Monte Carlo simulation of X-ray space telescopes

Building a high energy mission

X-ray and Gamma-ray space telescopes are characterized by:

- Intense and complex instrumental background
- A fainter signal from astrophysical sources

The development of a high energy space telescope requires:

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Astronomers

- Scientific goals

  ↓

- Top scientific requirements
  (e.g. sensitivity, angular and
  spectral resolution)

  ↓

- Top technological requirements
  (e.g. background level,
  effective area, focal length)

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Engineers

- Mass budget
- Payload design
- Feasibility study (e.g. materials, tolerances, thermal control)

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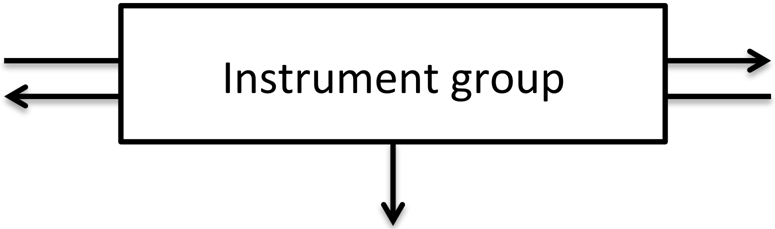

Astronomers

- Scientific goals

  ↓

- Top scientific requirements (e.g. sensitivity, angular and spectral resolution)

  ↓

- Top technological requirements (e.g. background level, effective area, focal length)

✓ Study of the space radiation environment and evaluation of the background level

✓ Definition of the shielding system and focal plane design

(engineering feasibility study)

✓ Calibration phase and data filtering

Engineers

- Mass budget
- Payload design
- Feasibility study (e.g. materials, tolerances, thermal control)

Building a high energy mission

X-ray and Gamma-ray space telescopes are characterized by:

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- A fainter signal from astrophysical sources

The development of a high energy space telescope requires:

Instrument group

We can not reproduce the space environment in laboratory, and we can not repair the telescope once in space.
The simulation of the telescope and spacecraft with the space environment is fundamental for the development of a space mission!

↓

- Top scientific requirements
  (e.g. sensitivity, angular and spectral resolution)

↓

- Top technological requirements
  (e.g. background level, effective area, focal length)

✓ Definition of the shielding system and focal plane design
(engineering feasibility study)

✓ Calibration phase and data filtering

Mass budget

- Payload design
- Feasibility study
  (e.g. materials, tolerances, thermal control)

Monte Carlo simulations

The **Monte Carlo** method generally refers to a stochastic computational algorithm based on the use of randomly generated numbers to solve a problem with a well known probability distribution that can not be analytically computed (Metropolis & Ulam 1949). An example is the angular direction of a photons after it is Compton scattered by the interaction with an electron.

The development of Monte Carlo based simulations of the particles interaction with matter, coupled with computer 3D models of the spacecraft and instruments design, allows

- to track the particle from the first hit to the final energy deposit on the detection plane
- To produce the spatial and energy distribution of the detected background counts with the resolution of a real observation in space
- All this, before even building the real telescope!

The possibility of creating **a virtual model of the telescope** and exposing it to the space radiation environment has fundamental benefits along the entire project development:

- the shielding optimization
- The production and characterization of the background flux
- the calibration validation, the treatment and filtering of the observation data sets.

The Geant4 toolkit

The accuracy of the background Monte Carlo simulations depends on many factors:

- the modelling of the space radiation environment;
- the reliability of the interaction cross sections and parameterization of the physics processes;
- the building of the spacecraft and instruments geometry and composition model.

One of the most used nuclear and particles physics codes is the open source C++ based **Geant4** Monte Carlo toolkit (Agostinelli et al. (2003), Allison et al. (2006)).

Developed by CERN and maintained by a large, international collaboration, the Geant4 toolkit was first conceived for the high energy experiments involved at particles accelerators and then extended to “lower” energy ranges, i.e. the X-ray and Gamma-ray domain, and it is now a widely used particle transport code for astrophysics missions.

On the basis of Geant4 libraries, at the INAF/IASF Bologna we developed the BoGEMMS project, a multi-mission tool for the simulation of high energy mission. The exercise will use BoGEMMS.

BoGEMMS – the Bologna Geant4 Multi-Mission Simulator

Background/calibration study main issues:

1. Unprecedented scientific requirements → New background sources
2. Unprecedented mission design → New shielding solutions
3. Evolution of the mission design (budget) along the years → Customizable simulations
4. Detailed background evaluation → Background spectra as a real observation in space
5. Cross-checking with real data → Analysis and filtering as a real observation in space

---

What makes BoGEMMS an innovative, unique instrument?

- The BoGEMMS architecture takes care of the Geant4 libraries (no need to program in C++!)
- It is totally parametrized and customizable by the user:
  - Physics processes
  - Geometry
  - Input particles
  - Output files
- The output (e.g. energy deposits in the detector) is saved in FITS files, a format widely used in Astronomy and easily processed by IDL/Python/ROOT based tools.

(see Bulgarelli+ 2012, Fioretti+ 2012)

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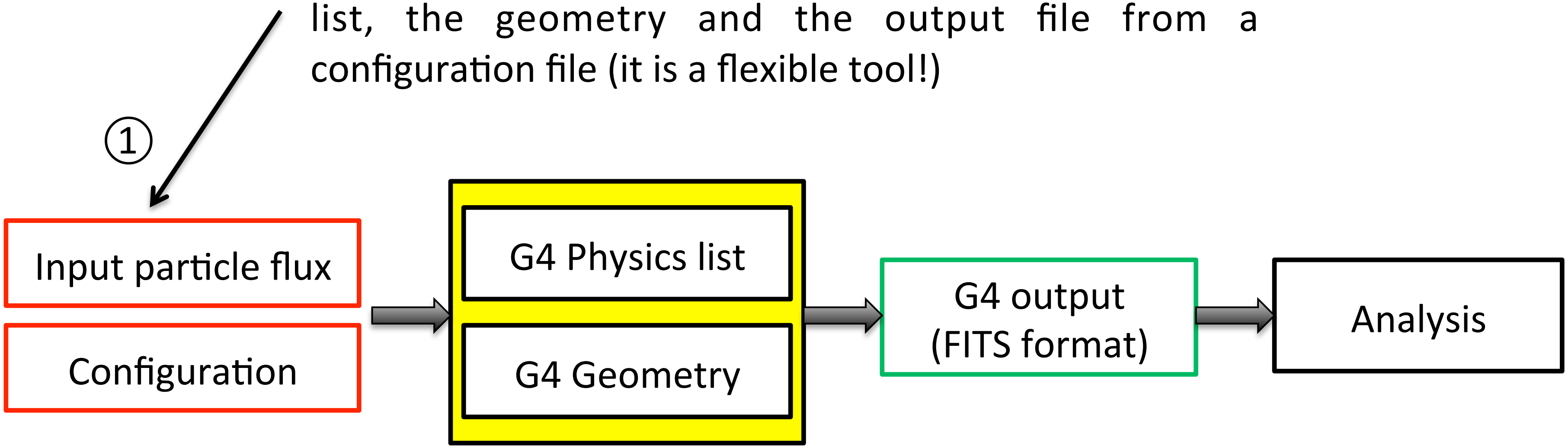

The user sets the radiation environment, the physics list, the geometry and the output file from a configuration file (it is a flexible tool!)

