ICSC

Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

BoGEMMS-HPC: development of Geant4 simulations in High-Performance Computing environments

ICSC and Spoke 2 - Where Are We Now?
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WP3.4 Flagship UC: Pipeline optimization for space and ground based experiments

- Collecting the requirements and efforts of four subtasks into pipeline frameworks for data simulation and analysis based on a selected ICSC infrastructure (e.g. data clouds, HPC);
- Building pipeline prototypes, which includes the definition of the technological solutions for the containerization, data and metadata management, pipeline tools and software repository and the selection of the target infrastructure (e.g. the INFN Cloud infrastructure). This activity will be performed in collaboration with WP 5, 6.

WP3.4 Flagship UC subtask: Pipeline for GEANT4 simulations in HPC environments, with the simulation of the NASA COSI Anti-Coincidence System (ACS) as a test case

- The goal of the project is applying new methodologies for multi-threading and multi-node computation in a pipeline for Geant4 simulations in HPC architectures while exploring new I/O interfaces (e.g. CAD geometries, databases). The pipeline will use the Bologna Geant4 Multi-Mission Simulator (BoGEMMS) as baseline simulation framework to validate the results and as starting point for the implementation of new HPC-oriented features.

  - **Members:**
    - **V. Fioretti (INAF, 3m/yr) - coordinator**
    - **A. Ciabattoni (ICSC PhD, UniBo & INAF)**

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BoGEMMS-HPC
(Bologna Geant4 Multi-Mission Simulator for HPC applications)

- Geant4 (Allison+ 2016) is an open-source C++ toolkit library for particle transport in Monte Carlo simulations
- **BoGEMMS** is a Geant4-based simulation project started at INAF OAS in 2010 (Bulgarelli+2012, Fioretti+2012, Fioretti+2014), with the aim of building an **Astronomy-oriented** multi-application simulation framework
- **BoGEMMS-HPC**, based on BoGEMMS, is being developed within the WP3 Flagship UC PIPELINE

NEW GENERAL FEATURES

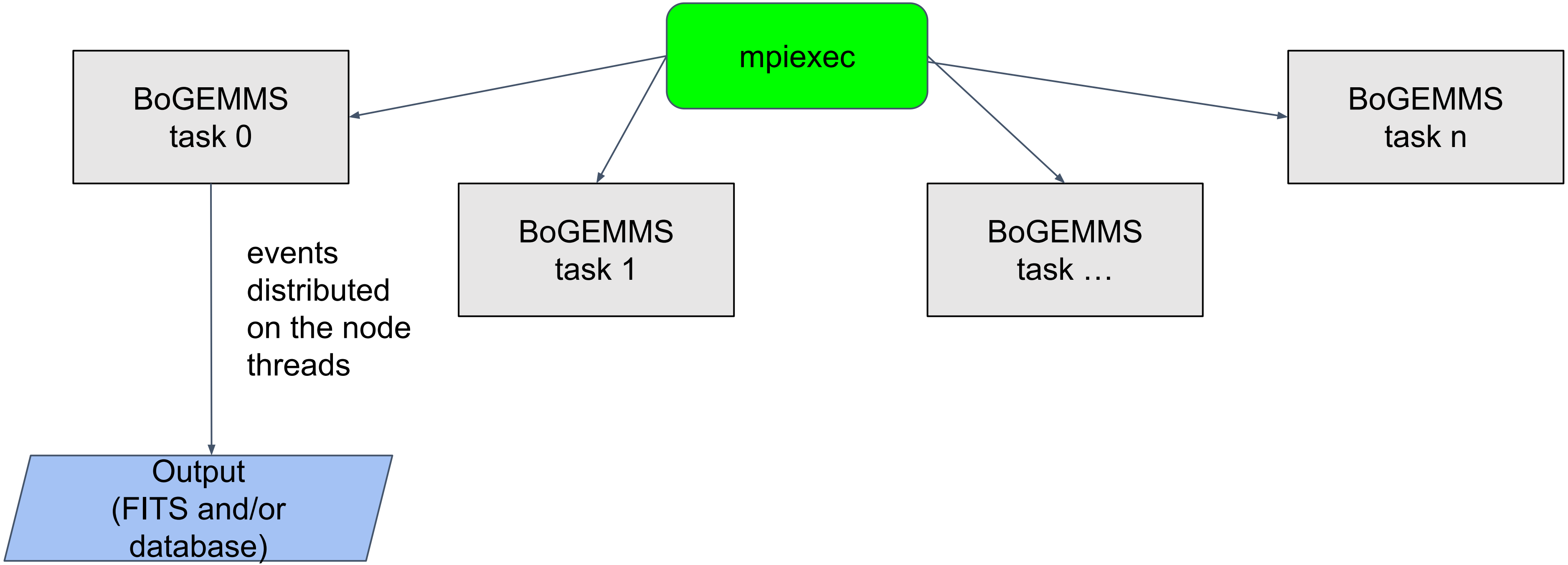
- Input interface: the user can simulate from a list of particles provided in ASCII, FITS, or ROOT format, in addition to the Geant4 standard inputs
- Output: an event list, with each row describing the particle interaction with selected sensitive volumes, is written using FITS file or **SQLite databases**
- Modularity: new geometry and physics classes can be added by the user without modifying the framework code
- Geometry: within the geometry classes the user can read CAD and GDML geometry files

