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

### BoGEMMS-HPC: development of Geant4 simulations in High-Performance Computing environments (WP3 Flagship UC PIPELINE)

**ICSC Spoke 2 Annual Meeting 2023** 

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Pipeline for GEANT4 simulations in HPC environments, with the simulation of the NASA COSI Anti-Coincidence System (ACS) as a test case

- subproject of the WP3 Flagship UC "Pipeline optimization for space and ground based experiments (PSGE)"
- 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).
- Bologna Geant4 Multi-Mission Simulator (BoGEMMS) as baseline simulation framework
- **WPs:** WP3, WP6
- Flagship UC: WP3.4 PIPELINE
- Members:
  - V. Fioretti (INAF OAS Bologna) coordinator
  - A. Ciabattoni (ICSC PhD, UniBo & INAF OAS Bologna)
  - S. Lotti (INAF IAPS)



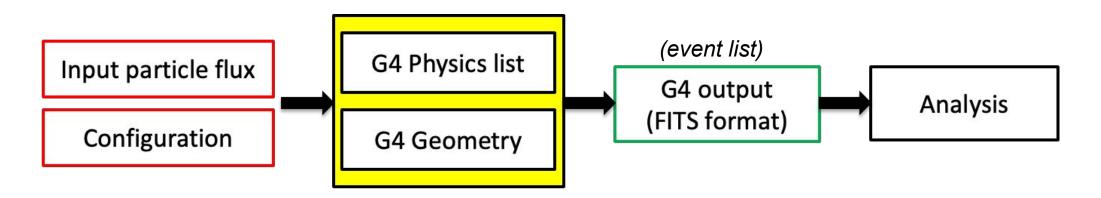






# **BoGEMMS - Bologna Geant4 Multi-Mission Simulator**

- **Geant4** (Allison+ 2016) is an open-source C++ toolkit library for particle transport, developed by CERN and currently maintained by a large scientific collaboration
- 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 that handles the configuration of the input particles, geometry, output data format (formatted in FITS files) with configuration files at runtime











# **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
- <u>The ICSC funding represented the perfect opportunity to port BoGEMMS to HPC</u> <u>architectures with multi-threading and multi-node computation and adding new</u> <u>features</u> (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 a testcase for the new BoGEMMS, and the Flagship PIPELINE UC hosts the BoGEMMS pipeline









# **BoGEMMS-HPC**

- New geometry features:
  - the user can read CAD geometry files using the open-source library CADmesh
    - future implementation: reading and configuring CAD geometries with a configuration file at runtime
  - the user can read GDML (Geometry Description Markup Language) geometries and assign the sensitive volumes using a configuration file at runtime
- New output data format:
  - data format: FITS files, database (SQLite currently being tested)
- New multi-threading (MT) (using Geant4 built-in feature)
  - when a thread writes on FITS files, the other threads are placed on hold
- New implementation of parallel computing
  - using the G4-mpi library (K. Murakami (KEK)) tested with open MPI
  - BoGEMMS runs independent applications (with separated output) on different nodes.



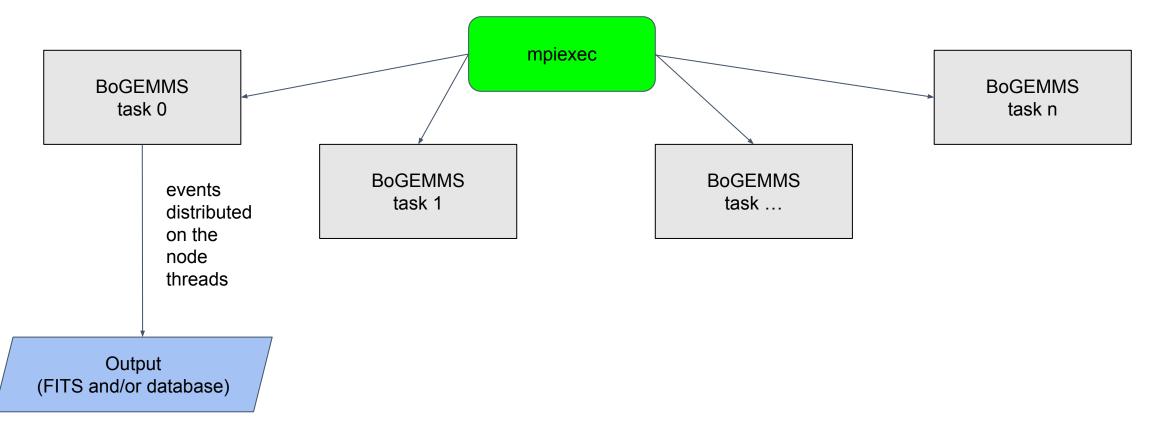
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#### **BoGEMMS-HPC**





