Simulation of X-ray fluorescence from planetary surfaces

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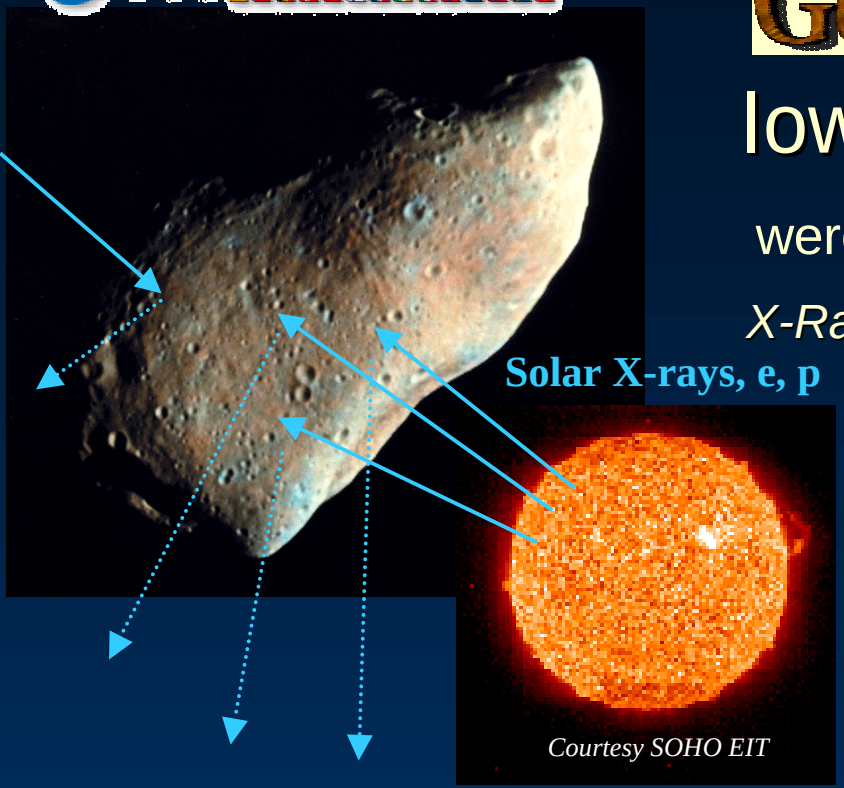
Geant 4

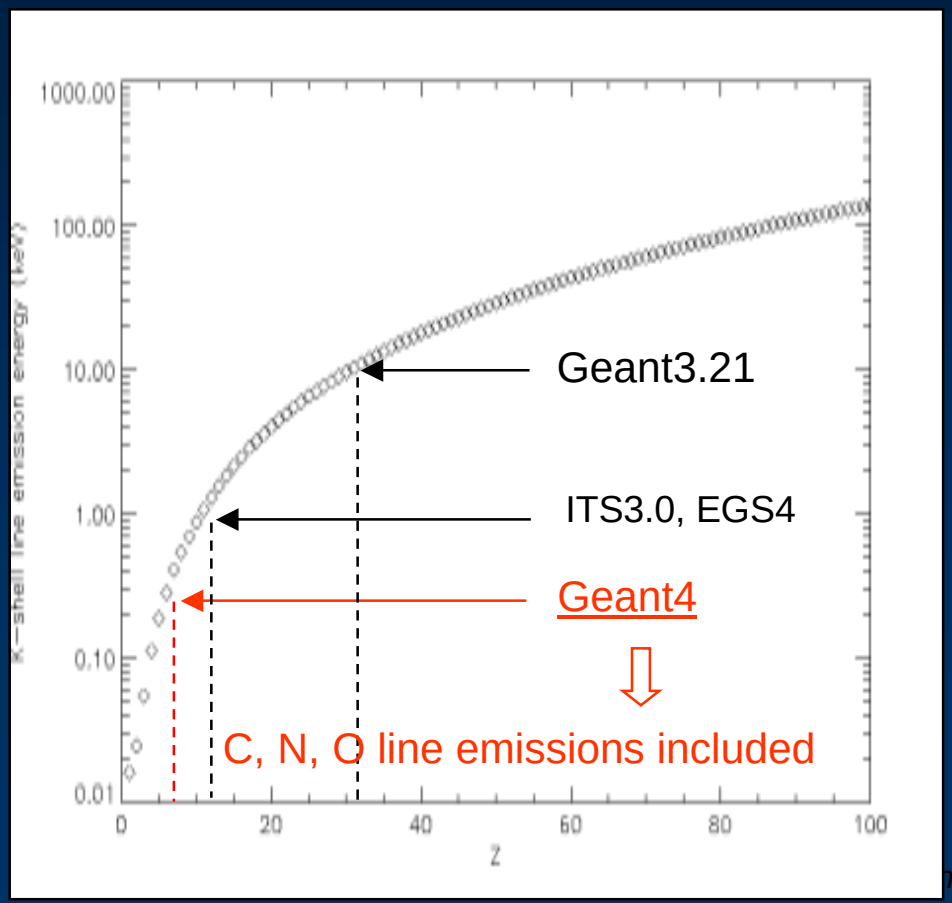
low energy e/γ extensions

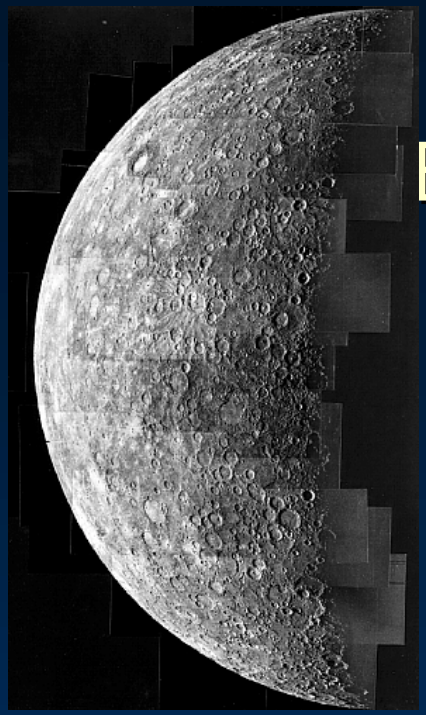
were triggered by astrophysics requirements

X-Ray Surveys of Planets, Asteroids and Moons



Induced X-ray line emission:
indicator of target composition
(~100 μm surface layer)

