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

BoGEMMS-HPC
The Bologna Geant4 Multi Mission Simulator (BoGEMMS) updated to HPC architectures and new I/O interfaces

MS7 KPI Status update (28/02/2024)

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Outline

1. UC overview
2. BoGEMMS-HPC new release (private INAF repo)
3. Flagship UC KPI update
    - preliminary performance tests

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UC overview

- **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 multi-purpose 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 [5]) as baseline simulation framework to validate the results and as starting point for the implementation of new HPC-oriented features.

- **WPs: WP3, WP6**
- **Flagship UC: WP3.4 PIPELINE**
- **Members:**
  - **V. Fioretti (INAF, 3m/yr) - coordinator**
  - **A. Ciabattoni (ICSC PhD, UniBo & INAF)**
  - **S. Lotti (INAF, 1m/yr)**

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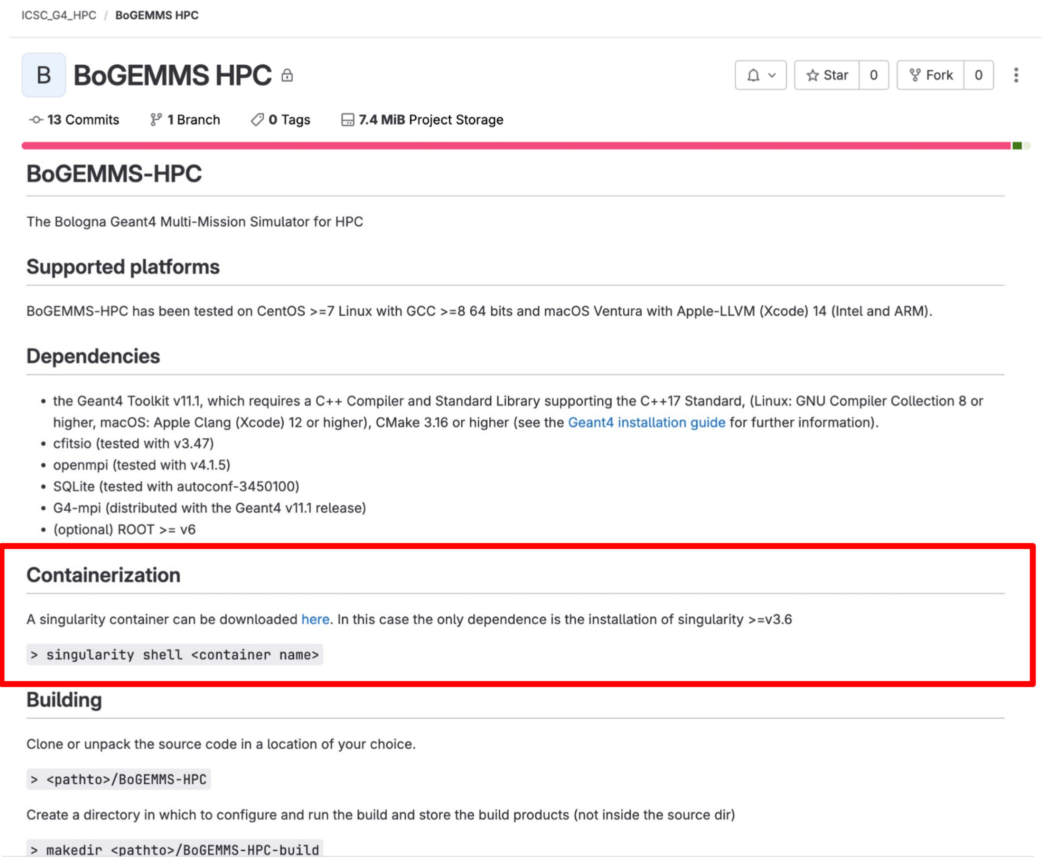
BoGEMMS-HPC main features

- BoGEMMS-HPC kernel is now separated from the user-defined classes
  - **the architecture can be published in the public repository** NEW
- input particles:
  - **the user can simulate from a list of particles provided in ASCII, FITS, or ROOT format** NEW
- geometries and physics:
  - **the user can select the geometry and physics classes using the name of the class** NEW
  - within the geometry classes the user can read CAD geometry files
  - the user can read GDML (Geometry Description Markup Language) geometries BoGEMMS output: FITS files, SQLite database
- BoGEMMS now 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 now 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 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.**

INAF gitlab repository

singularity container available to the user for running applications in HPC environments



ICSC_G4_HPC / BoGEMMS HPC

B BoGEMMS HPC

Star 0 Fork 0

13 Commits 1 Branch 0 Tags 7.4 MiB Project Storage

BoGEMMS-HPC

The Bologna Geant4 Multi-Mission Simulator for HPC

Supported platforms

BoGEMMS-HPC has been tested on CentOS >=7 Linux with GCC >=8 64 bits and macOS Ventura with Apple-LLVM (Xcode) 14 (Intel and ARM).