BoGEMMS-HPC: NEW HPC FEATURES

- BoGEMMS-HPC supports the Geant4 multi-threading (MT) built-in feature that distributes each event on different threads
  - when a thread writes on FITS files **and SQLite***, the other threads are placed on hold
- BoGEMMS-HPC supports the G4-mpi library (K. Murakami (KEK)) for parallel computation, distributed by Geant4 but not included in the Geant4 installation
  - tested with open MPI
  - BoGEMMS-HPC runs independent applications (with separated output) on different nodes.

***SQLite can be safely used by multiple threads provided that no single database connection nor any object derived from database connection, such as a prepared statement, is used in two or more threads at the same time.**

BoGEMMS-HPC


mpiexec
BoGEMMS task 0
BoGEMMS task 1
BoGEMMS task …
BoGEMMS task n
events distributed on the node threads
Output (FITS and/or database)

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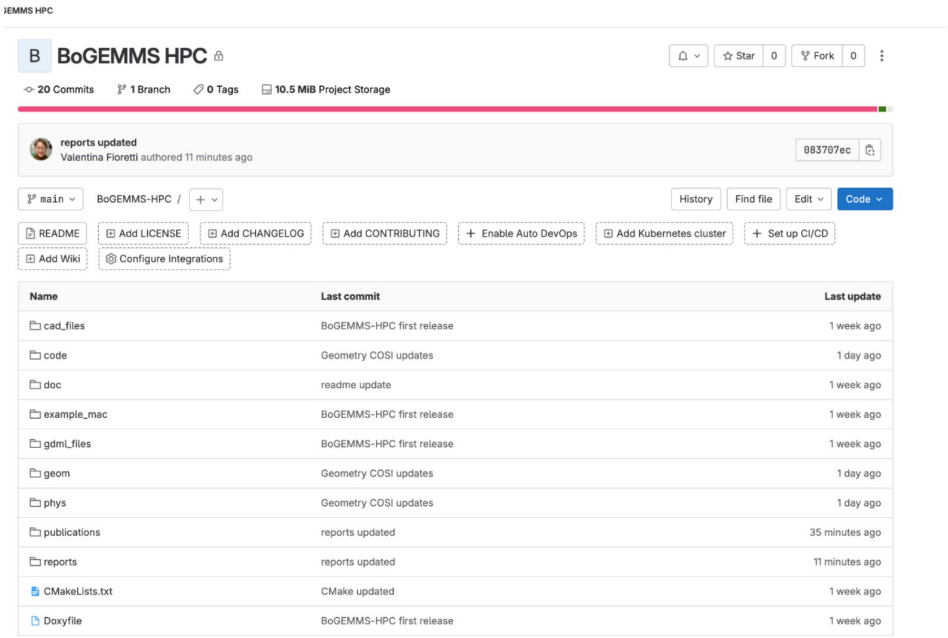
BoGEMMS-HPC repository