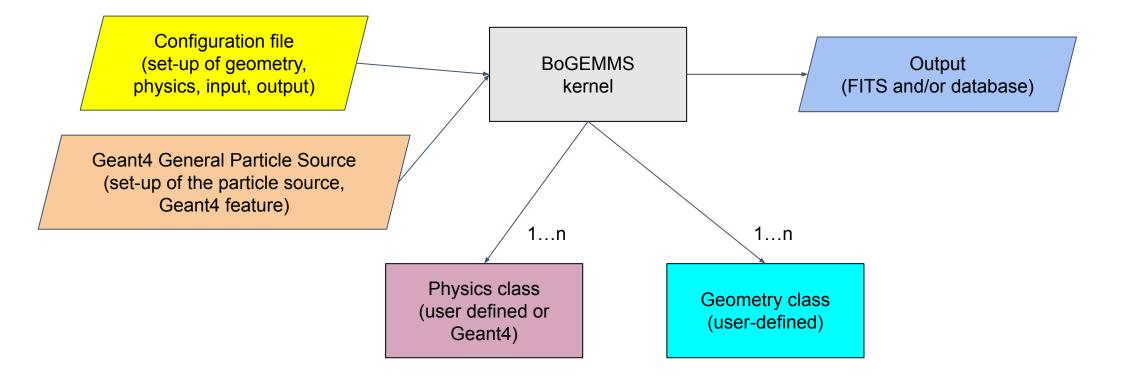
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# **BoGEMMS-HPC**





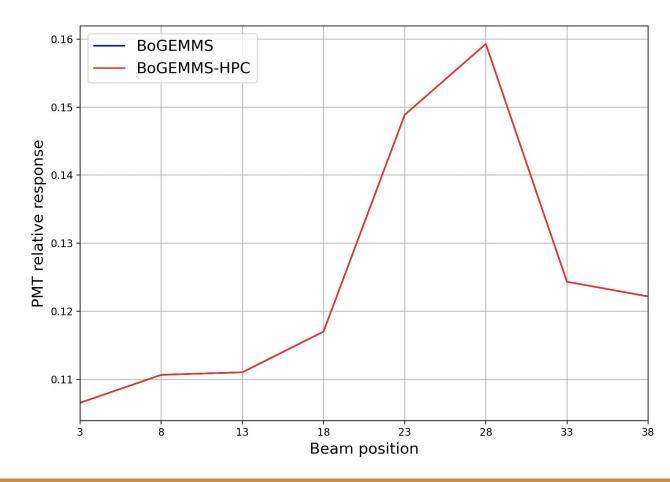






## **Testing BoGEMMS-HPC without HPC features**

- BoGEMMS-HPC tested on local machine without MT and MPI against the standard BoGEMMS (v2.1.2)
- Same random seed, so that we expect the exact same result
- Test case: COSI anticoincidence system











## Next steps

- Testing BoGEMMS-HPC performance on HPC architecture
  - a singularity container with cfitsio, openmpi, SQLite, Geant4 v11.1, G4-mpi has been prepared
  - ICSC RAC proposal submitted
  - The performance requirement is the reduction of the computing time of at least 20% (goal 30%) with respect to the BoGEMMS architecture, using the simulation of the COSI Anticoincidence prototype as test-case.
- Adding modularity for using CAD files as input to the simulation, selecting geometries and physics lists
- Optimization if needed of the parallelization methods and database engine