①

Input particle flux

Configuration

G4 Physics list

G4 Geometry

G4 output (FITS format)

Analysis

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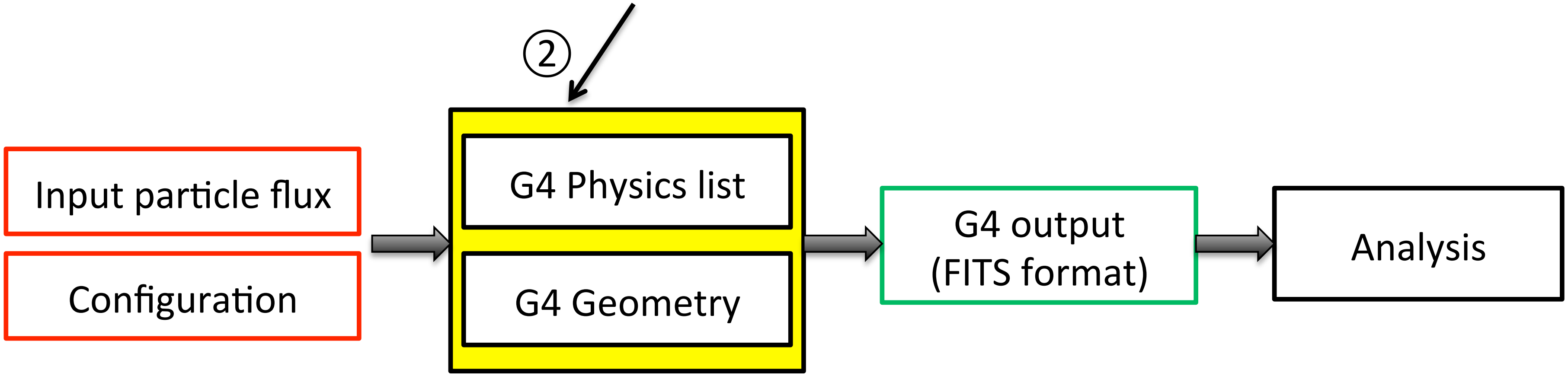
The BoGEMMS core, where the Geant4 libraries are called, produces the simulation output in FITS format. It allows to create a 3d model of the spacecraft.



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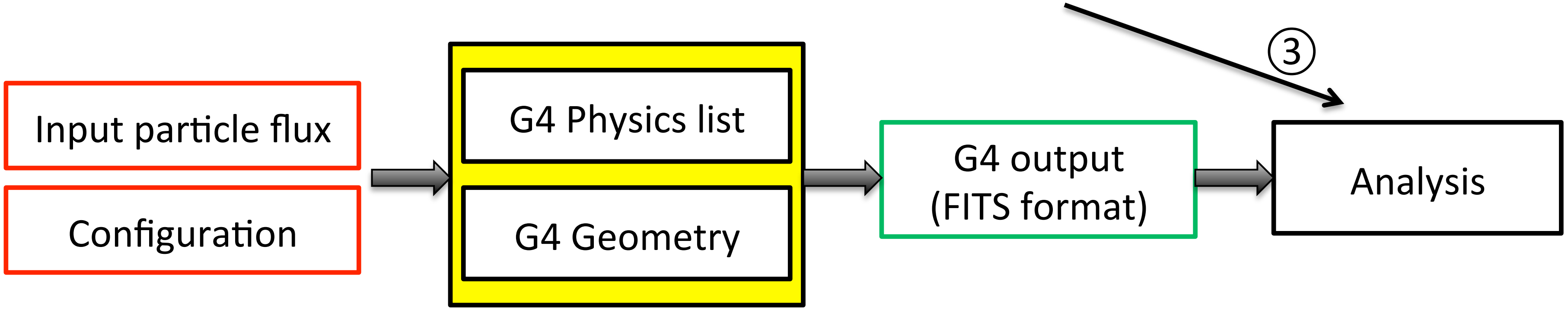
The analysis software filters the output (e.g. energy range, removal of the active shields concidence counts, pattern analysis) as a real observation in space and produces the expected background spectrum, the detection efficiency, etc.



A cook-book for background evaluation

Ingredients:

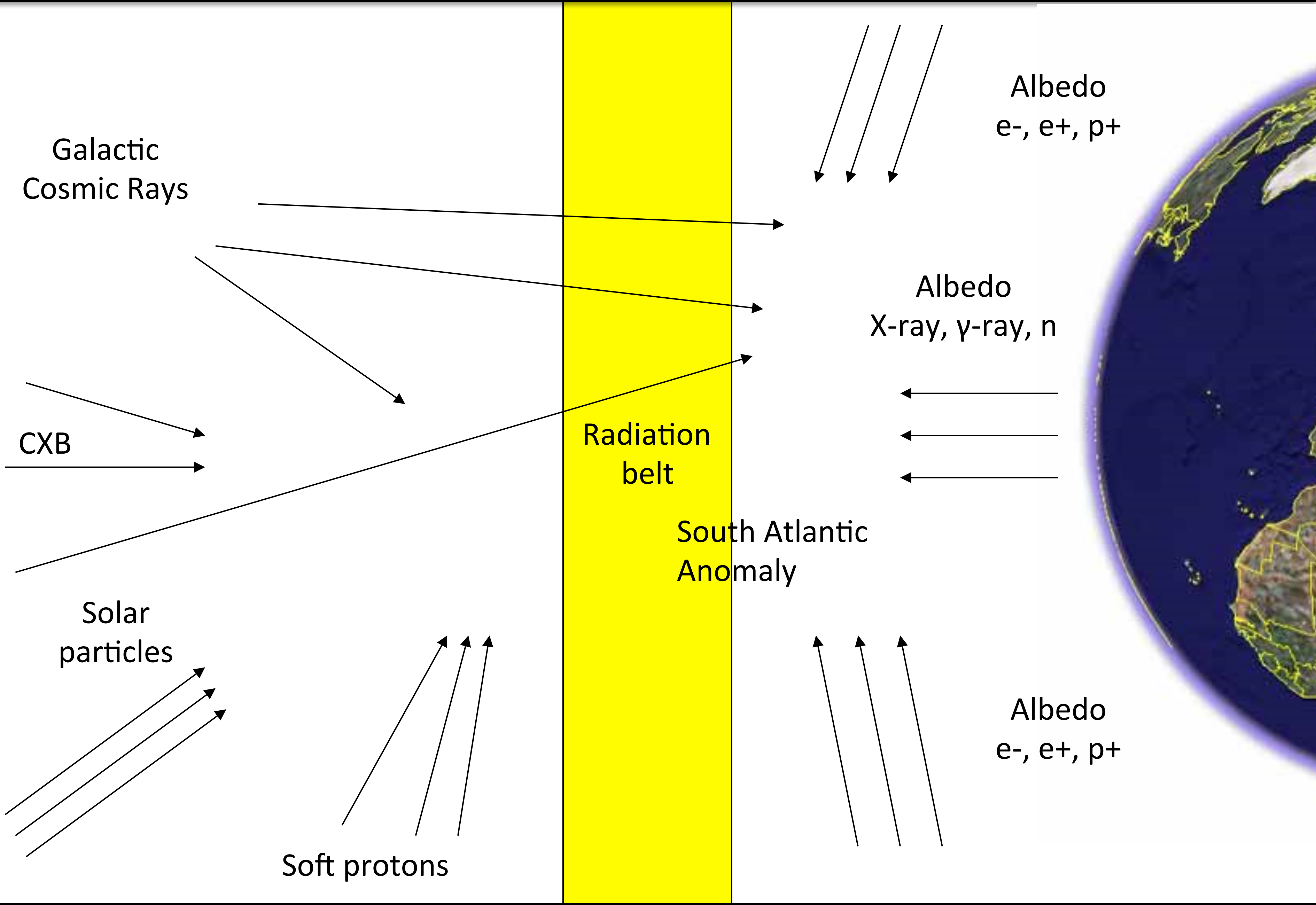
- ✓ Background requirement as the goal
- ✓ Modeling of the space radiation environment
- ✓ Shielding and detectors design
- ✓ Development of a Monte Carlo simulator for particle trasport