The first release of BoGEMMS-HPC is currently stored in a **private INAF gitlab repository**

The repository includes directories storing publications and reports

A Singularity container is also distributed with the repo to run BoGEMMS-HPC on CINECA HPC resources



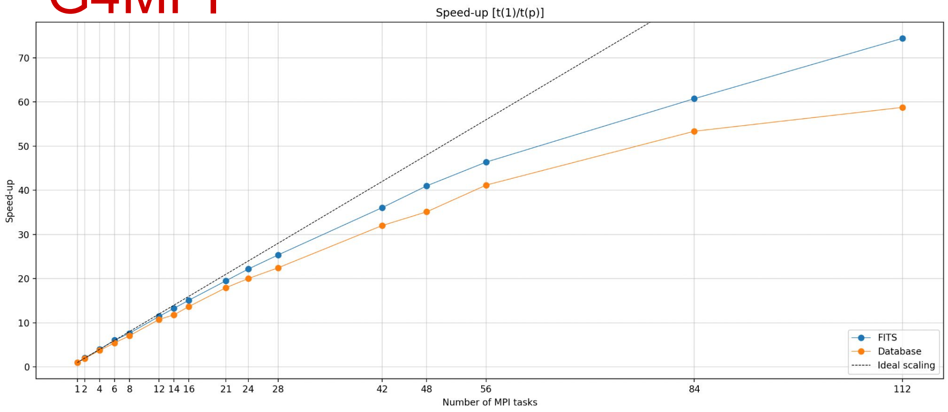
BoGEMMS-HPC performance test

- BoGEMMS-HPC performance already verified and tested on local Mac OS and INAF OAS computing node
- We now present the performance of BoGEMMS-HPC on the CINECA Leonardo supercomputer
- We evaluate the speed-up of the code with respect to a serial simulation, by incrementally increasing the number of threads/MPI tasks for both FITS and SQLite output data formats
- The test case chosen for this evaluation is the NASA COSI anticoincidence system, where an X-ray photon is emitted towards a scintillation panel and the optical photons hitting the read-out device are collected to form the signal. A total number of 336 photons is simulated in each run.

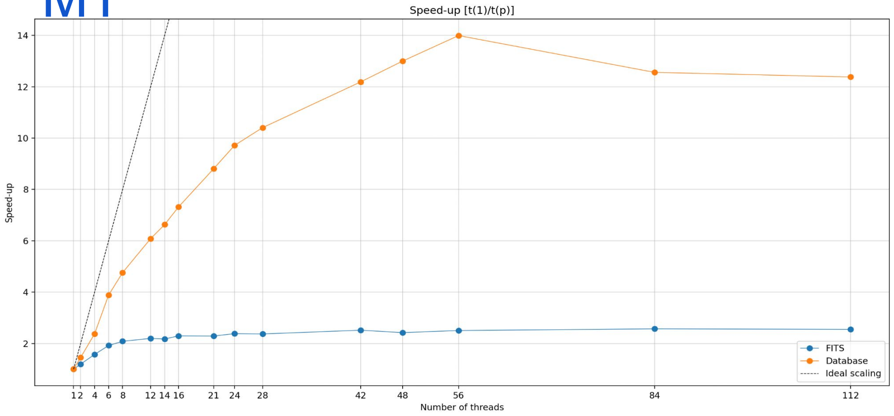
- **RAC resources:**
  - **CINECA/LEONARDO DCGP partition**
  - **Total of 100000 core-hours requested in proposal**
  - **in the performance test, using 1 node and up to 112 parallel cores (1 task = 1 core)**