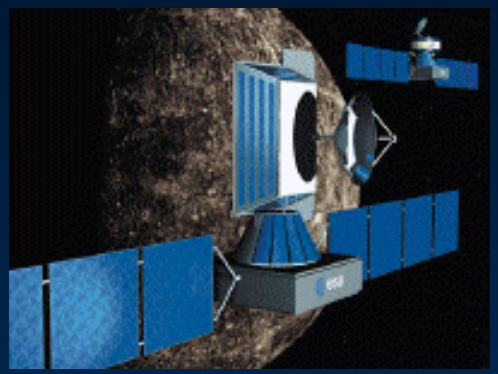


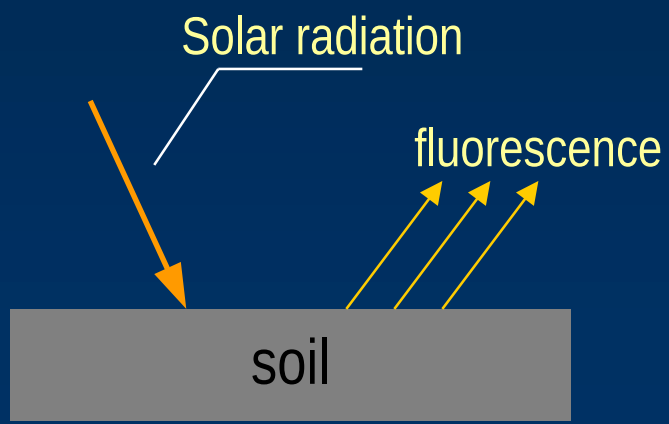


Bepi Colombo mission to Mercury

ESA cornerstone mission

- multi-disciplinary
- wide scientific programme





As part of the physics programme:

measurement of the elemental composition of the planet crust through the analysis of the X-ray spectra induced by the solar radiation

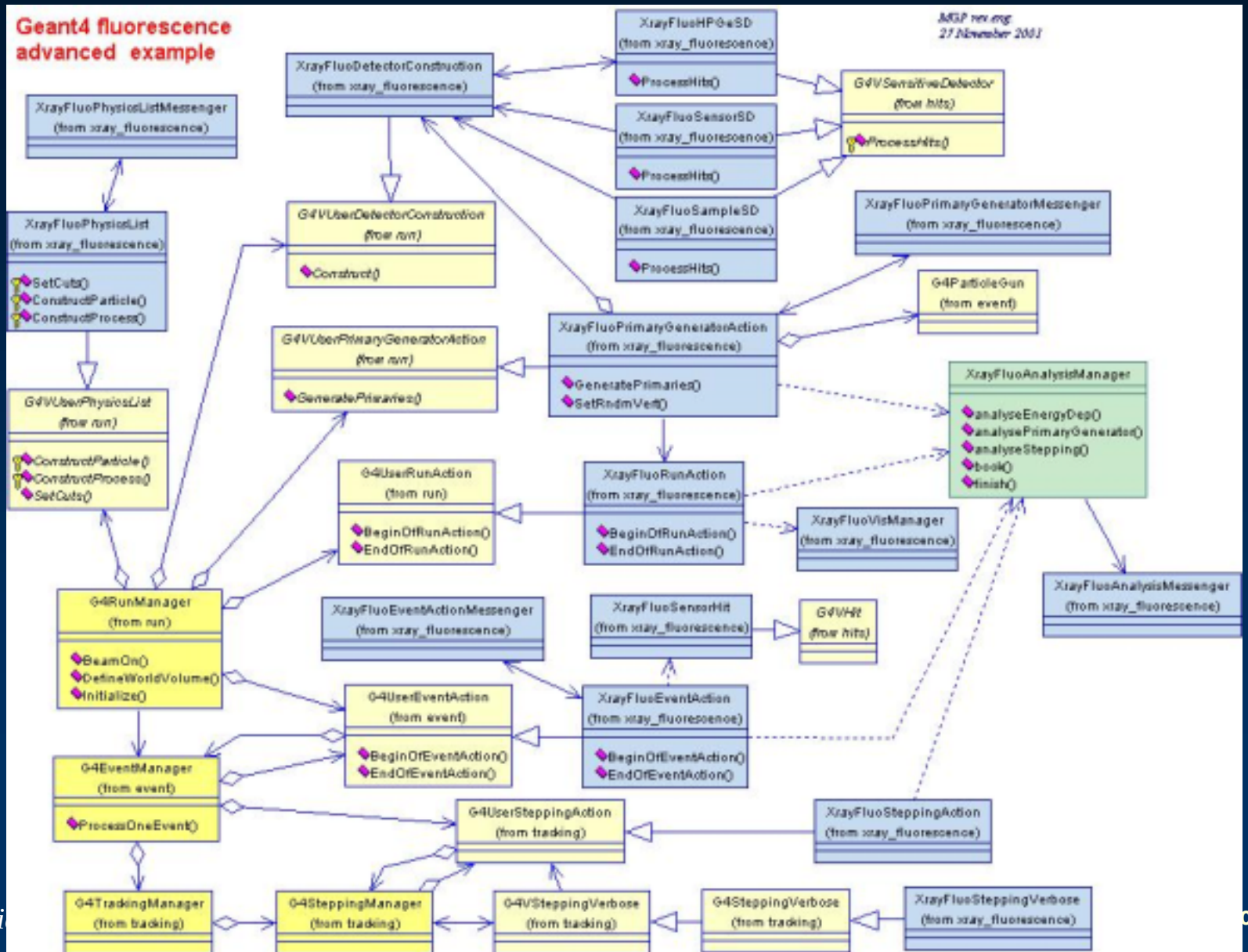
Geant4 simulation of the X-ray spectrometer

- Evaluate the physics reach of the measurement
  - is a XRF measurement feasible in the mission?
  - which elemental components are visible?
  - what is the effect of detector resolution?
- Optimisation of the choice of the detector
  - Si versus compound semiconductor detectors
- What is the expected yield?
  - from solar X-rays
  - from solar protons

Preparing a correct and detailed simulation is a crucial part of the risk mitigation strategies of the mission