Cooking time: it depends on the statistics you want and on the CPU power

Final products:

- ✓ Background spectra
- ✓ Shielding feasibility study
- ✓ Instruments performances
- ✓ …

1. The modeling of the space radiation environment



Galactic Cosmic Rays

CXB

Solar particles

Soft protons

Radiation belt

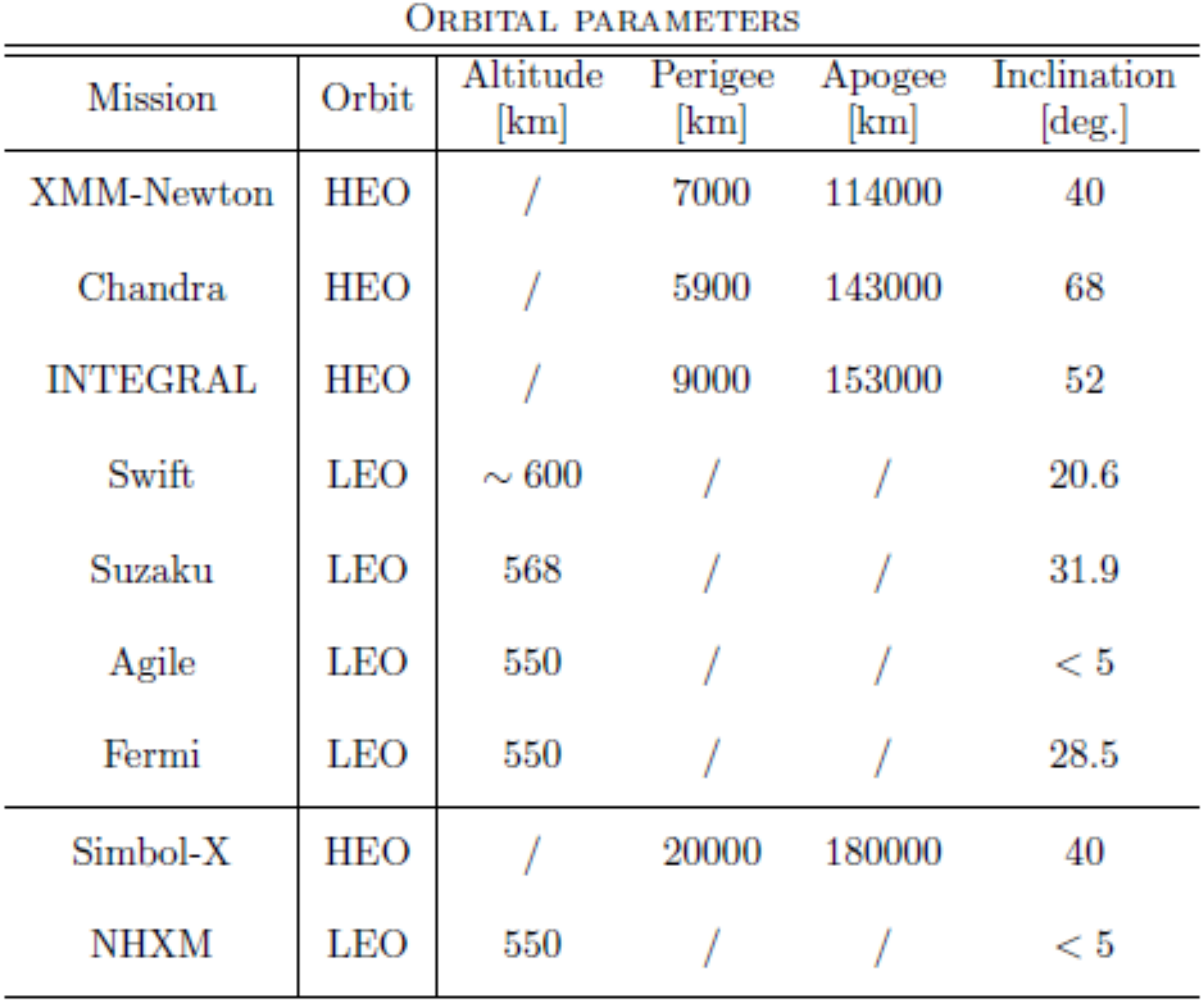
South Atlantic Anomaly

Albedo
e-, e+, p+

Albedo
X-ray, γ-ray, n

Albedo
e-, e+, p+

1. The modeling of the space radiation environment – Highly Elliptical Orbit (XMM, Chandra)



ORBITAL PARAMETERS

Mission	Orbit	Altitude [km]	Perigee [km]	Apogee [km]	Inclination [deg.]
XMM-Newton	HEO	/	7000	114000	40
Chandra	HEO	/	5900	143000	68
INTEGRAL	HEO	/	9000	153000	52
Swift	LEO	~ 600	/	/	20.6
Suzaku	LEO	568	/	/	31.9
Agile	LEO	550	/	/	< 5
Fermi	LEO	550	/	/	28.5
Simbol-X	HEO	/	20000	180000	40
NHXM	LEO	550	/	/	< 5