Dependencies

- the Geant4 Toolkit v11.1, which requires a C++ Compiler and Standard Library supporting the C++17 Standard, (Linux: GNU Compiler Collection 8 or higher, macOS: Apple Clang (Xcode) 12 or higher), CMake 3.16 or higher (see the Geant4 installation guide for further information).
- cfitsio (tested with v3.47)
- openmpi (tested with v4.1.5)
- SQLite (tested with autoconf-3450100)
- G4-mpi (distributed with the Geant4 v11.1 release)
- (optional) ROOT >= v6

Containerization

A singularity container can be downloaded here. In this case the only dependence is the installation of singularity >=v3.6

```
> singularity shell <container name>
```

Building

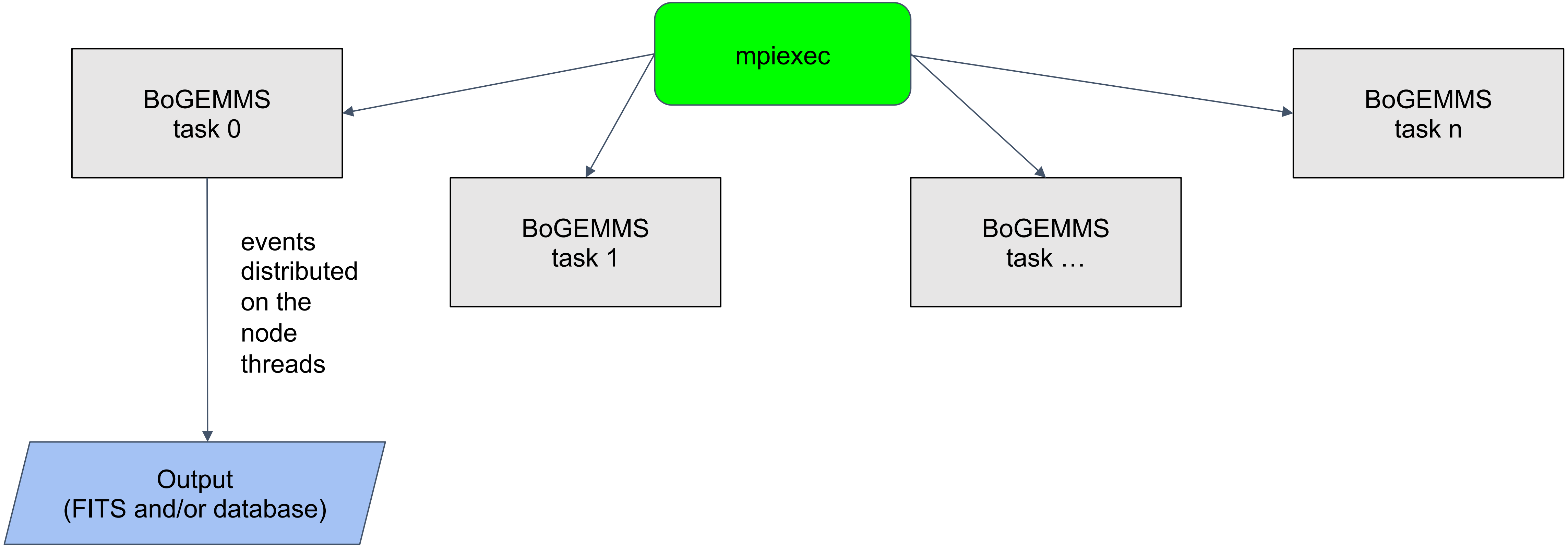
Clone or unpack the source code in a location of your choice.

```
> <pathto>/BoGEMMS-HPC
```