Speed-up test

G4MPI



MT



MPI vs MT:

We obtain a **maximum speed-up of ~ 70** using G4MPI and all the 112 cores available, while with MT we obtain a **maximum speed-up of ~ 12**

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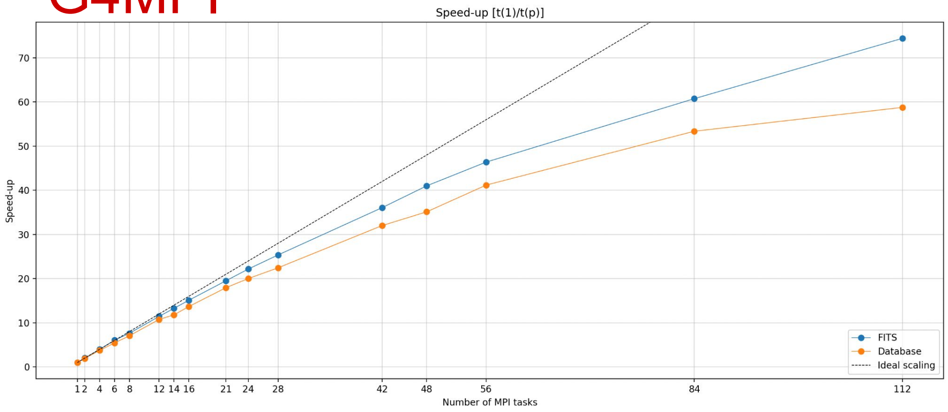
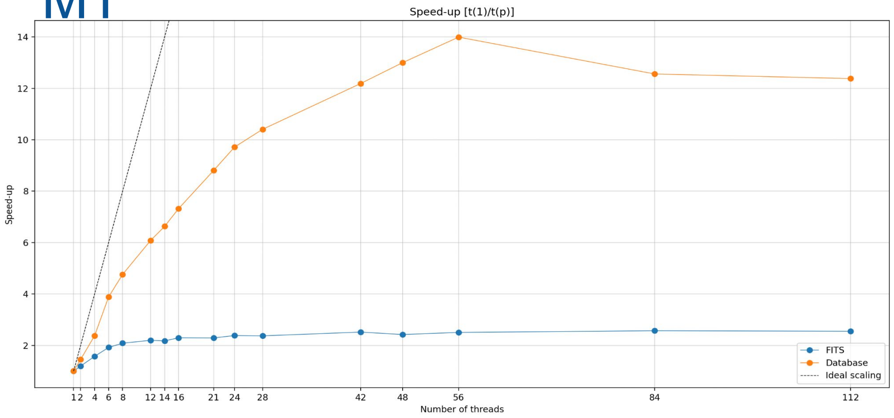
Speed-up test

G4MPI



MT



MPI vs MT:

The G4-mpi library allows to distribute the time of the output opening, writing and closing

→ maximum speed-up about 5 times higher than using multi-threading with SQLite, and more than 30 using FITS files.