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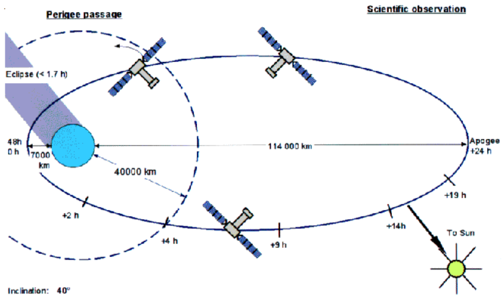
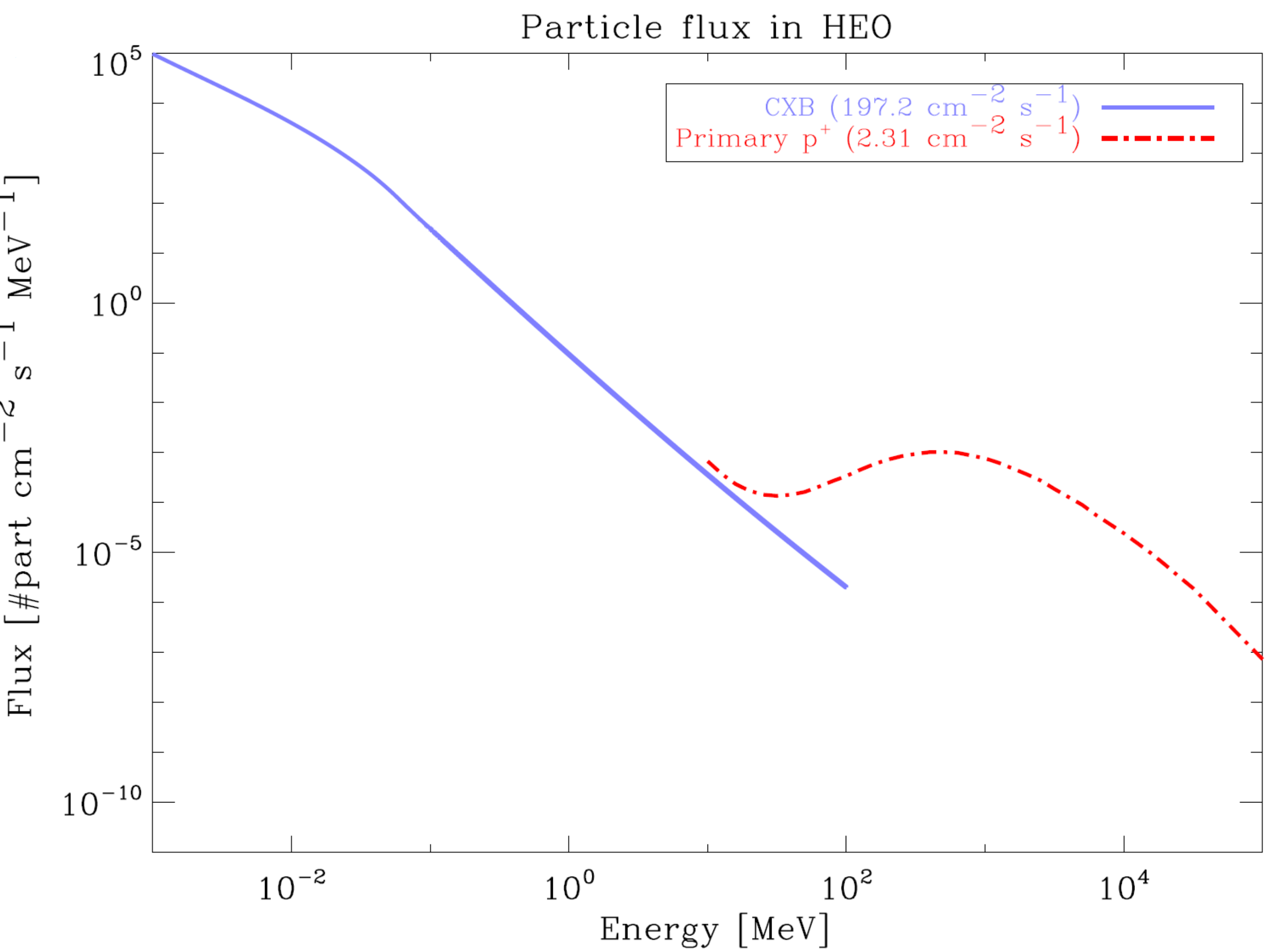
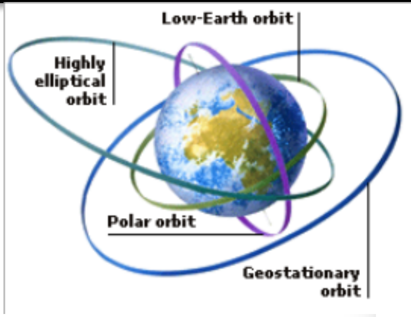
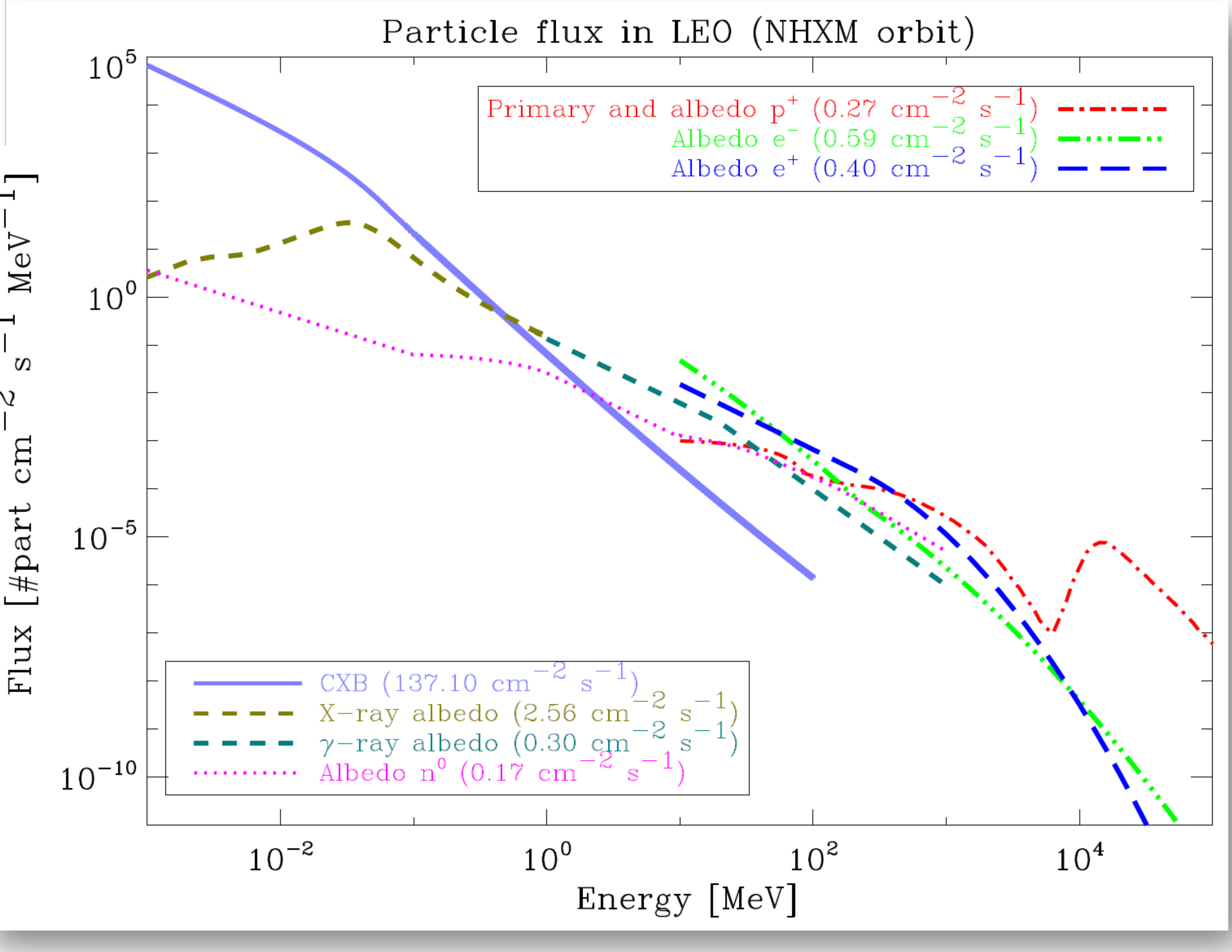