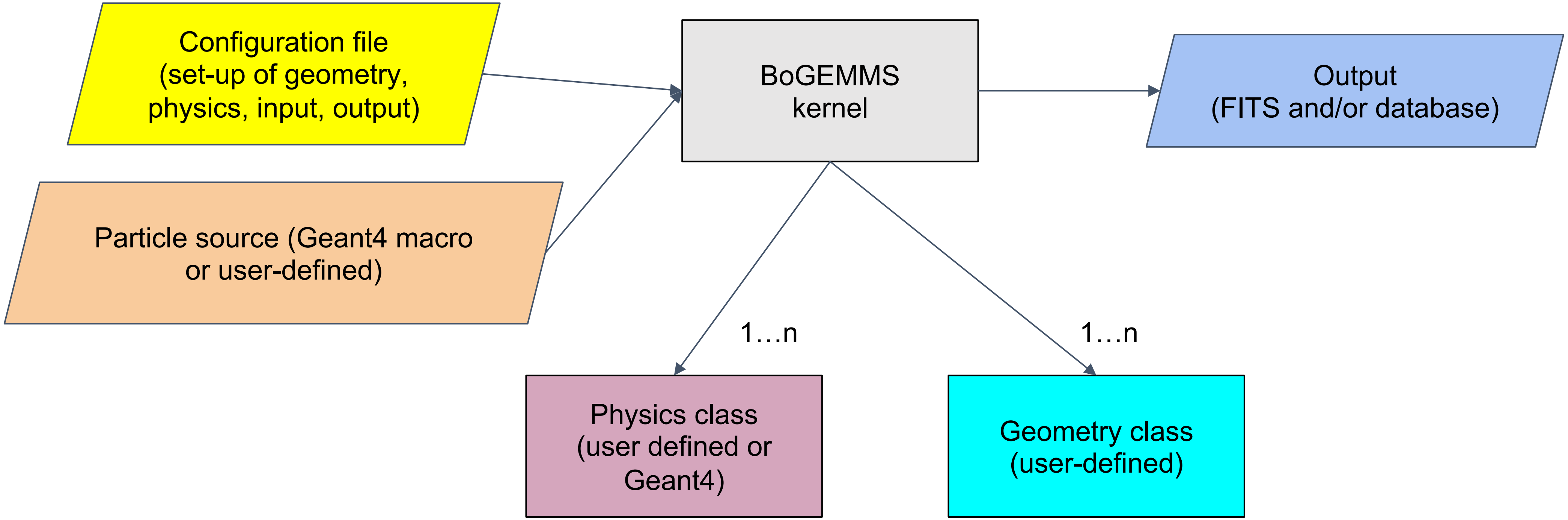
Create a directory in which to configure and run the build and store the build products (not inside the source dir)

```
> makedir <pathto>/BoGEMMS-HPC-build
```