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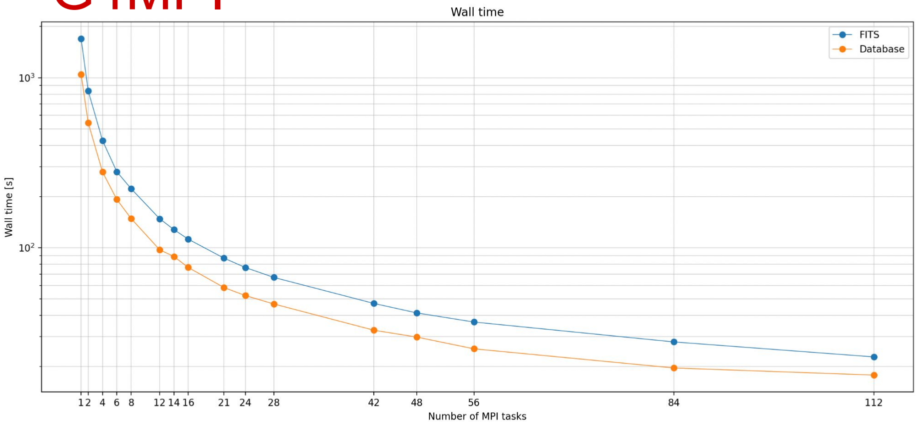
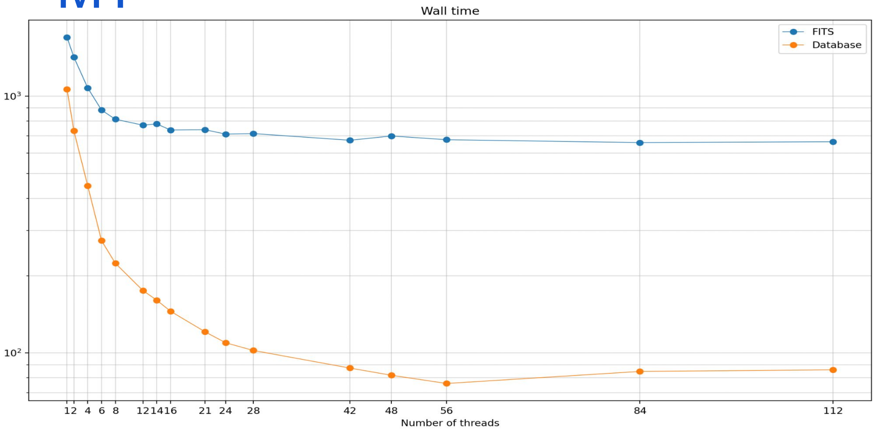
Wall-time test

G4MPI



MT



MPI vs MT:

using MPI and SQLite we are able to conclude the simulation in less than 20 seconds, instead of about 85 s with multi-threading.

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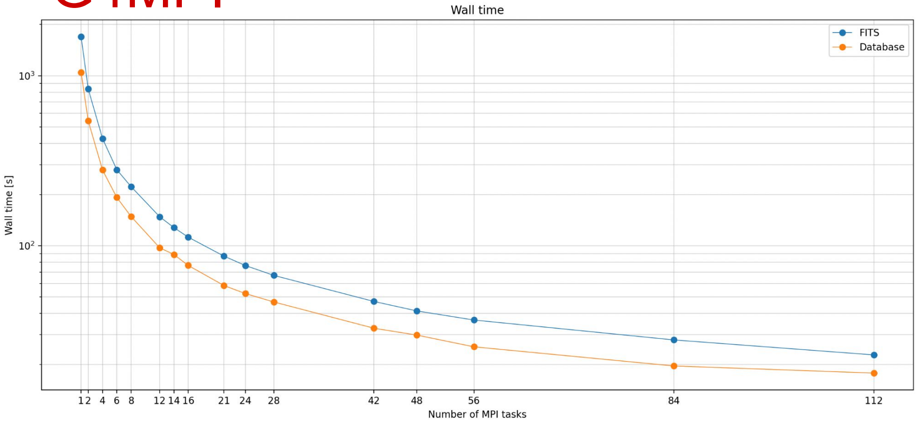
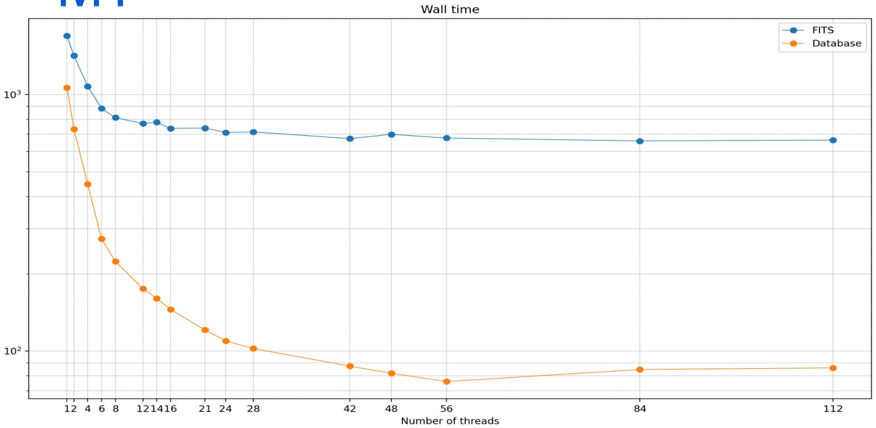
Wall-time test