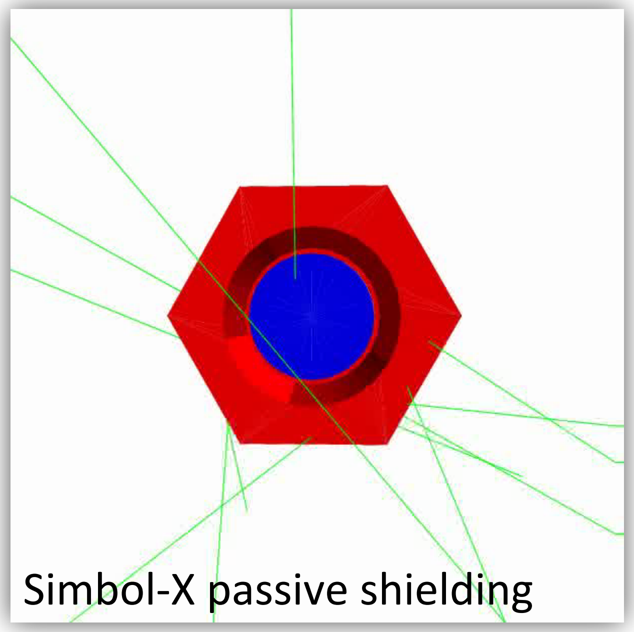


1. The modeling of the space radiation environment – Low Earth Orbit (AGILE, FERMI)

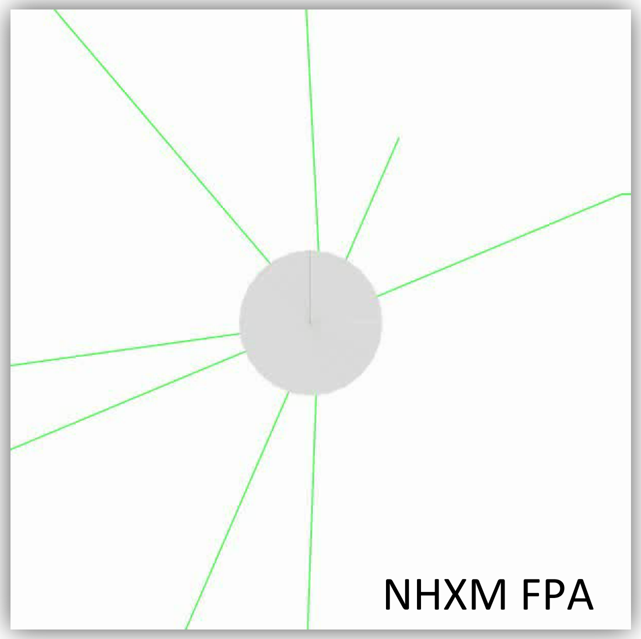




2. Shielding design



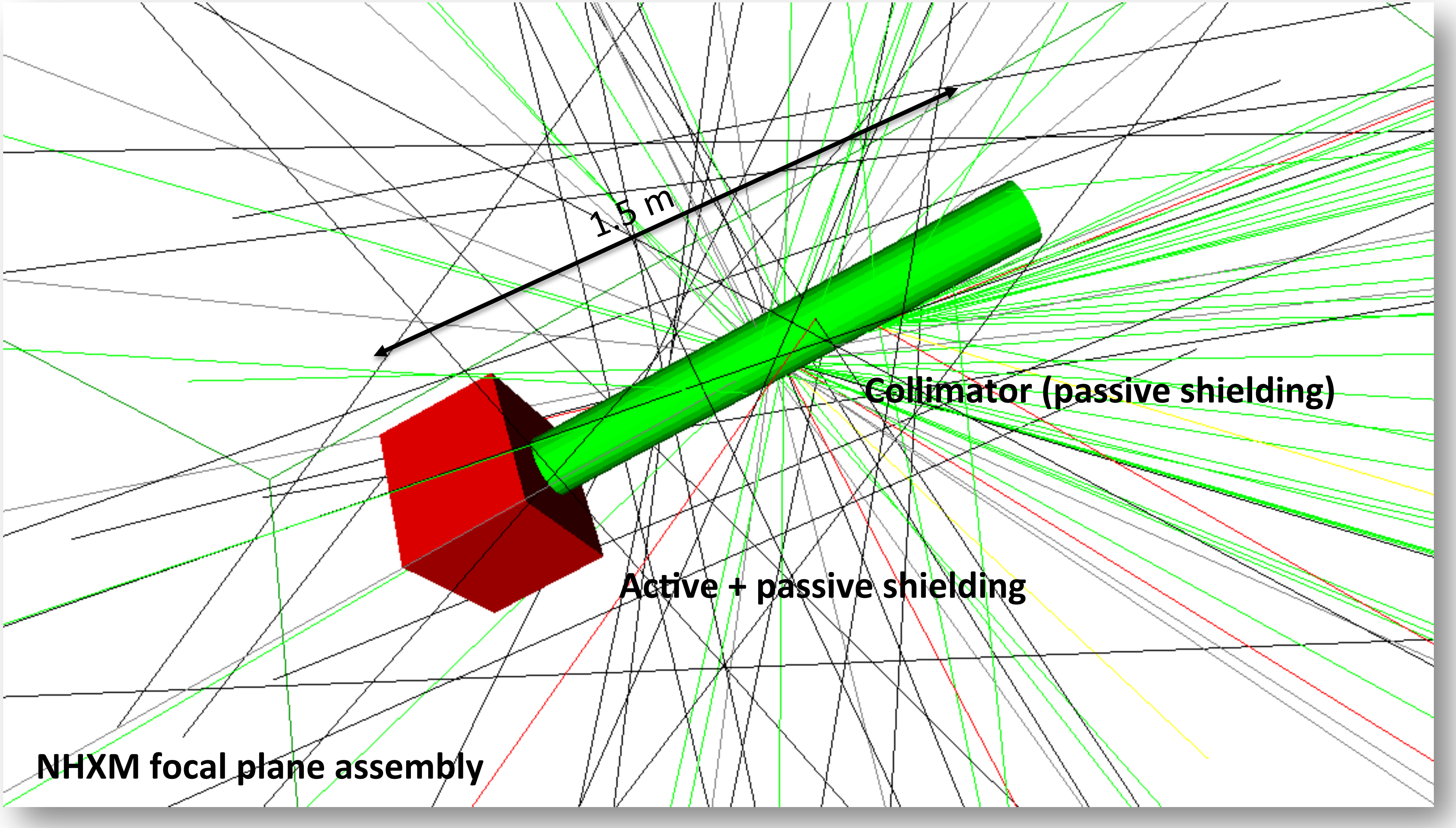
Simbol-X passive shielding



NHXM FPA

GAMMALight

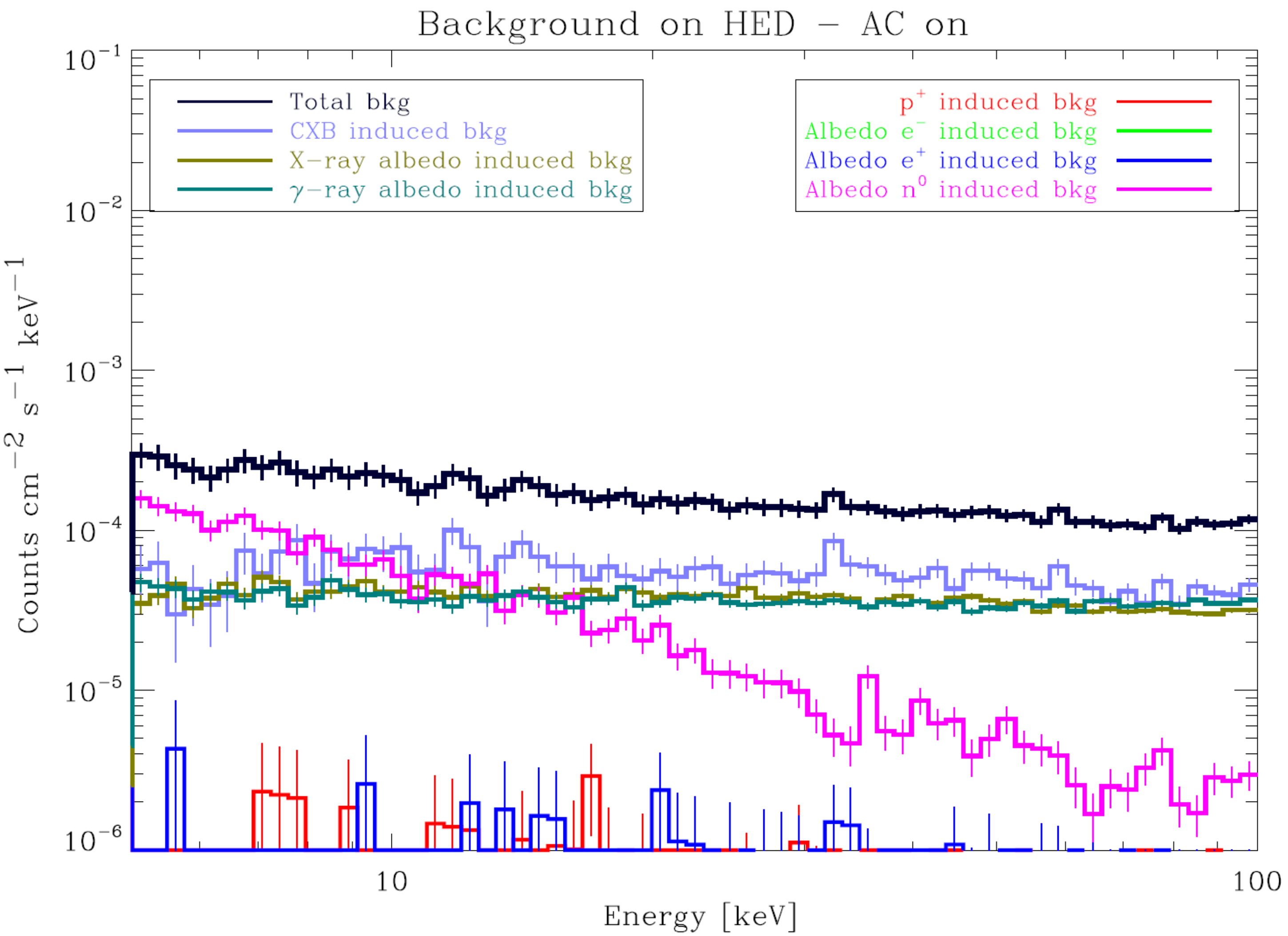
2. Shielding design



3. Background evaluation

Background spectra on a CdTe based hard X-ray detector (HED):

- Energy range = 5 – 100 keV
- Telescope geometry = BOX



Monte Carlo Geant4 simulation of X-ray space detectors: LABX 2014 exercise with BoGEMMS

Setting up the environment

```
> ssh –X userdev6@ice.giano.iasfbo
> cd LABX
> source profile
> . profile_sh
```

To copy the simulation output in your directory:

```
> scp xyz.0.fits.gz <gruppoXX>@tonno:/path-to-your-dir
```

To run the Simulation:

```
> ./bogemms simple_geo.conf 0 MCG6_input.mac
```

The random number seed generator

currentEvent.rndm

This file contains the seed for the random number generator of the Monte Carlo simulation. You have to change the bold numbers for each simulation.

Uvec
1625399437
0
487895547
4579454