Application design

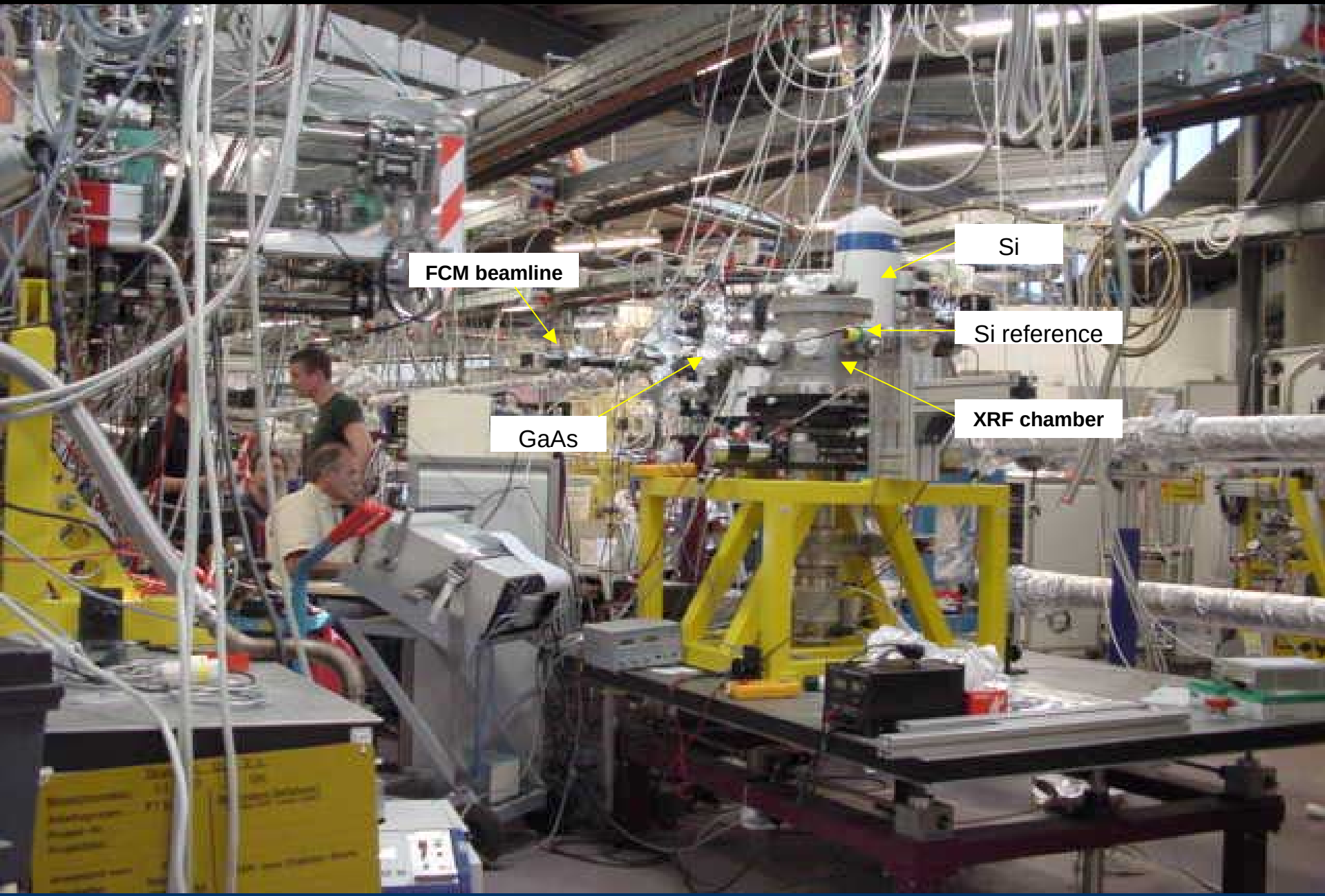
Geant4 advanced example
xray_fluorescence



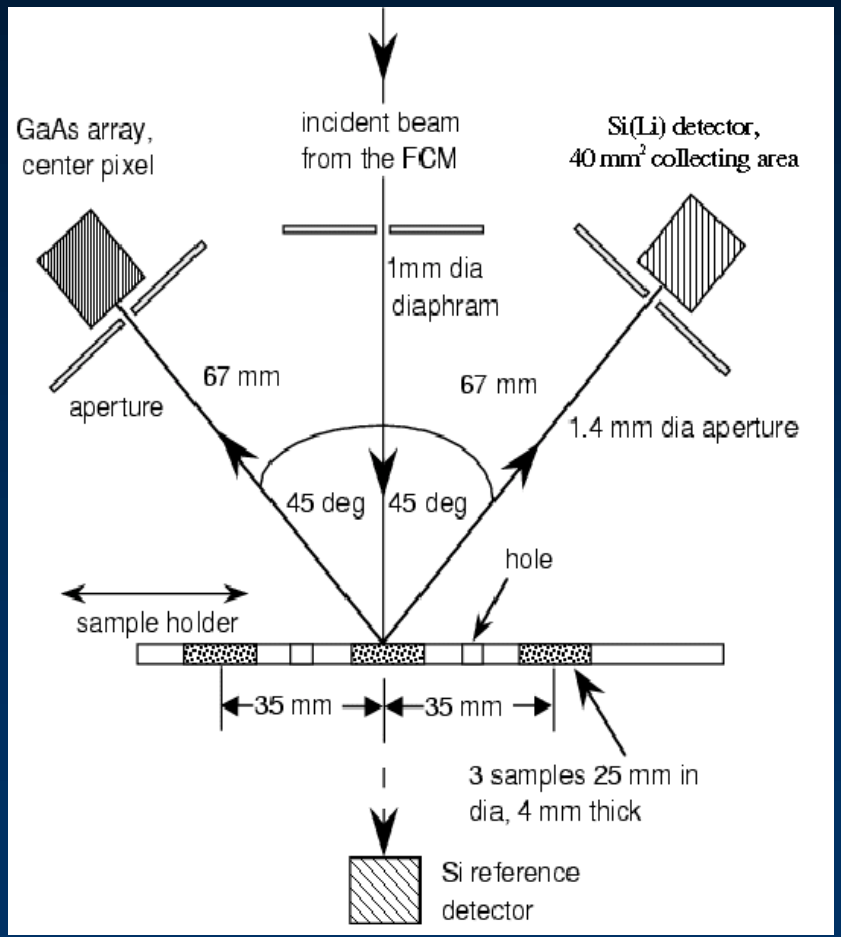
First phase: test beam simulation

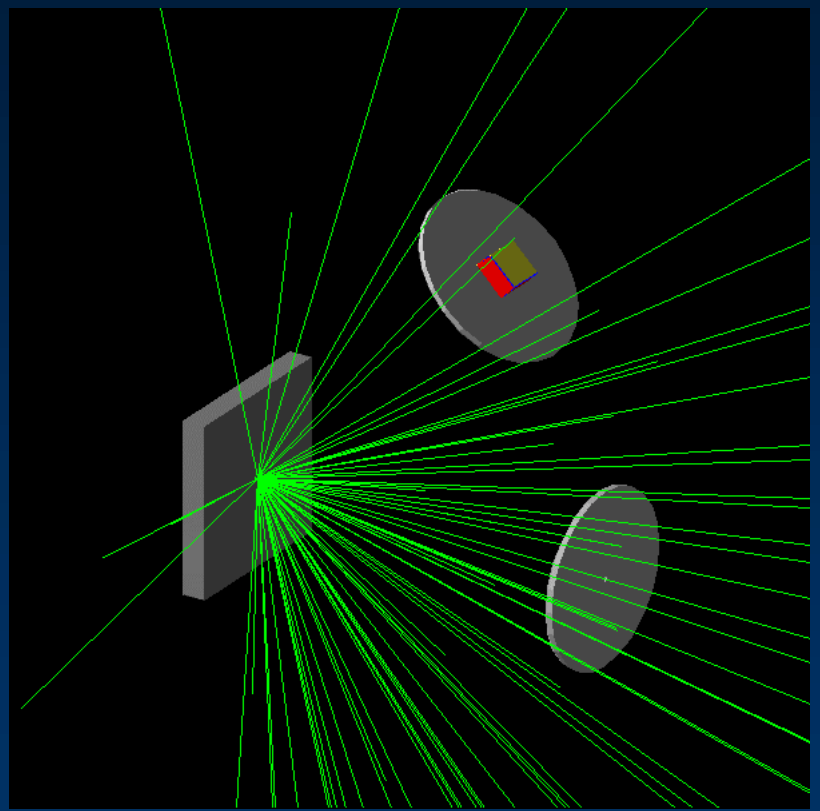
- Test beam at Bessy
  - validation of Geant4 capabilities to simulate X-ray fluorescence
- Rock samples
  - various rock samples prepared by a geological institute
  - reproduction of geological materials of astrophysical interest
  - controlled material composition of the samples
- Detector response
  - well known from lab tests at ESTEC

The experimental set-up at the PTB laboratory at BESSY-II.
The XRF chamber can be seen to be attached to the end of the Four Crystal Monochromator (FCM) beamline.



