed in all cases on both machines (standalone and cluster).

Inner detector geometry: execution time vs number of threads



- The number of events per thread has been set to 12500 events for each configuration. GCC 8.2.0 has been used.
- The improvement between static and dynamic linking is confirmed in all cases on both machines (standalone and cluster).

Future steps

- Perform measurements with other detector configurations (*in progress*).
- Perform measurements with different physics (consider different generated particles).
- Consider different compilers beyond GCC:
    1. clang *(in progress*);
    2. icc (intel);
    3. pgf (portland).
- Consider more advanced methods of compile-time optimization (e.g. link-time optimization (LTO)).
- GDML-based geometries, used for these studies, are not compatible with all the detector components. We need to adapt our benchmark simulation to support newer geometry definitions.

Conclusions

- Execution time for simulations based on Geant4 can be significantly improved by changing the default build method: linking Geant4 and its associated libraries statically can produce binaries that run even **10% faster**.

- Switching from gcc 4.8.5 to 8.2.0 results in a reduction of the execution time up to **25%**.

- Static libraries are embedded into the executable, resulting in a much larger size (~700 MB) than the corresponding dynamically-linked code (~ 2.5 MB).

- The different GCC optimizations do not seem to have visible effects on the execution time.

Thank you for your attention

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Optimization levels [Backup]

option	optimization level	execution time	code size	memory usage	compile time
-O0	optimization for compilation time (default)	+	+	-	-
-O1 or -O	optimization for code size and execution time	-	-	+	+
-O2	optimization more for code size and execution time	--		+	++
-O3	optimization more for code size and execution time	---		+	+++
-Os	optimization for code size		--		++
-Ofast	O3 with fast none accurate math calculations	---		+	+++

+increase ++increase more +++increase even more -reduce --reduce more ---reduce even more

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