Input source set-up

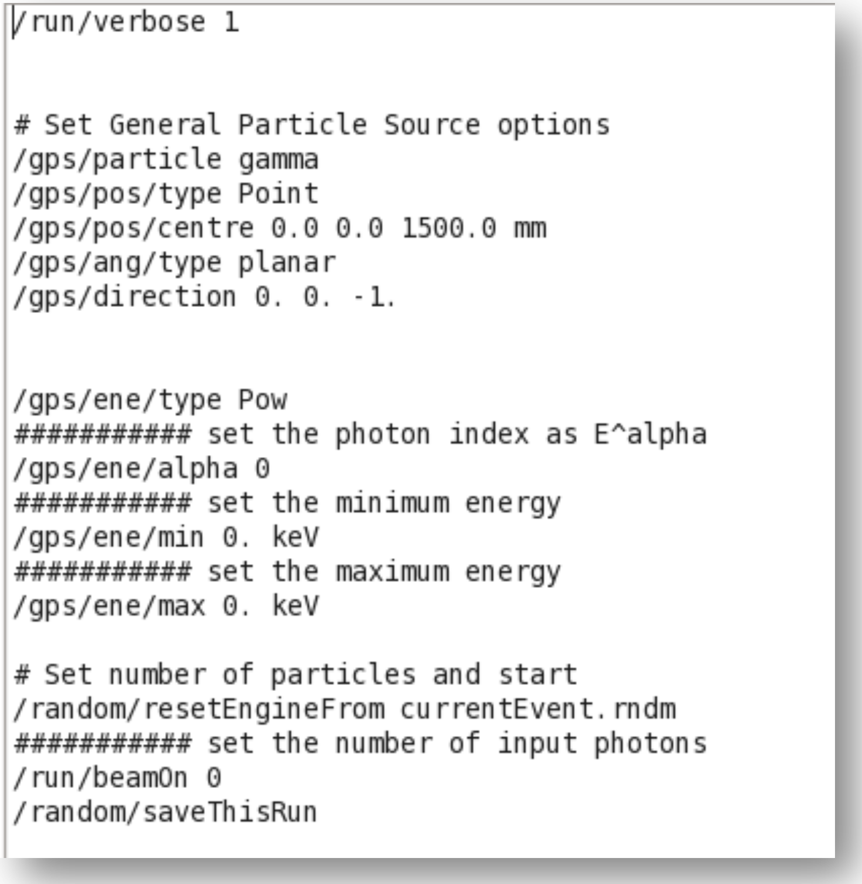
MCG6_input.mac

This macro configures the simulated input photons:

- Geometry of the source (e.g. point source, spherical source)
- The particle type (e.g. gamma for photons)
- The particle angular distribution and direction
- The particle energy range
- The particle spectral distribution
- The number of simulated particles

BoGEMMS uses the Geant4 General Particle Source toolkit for the configuration of the input particles

https://geant4.web.cern.ch/geant4/UserDocumentation/UsersGuides/ForApplicationDeveloper/html/ch02s07.html



```
/run/verbose 1


# Set General Particle Source options
/gps/particle gamma
/gps/pos/type Point
/gps/pos/centre 0.0 0.0 1500.0 mm
/gps/ang/type planar
/gps/direction 0. 0. -1.


/gps/ene/type Pow
########### set the photon index as E^alpha
/gps/ene/alpha 0
########### set the minimum energy
/gps/ene/min 0. keV
########### set the maximum energy
/gps/ene/max 0. keV

# Set number of particles and start
/random/resetEngineFrom currentEvent.rndm
########### set the number of input photons
/run/beamOn 0
/random/saveThisRun
```