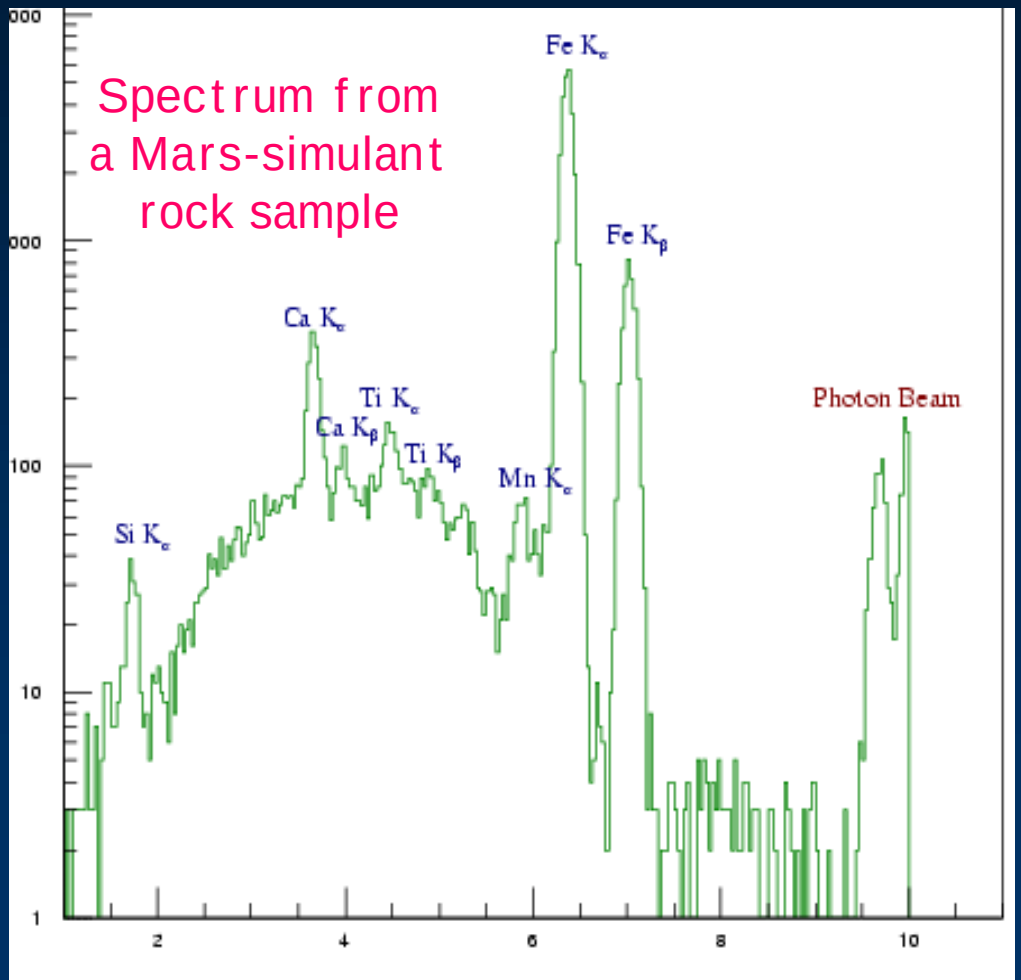
Test beam: geometry





Fluorescence

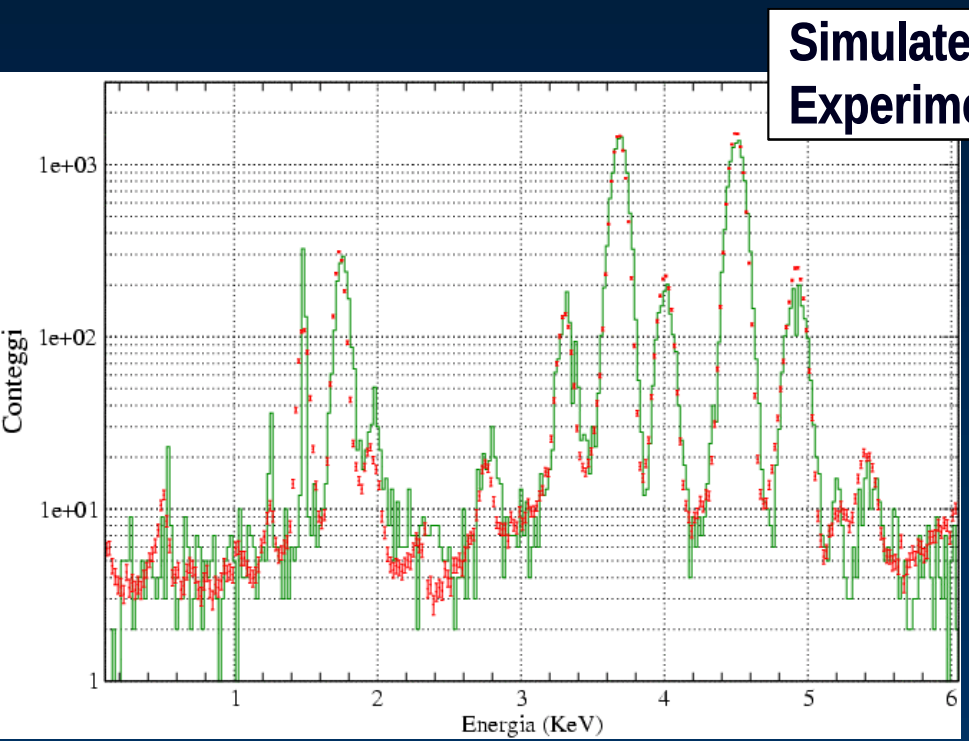
Experimental data: fluorescent spectra from various rock samples, at various energies