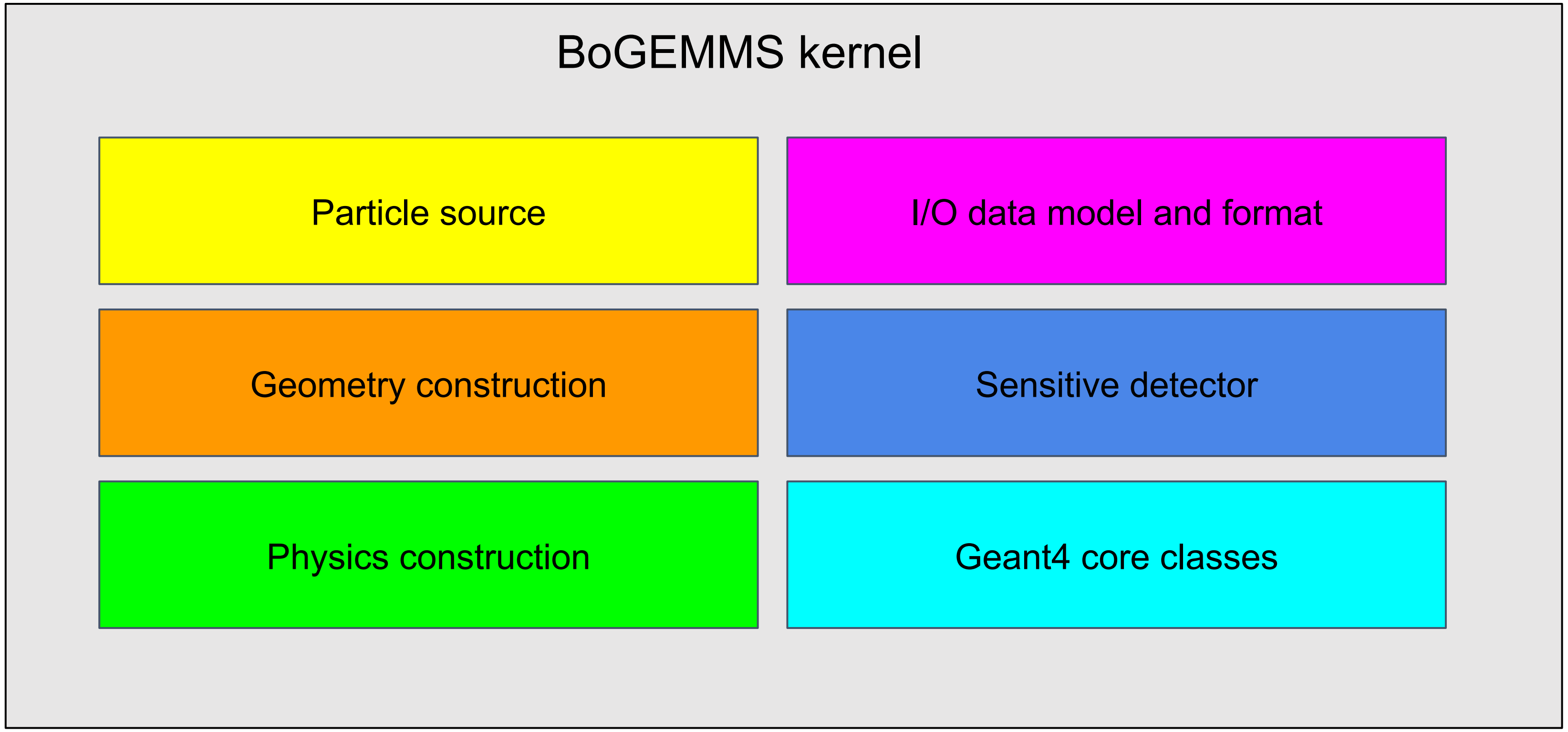
BoGEMMS-HPC


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

BoGEMMS-HPC


Configuration file
(set-up of geometry,
physics, input, output)
Particle source (Geant4 macro
or user-defined)
BoGEMMS
kernel
Output
(FITS and/or database)
1…n
1…n
Physics class
(user defined or
Geant4)
Geometry class
(user-defined)

BoGEMMS-HPC


BoGEMMS kernel
Particle source
I/O data model and format
Geometry construction
Sensitive detector
Physics construction
Geant4 core classes

I/O data format

- input particle source:
  - Geant4 GPS
  - list of particles/positions/energy read from ASCII/FITS/ROOT file

- simulation output:
  - the user can selects in the geometry class which volumes are sensitive (i.e. record the track information)
  - each row of the output file records the entrance and exit information (position, energy, volume ID, etc) through the sensitive volume
  - the user can select which columns to write

	EVT_ID	TRK_ID	PARENT...	VOLUM...	VOLUME_NAME	MOTHE...	E_DEP	X_ENT	Y_ENT	Z_ENT	X_EXIT	Y_EXIT	Z_EXIT	E_KIN_ENT	E_KIN_EXIT	MDX_ENT	MDY_ENT	MDZ_ENT	MDX_EXIT	MDY_EXIT
1	0	1	0	4	pDummySphere	0	0.	-0.00178	0.00186	-4999.8999	-0.00178	0.00186	-5000.	50.	50.	0.	0.	-1.	0.	0.
2	1	1	0	4	pDummySphere	0	0.	0.00173	-0.00181	-4999.8999	0.00173	-0.00181	-5000.	50.	50.	0.	0.	-1.	0.	0.
3	2	1	0	4	pDummySphere	0	0.	0.00088	-0.00034	-4999.8999	0.00088	-0.00034	-5000.	50.	50.	0.	0.	-1.	0.	0.
4	3	1	0	4	pDummySphere	0	0.	0.00094	0.00034	-4999.8999	0.00094	0.00034	-5000.	50.	50.	0.	0.	-1.	0.	0.
5	4	1	0	4	pDummySphere	0	0.	-0.00121	-0.00128	-4999.8999	-0.00121	-0.00128	-5000.	50.	50.	0.	0.	-1.	0.	0.
6	5	1	0	4	pDummySphere	0	0.	0.00016	-0.00053	-4999.8999	0.00016	-0.00053	-5000.	50.	50.	0.	0.	-1.	0.	0.
7	6	1	0	4	pDummySphere	0	0.	-0.00186	0.00046	-4999.8999	-0.00186	0.00046	-5000.	50.	50.	0.	0.	-1.	0.	0.
8	7	1	0	4	pDummySphere	0	0.	-0.002	0.002	-4999.8999	-0.002	0.002	-5000.	50.	50.	0.	0.	-1.	0.	0.
9	8	1	0	4	pDummySphere	0	0.	0.00175	0.00122	-4999.8999	0.00175	0.00122	-5000.	50.	50.	0.	0.	-1.	0.	0.
10	9	1	0	4	pDummySphere	0	0.	0.00096	0.00037	-4999.8999	0.00096	0.00037	-5000.	50.	50.	0.	0.	-1.	0.	0.