G4MPI



MT



FITS vs database:

The FITS files are compressed at the end of the simulation, databases are not. For MT, a single FITS file is compressed serially, and the compression time becomes rapidly dominant of the total execution time. For MPI, the compression is shared among the tasks and the difference is smaller (with the database still being slightly better).

Simulation campaign on Leonardo for the COSI Anti-Coincidence system

We used the CINECA Leonardo resource to launch a simulation campaign for the COSI Anti-Coincidence System (ACS), to characterize:

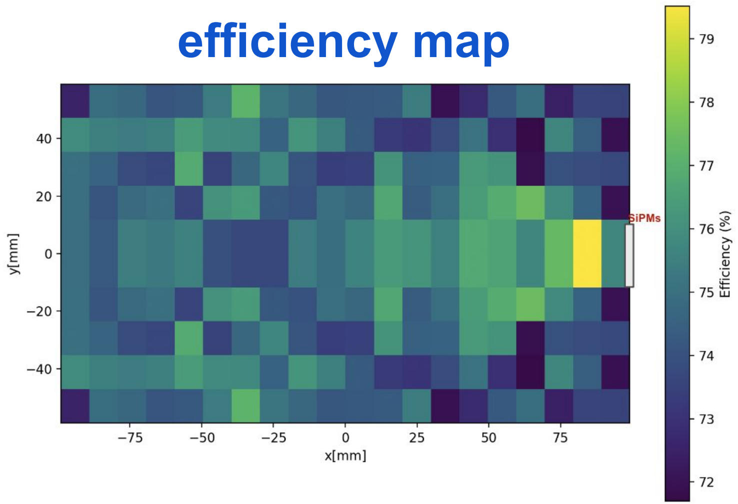
- ❑ the **optical light collection efficiency** (i.e. the probability for th optical photons generated in the scintillator to reach the readou device)
- ❑ the **energy resolution**

We used **G4MPI** as it provides the best speed-up.

Each run:

- ❑ **Events**: 5000 photons (1-10 MeV divided in 1 MeV bins)
- ❑ **Resources**: from 20 cores to 100 cores
- ❑ **Wall-time**: from few hours to 4 days (limit for dcgp_usr_prod partition)

BGO detection efficiency map



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Next steps

- ❑ Include more efficient database library
  - ❑ SQLite does not allow a simultaneous writing of the output to the same file
  - ❑ **MongoDB** is currently under implementation

- ❑ Clean up the code and prepare a public repository to be delivered to the community

Reports:

- ❑ **Ciabattoni** et al., *Verification of optical processes in Geant4 for the simulation of the COSI mission: using simple slabs as test case*
- ❑ **Ciabattoni** et al., *Validation of optical processes in Geant4 for the simulation of the COSI mission: the CLAIRE simulation*
- ❑ **Ciabattoni** et al., *BoGEMMS-HPC validation test: comparison with standard BoGEMMS with no MT and MPI*

Poster & Proceedings:

- ❑ **Ciabattoni** et al., *Towards a response function for the COSI anticoincidence system: preliminary results from Geant4 simulations*, SPIE Proc., 2024 (poster + proceedings)

Experience abroad:

- ❑ **3-months visit (June-September 2024) at Space Sciences Laboratory (Berkeley, USA) under the supervision of John Tomsick (COSI P.I.) on benchmarking the COSI ACS simulations**