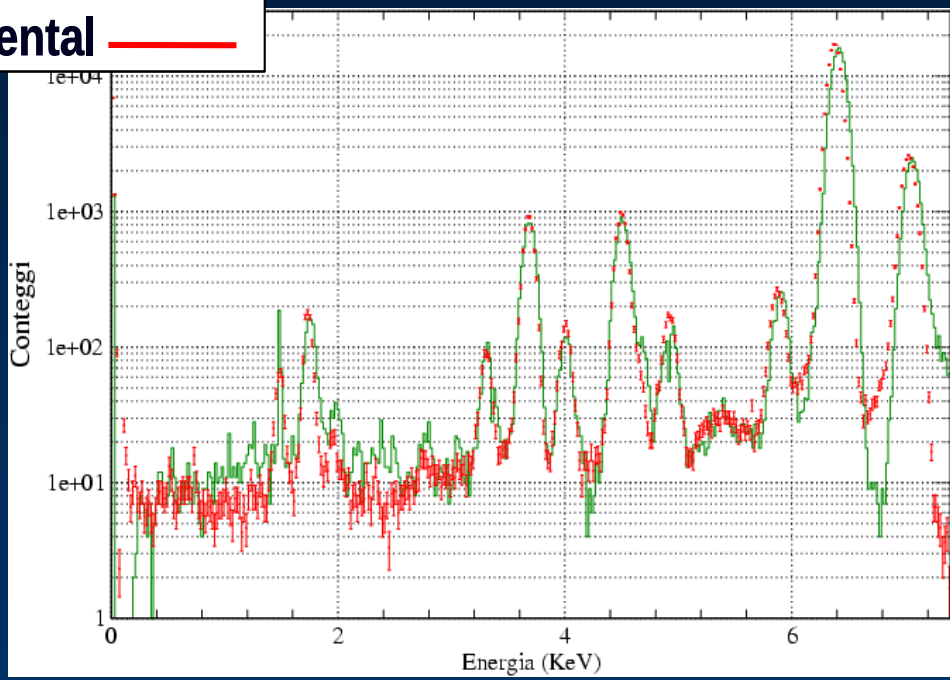


- Anorthosite (Harris)
- Dolerite (Madagascar)
- Dolerite (Whin Sill)
- Basalt (Madagascar)
- Basalt(Icelandic)
- Hematite (Sishen)
- Gabbro (Mount Royal)
- Mars-1
- Obsidian