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Running BoGEMMS-HPC

- Single node (no mpi): `bogemms <conf file> <starting number> <mac file>`
- multinode (with mpi): `mpiexec -n <task number> bogemms <conf file> <starting number> <mac file>`

- conf file:
  - geometry, physics, MT, output data format configuration file

```
############################################################
# Volume ID handling

# 1 = summing mother and grandmother ID in case of replicas
GEOM.VOLID.TYPE = 0

############################################################
# Multithreading
RUN.MT.ACTIVATE = 1


############################################################
# physical process

ENERGYPROCESS.VERSION = AREMBESPhys
HADRONPHYS.NAME = emstandardSS_QBBC
PHYS.DEFAULT.CUT = 0.001

# activating SS for all regions
SPACEPHYS.ACTIVATE = 1
SSPHYS.ACTIVATE = 0

# region cuts
REGION.TARGET.CUT = 0.1
REGION.TARGET.PROTON.CUT = 0.1

# not applying SS to region
REGION.TARGET.SS.ACTIVATE = 0

# user limit
GEOM.EXACRAD.4.MAXSTEP = 0.00000001

# Energy in MeV, angle in deg.
FIRSOVPHYS.ACTIVATE = 0
```

```
############################################################
# geometry configuration
# Print the current geometry to output
GEOM.PRINT_GEOMETRY = false
GEOM.WRITE.GDML = false
GEOM.WRITE.GDML.NAME = WFI.gdml

# setting the world dimension [mm]
WORLD.BOX.SIDE = 5000

GEOM.VERSION = EXACRAD

# Experiment type
# 0: full set-up with degrader foil and collimator
# 1: only target and detecto
# 2: degrader and collimator
# 3: target and detector (WP 6.1)
# 4: EXACRAD2 experiment

GEOM.EXACRAD.EXPERIMENT = 4

# Experiment = 4
#

# selecting the chamber material
GEOM.EXACRAD.4.VACUUM = 1

# degrader foil distance (from foil face to target center) in mm
#GEOM.EXACRAD.0.FOIL.DISTANCE = 1567.
```

Running BoGEMMS-HPC

- Single node (no mpi): `bogemms <conf file> <starting number> <mac file>`
- multinode (with mpi): `mpiexec -n <task number> bogemms <conf file> <starting number> <mac file>`

- mac file:
  - Geant4 General Particle Source

```
/run/verbose 0

/gps/particle geantino

/gps/pos/type Plane
/gps/pos/shape Rectangle
/gps/pos/halfx 0.002 mm
/gps/pos/halfy 0.002 mm
/gps/pos/centre 0.0 0.0 10.0 cm
/gps/direction 0 0 -1



/gps/ene/mono 50 keV



# Set number of particles and start
/random/resetEngineFrom currentEvent.rndm
/run/beamOn 10
/random/saveThisRun

```

Flagship UC KPI for MS7 (end of February 2024)