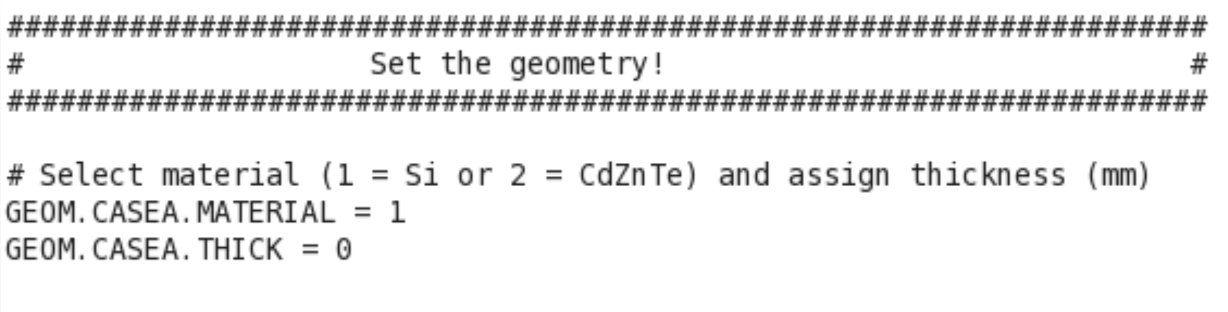
Geometry set-up

simple_geo.conf

The geometry configurator is a built-in feature of the BoGEMMS framework.
It allows to change, among many things, the detector material and thickness:

- Material:
    - 1 = Silicon
    - 2 = CdZnTe

- Thickness in mm



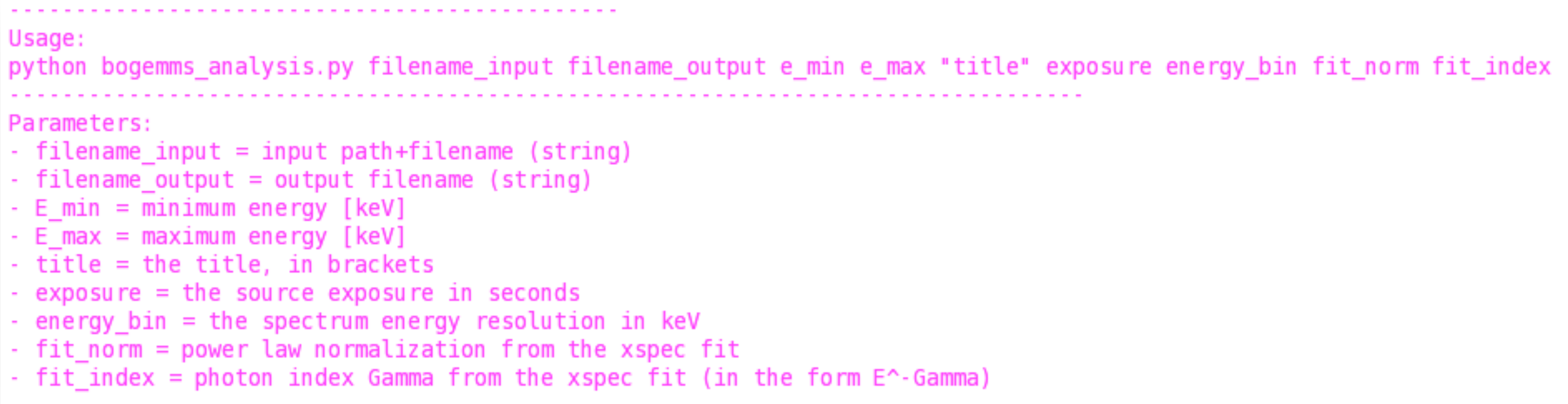
```
######################################################################
#                    Set the geometry!                               #
######################################################################

# Select material (1 = Si or 2 = CdZnTe) and assign thickness (mm)
GEOM.CASEA.MATERIAL = 1
GEOM.CASEA.THICK = 0
```

Analysis of the simulation output

bogemms_analysis.py

The Python script allows to:

- plot the X-ray spectrum of the simulated source as detected by a Silicon or CdZnTe detector
- create the txt file of the binned simulated spectrum to be used as input for the XSPEC analysis



```
----------------------------------------------
Usage:
python bogemms_analysis.py filename_input filename_output e_min e_max "title" exposure energy_bin fit_norm fit_index
---------------------------------------------------------------------------------
Parameters:
- filename_input = input path+filename (string)
- filename_output = output filename (string)
- E_min = minimum energy [keV]
- E_max = maximum energy [keV]
- title = the title, in brackets
- exposure = the source exposure in seconds
- energy_bin = the spectrum energy resolution in keV
- fit_norm = power law normalization from the xspec fit
- fit_index = photon index Gamma from the xspec fit (in the form E^-Gamma)
```

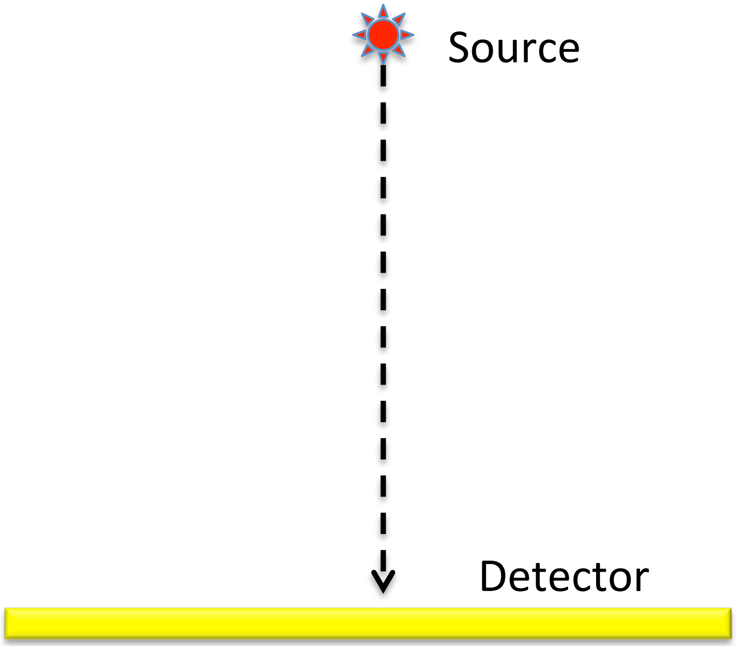
Example:

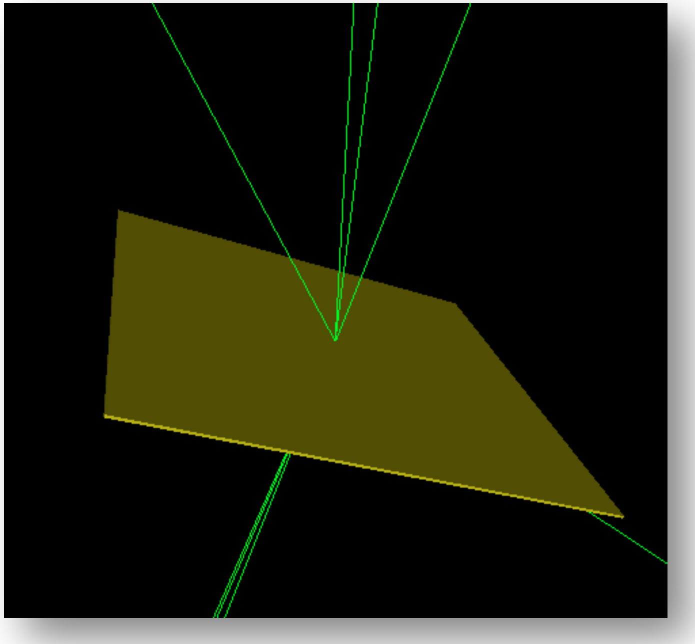
```
> python bogemms_analysis.py ./xyz.0.fits.gz mcg_xspec.txt 0.1 50. "MCG6 - CdZnTe”
1000 0.2 10. 2.1
```