Simulation of test beam configurations

Various rock sample irradiated, at various incident beam energies

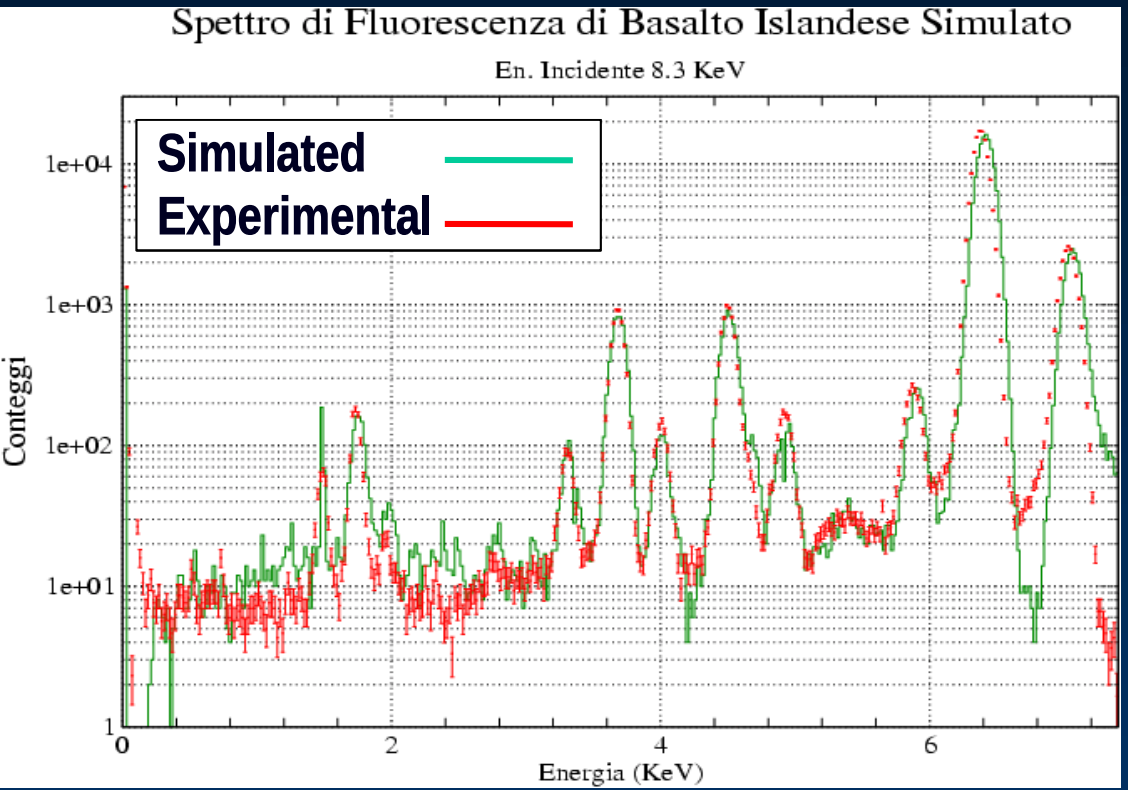




Icelandic basalt, E_{beam} = 6.5 keV

Icelandic basalt, E_{beam} = 8.3 keV

Comparison to experimental data



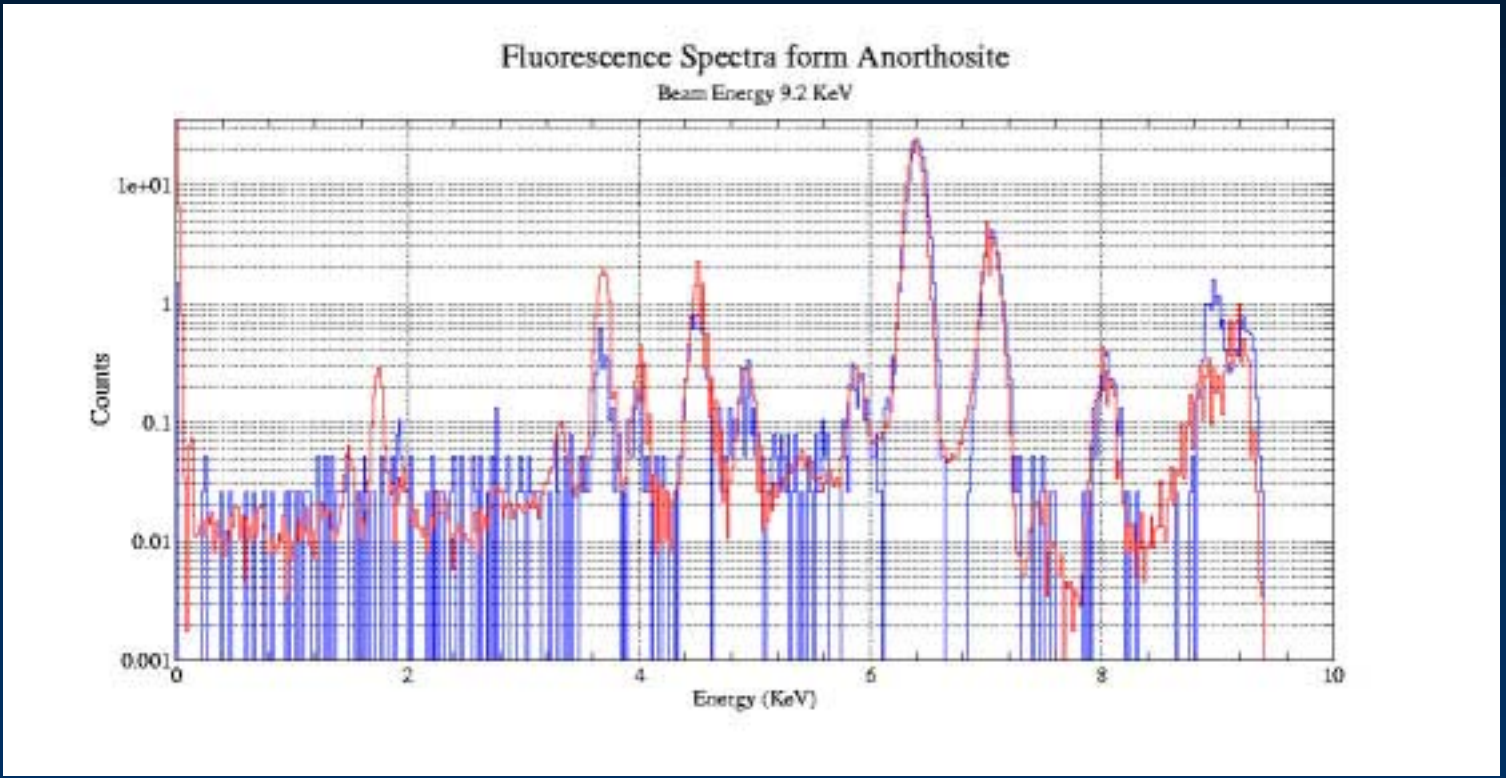
Anderson Darling test

Beam Energy	A2
4.9	0.04
6.5	0.01
8.2	0.21
9.5	0.41

Ac (95%) =0.752

Experimental and simulated X-Ray Spectra are statistically compatible at a 95% C.L.

Study of various material samples



9 materials irradiated at Bessy – simulation production in progress

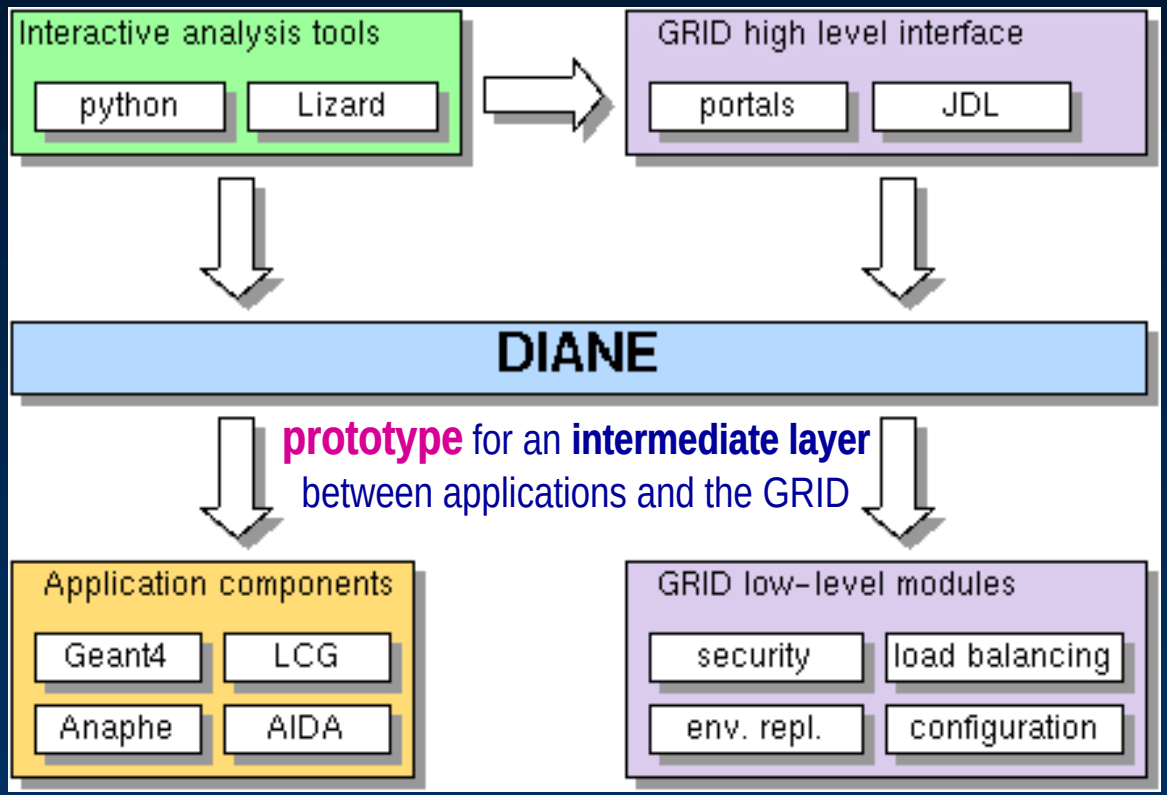
Performance

- Execution time: 5 days on a dual PIII 1.2 GHz for the simulation of a test configuration (one rock, at a given beam energy)
- CPU time necessary for a complete simulation of a rock sample irradiation: 5 days

- Integration into a distributed computing environment
  - parallelisation of the application
  - run on a PC farm
  - run on the GRID