- KPI2.3.4.2 (MS7): The design of the pipeline prototypes includes the software architecture, functions and I/O interfaces, the software implementation and the requirements (e.g. speed, data transfer, memory load, scalability) to satisfy in the verification phase
  - KPI: design and test of at least >= 2 pipelines containerized available on the repository with a subset of requirements operables
- KPI status:
  - report on the software architecture -> work in progress
  - report on testing BoGEMMS-HPC without multithreading and multi-core
    - DONE: Ciabattoni & Fioretti, “BoGEMMS-HPC validation test: comparison with standard BoGEMMS with no MT and MPI”, 2023
  - performance tests on MT and MPI: DONE, results in the MS7 report

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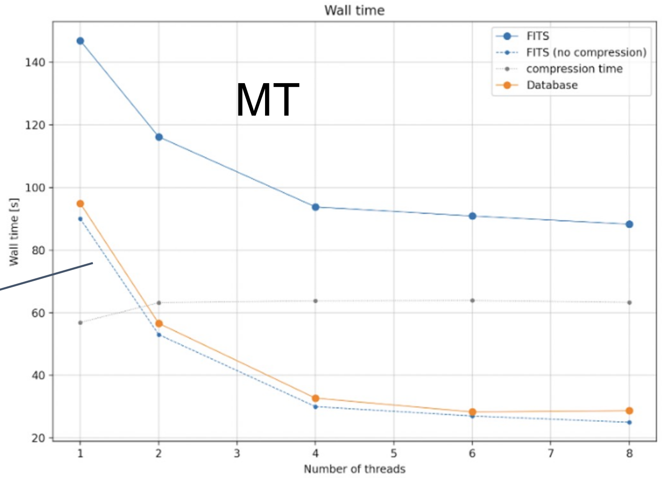
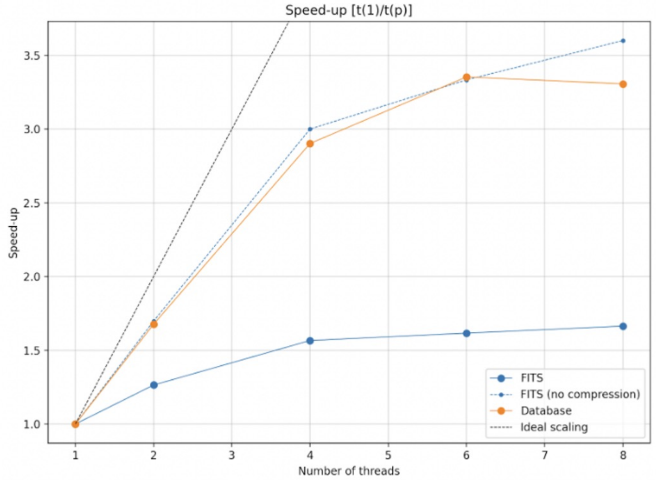
Preliminary performance tests

- target architectures:
  - local machine (Apple M2, macOS Sonoma,16 GB RAM, 8 cores)
  - computing node of the INAF OAS cluster (Centos Linux 7, x86_64 architecture, 2 sockets, 10 cores per socket) using the singularity container
- We conducted separate tests for multi-threading (MT) and MPI multi-task parallelism.
- For each case, we iteratively executed simulations while incrementally increasing the number of threads/tasks utilized. We then measured the wall time for each simulation run, enabling the evaluation of the performance gain of the code and its scalability across the number of resources.
- We tested both FITS and SQLite databases as output data format and we used a maximum of 8 threads/tasks in the local machine, and 20 threads/tasks in the computing node.

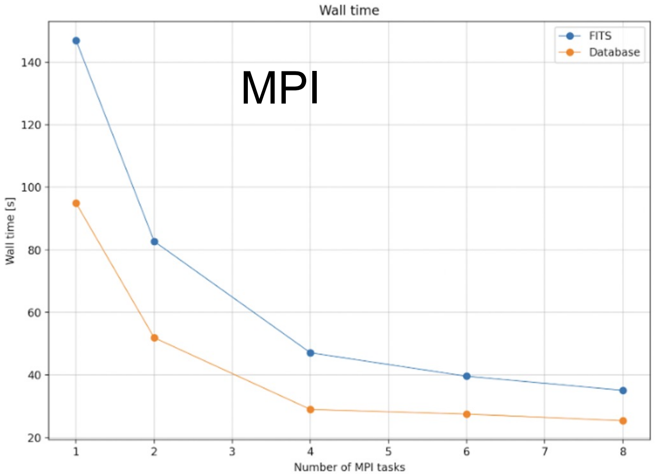
Wall time (left) and speed-up (right) on laptop