DIANE **DI**stributed **AN**alysis **E**nvironment

Hide complex details of underlying technology



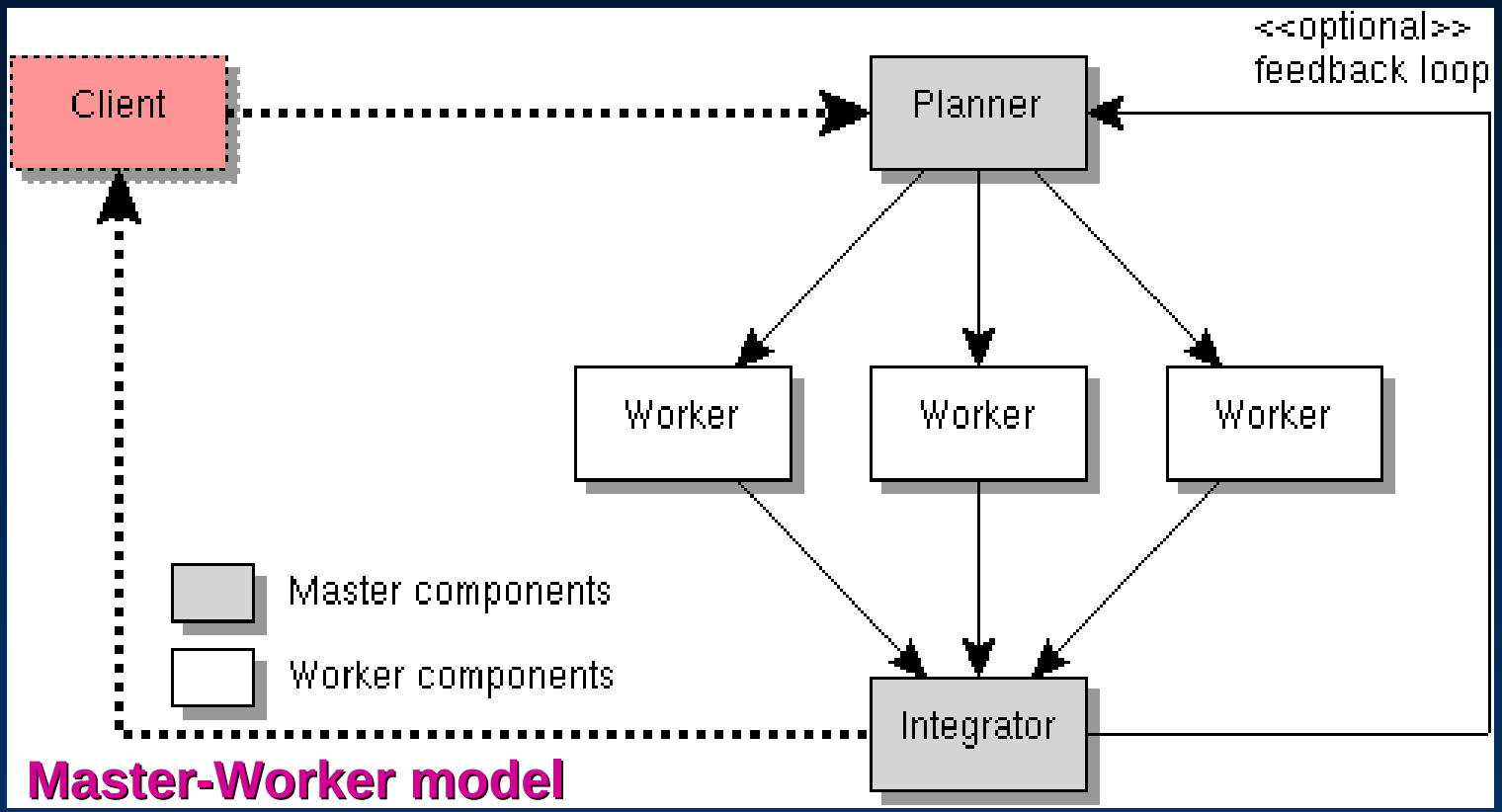
Developed by J. Moscicki, CERN

http://cern.ch/DIANE

Parallel cluster processing

- make fine tuning and customisation easy
- transparently using GRID technology
- application independent

DIANE architecture



Master-Worker model

Parallel execution of independent tasks

Very typical in many scientific applications

Usually applied in local clusters

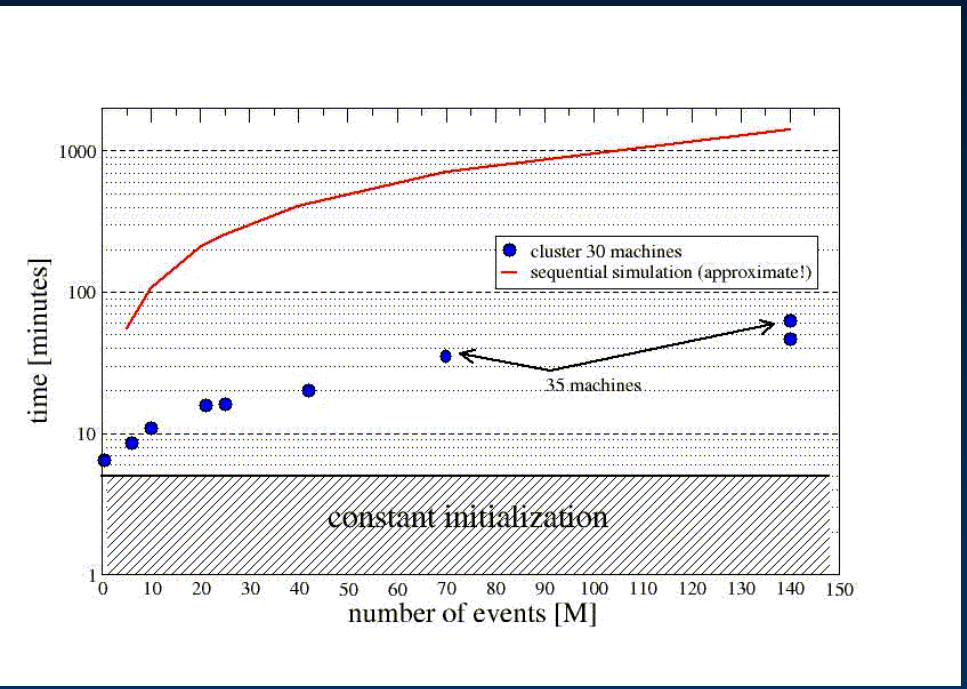
R&D in progress for Large Scale Master-Worker Computing

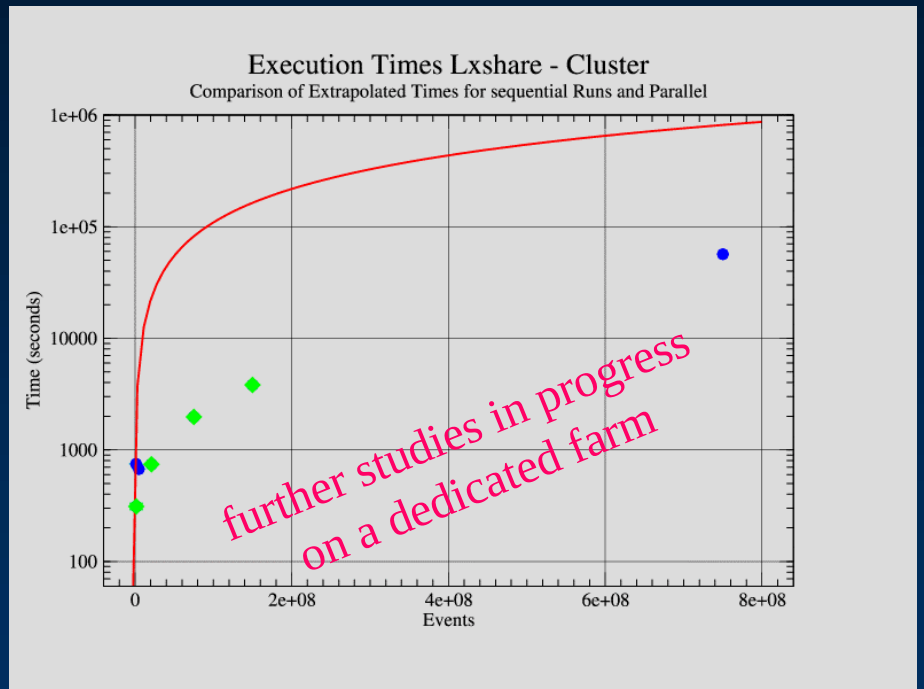
Running in a distributed environment

The application developer is shielded from the complexity of underlying technology via DIANE

- Not affecting the original code of application
  - standalone and distributed case is the **same code**
- Good separation of the subsystems
  - the application does not need to know that it runs in distributed environment
  - the distributed framework (DIANE) does not need to care about what actions an application performs internally