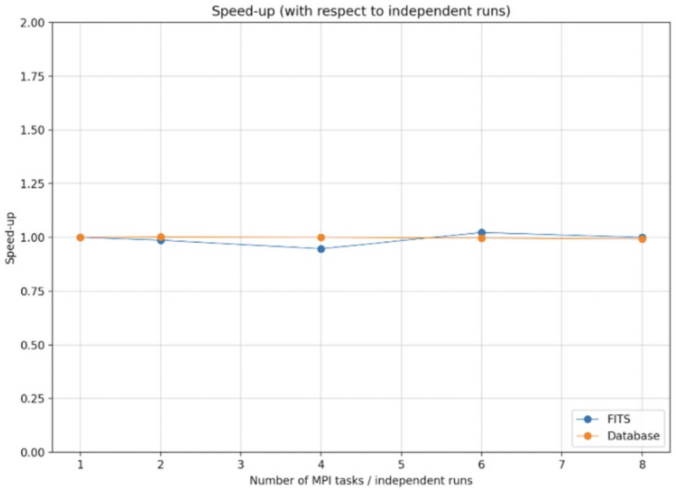
Without compression, FITS are a bit faster because SQLite does not allow simultaneous access





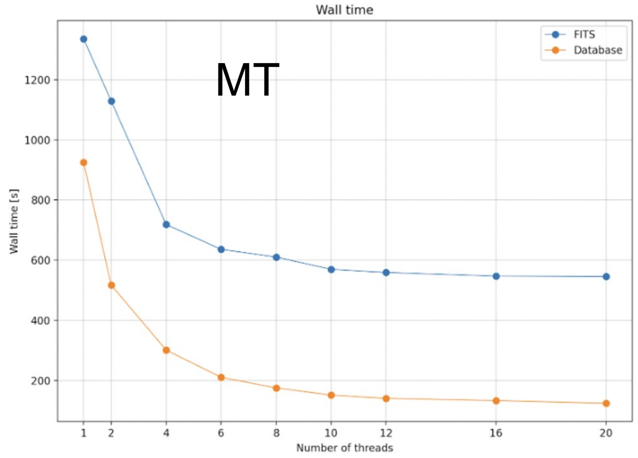
The speed-up is defined as the wall time using 1 process, divided by the wall time using p processes

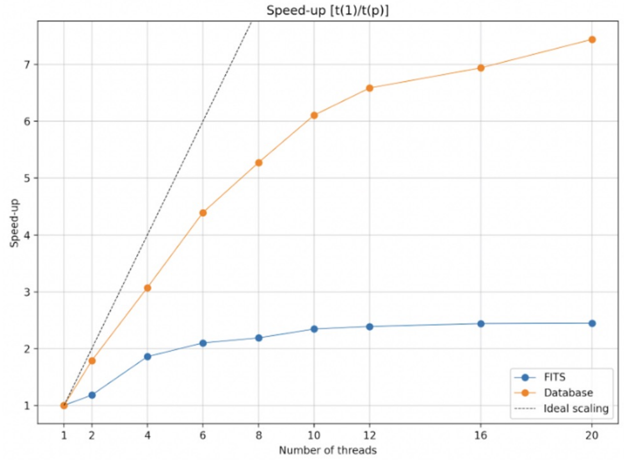




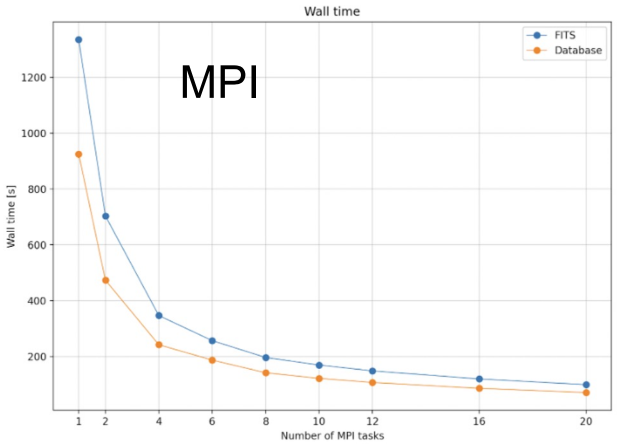
The speed-up of executing one run with p MPI tasks (simulating 240 events) with respect to simultaneously executing p independent runs each with 1 task (each simulating $240/p$ events)

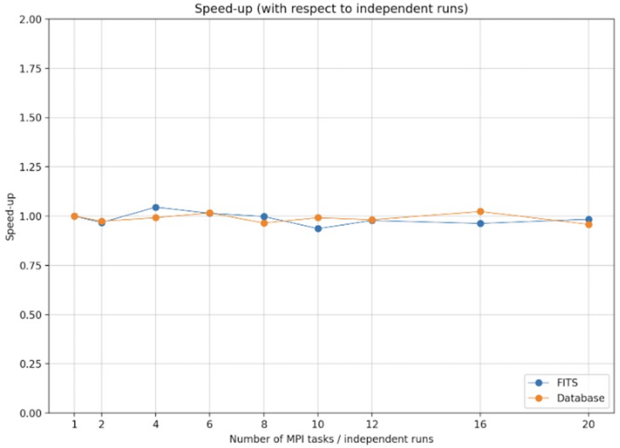
Wall time (left) and speed-up (right) on the computing node





The speed-up is defined as the wall time using 1 process, divided by the wall time using *p* processes





The speed-up of executing one run with *p* MPI tasks (simulating 240 events) with respect to simultaneously executing *p* independent runs each with 1 task (each simulating 240/*p* events)

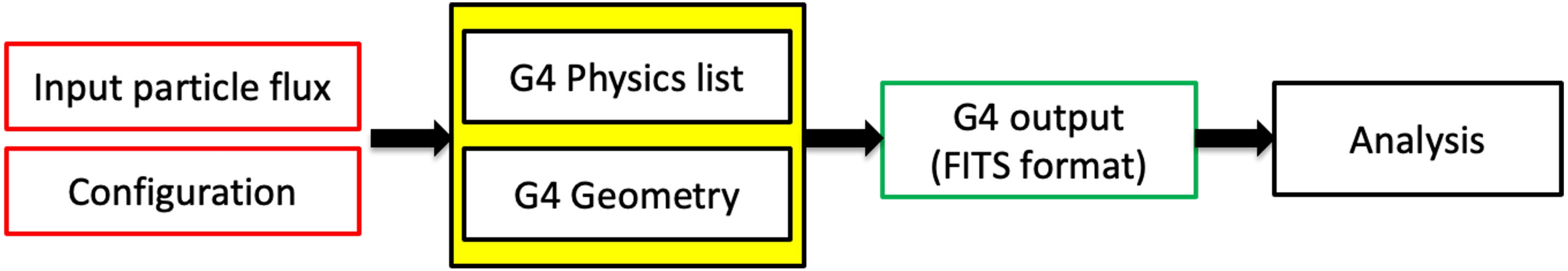
Next steps

- including mySQL
- extending the geometry and physics modularity
- testing BoGEMMS-HPC on the CN HPC resources

BACK-UP

BoGEMMS - Bologna Geant4 Multi-Mission Simulator

- Geant4 (Allison+ 2016) is an open-source C++ toolkit library for particle transport, developed by the CERN and currently maintained by a large scientific collaboration (with members from INFN and ESA)
- BoGEMMS is a Geant4-based simulation project started at INAF OAS in 2010 (Bulgarelli+2012, Fioretti+2012, Fioretti+2014), with the aim of building a multi-application simulation framework that handles the configuration of the input particles, geometry, output data format (formatted in FITS files) with configuration files at runtime
- The output data model is an “event list”, with each row describing the particle interaction with selected sensitive volumes



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BoGEMMS - Bologna Geant4 Multi-Mission Simulator

- BoGEMMS was used for the simulation of operating and proposed space missions such as XMM-Newton, AGILE, Simbol-X, NHXM, Athena, e-ASTROGAM, COSI
- The code was never released to the community because of lack of manpower to implement mandatory features, documentation, manuals, etc
- The ICSC funding represented the perfect opportunity to port BoGEMMS to HPC architectures with multi-threading and multi-node computation and adding new features (CAD and GDML geometry support, new output data format)
- The simulation of the COSI (Compton Spectrometer and Imager) mission (NASA Small Mission program) was selected as testbed for the code porting, and the Flagship PIPELINE UC hosts the BoGEMMS pipeline