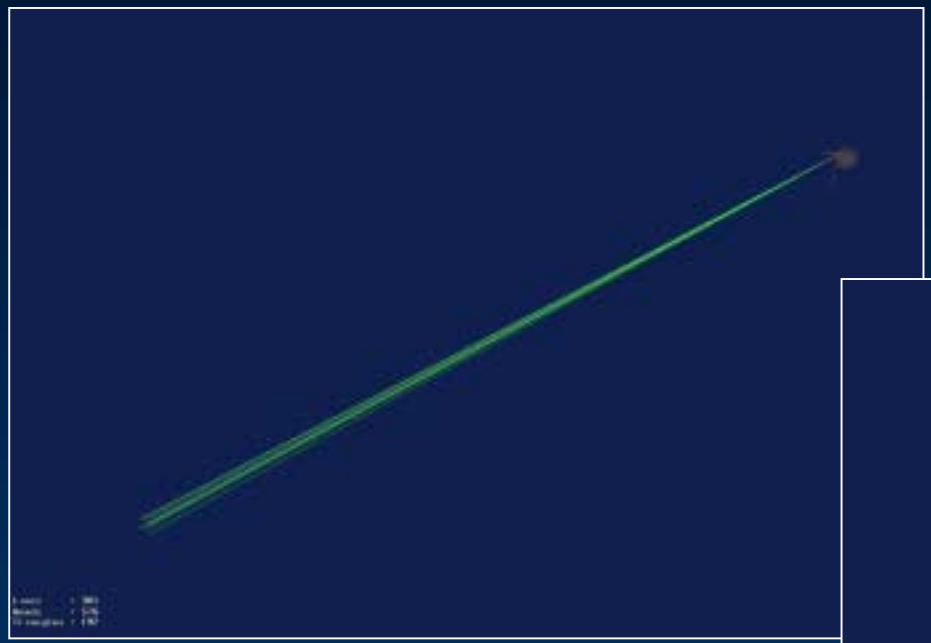
Running in parallel mode

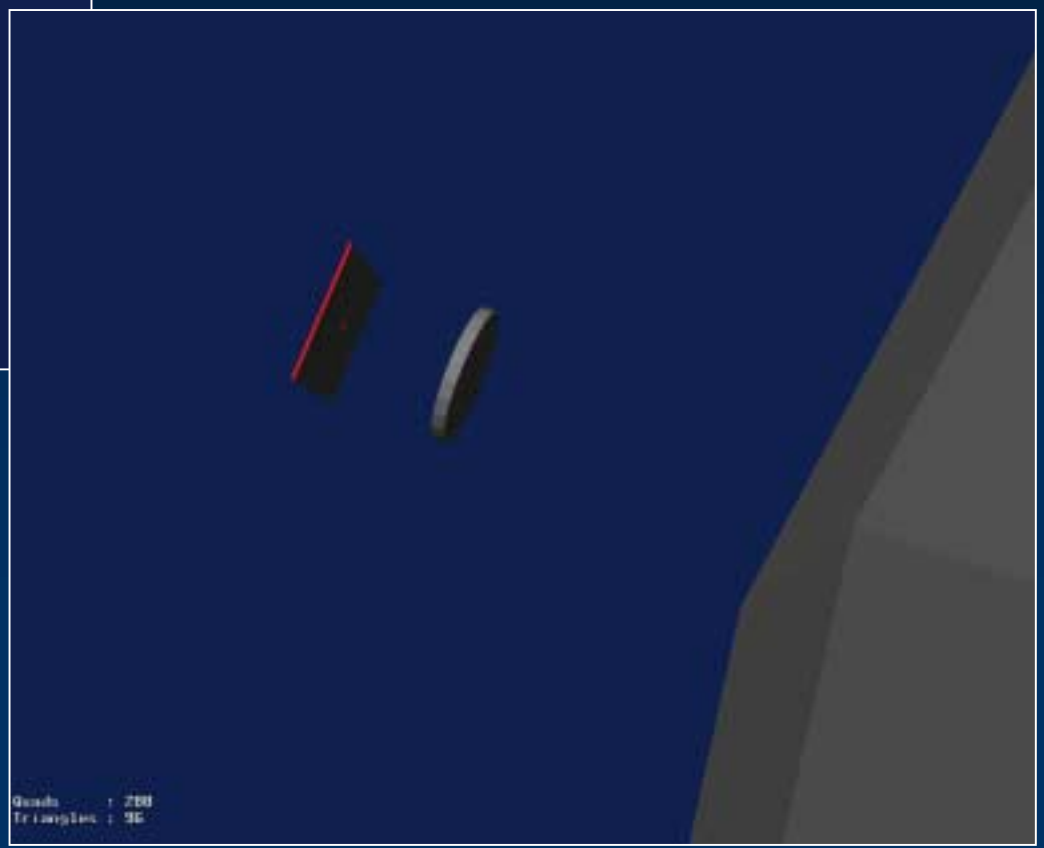




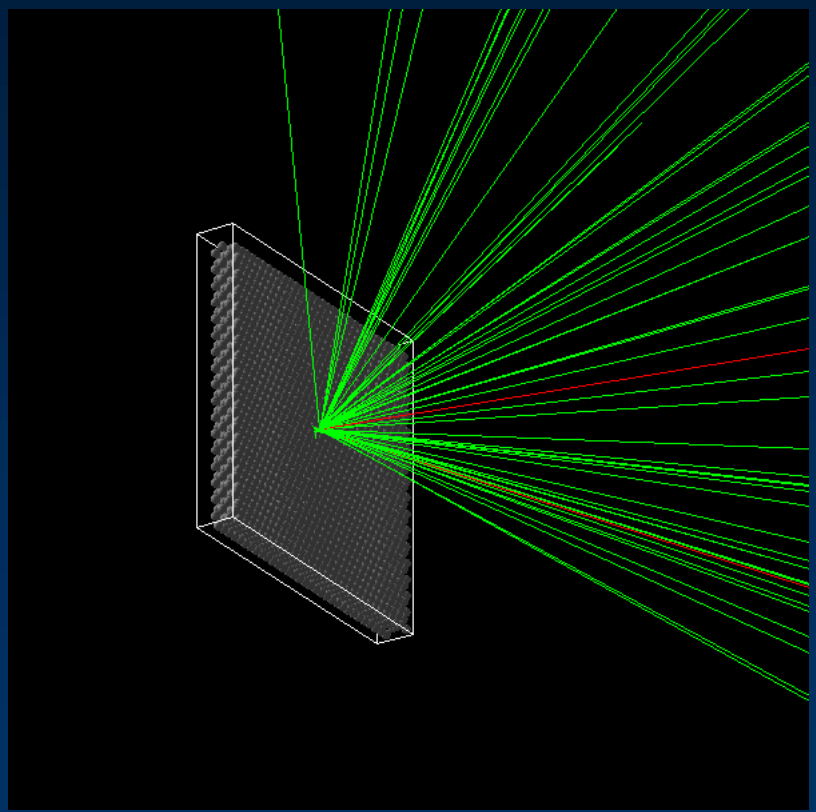
Execution time is reduced by an order of magnitude
(24 h – 750 M events)

Planetary configuration





Effects of material granularity



Further iterations, adding more realistic elements to the simulation

Work in progress to evaluate the effects of the granularity of the material

Summary

- Simulation of Geant4 Bepi Colombo mission to Mercury: study of X-ray fluorescence
- Simulation of a dedicated test beam at Bessy
  - validation of Geant4 atomic relaxation package
- Irradiation of various rock samples
  - creation of a “rock library” of Geant4 simulations
- Model of a more realistic set-up
  - in progress
- Integration in a distributed computing environment
- Valuable collaboration between ESA Astrophysics / Science Payload Division and Geant4 developers
- Work in progress, more to come...