The LABX 2014 Geant4 simulation

- X-ray photons are emitted from a point source placed above the detector
- The material are:
  - Silicon (e.g. the Wide Field Imager of Athena)
  - CdZnTe (e.g. the NuStar detector)

- The detector is planar, no pixels
- Since all the photons are directed to the same point, we consider a detection area of 1 cm^2





The LABX 2014 Geant4 simulation

General objectives:

- Learning the general procedure in the design/testing of X-ray detectors
- Learning how to play with input fluxes and normalization
- Learning how to handle a Monte Carlo simulation

Hands-on exercise:

- Use of the BoGEMMS Geant4 simulator
- Simulation of a set of detectors with different thickness/material
- Simulation of an input astrophysical source
- Analysis and production of:
  - X-ray spectrum
  - Quantum efficiency
  - S/N (signal-to-noise ratio)

The LABX 2014 Geant4 simulation

The exercise step-by-step:

1. Fit the real data set and find out the normalization (NORM) and photon index Γ of the power law in the form:

   $F(E) = NORM \times E^{-\Gamma}$ photons/cm^2/s/keV

2. Compute the integral in energy of F(E) from a minimum energy E_0 to a maximum energy E_1

3. The resulting energy integrated *f* is in units of photons/cm^2/s. For 1 cm^2 of detector (we simulate all the photons in 1 cm^2) we have f photons in 1 second. Given N the number of input simulated photons, compute the how many seconds of source you are simulating (the time exposure)

4. Using the .mac and .conf files, configure the input source and and the geometry, and run the simulation. Try to change the material and try at least two thicknesses for each material

5. Analyse the output and convert it to a txt file to be used as input for the XSPEC analysis (use the source exposure to normalize the flux)

6. Load the file from XPSEC, and compute the quantum efficiency and the Signal-to-Noise ration (S/N = S/sqrt(S))

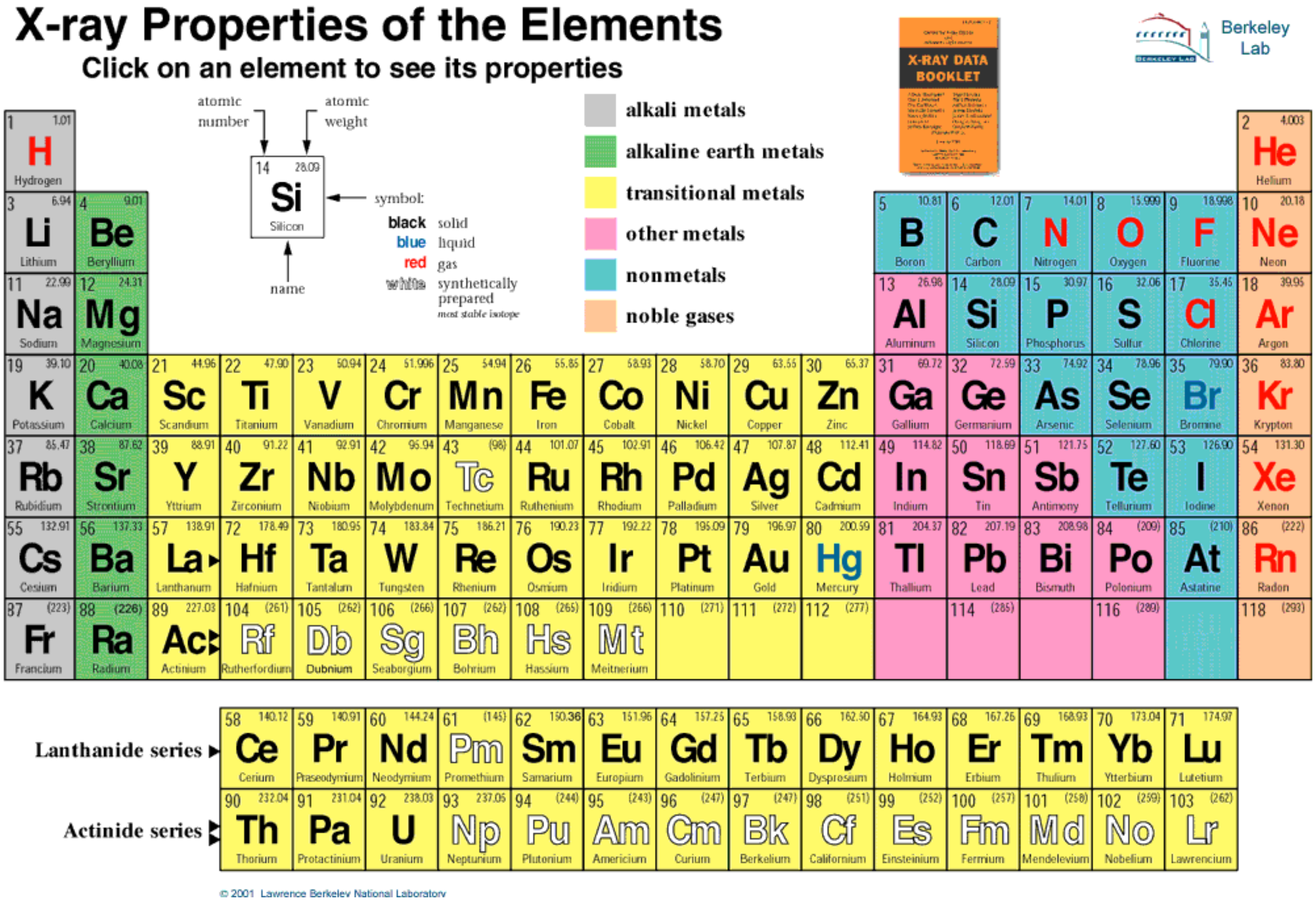
The LABX 2014 Geant4 simulation

Questions:

- What is the source best fit?
- What is the difference between the simulation and the input power law? Could you explain the simulated spectrum?
- What is the best detector material?
- How the thickness affects the result? What is the best thickness?
- What is the quantum efficiency at the Fe Kalpha fluorescence line? And in the 10-15 keV energy range?
- What is the best detector to observe the Fe fluorescence line?

1. X-ray properties of the elements - a useful link

http://xdb.lbl.gov/Section1/Periodic_Table/X-ray_Elements.html



X-ray Properties of the Elements

Click on an element to see its properties

atomic number
atomic weight

14 28.09 Si Silicon

symbol:
name

black solid
blue liquid
red gas
white synthetically prepared
most stable isotope

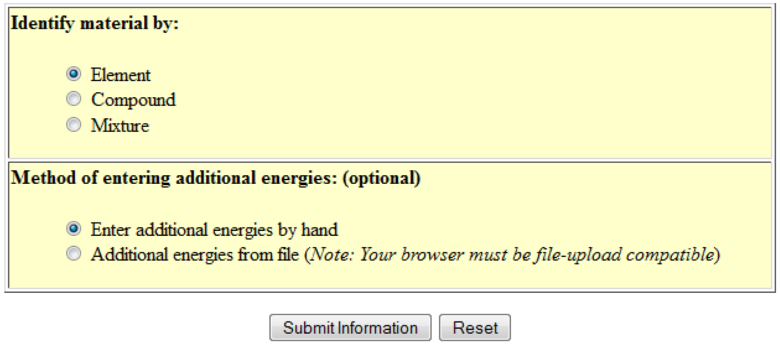
- alkali metals
- alkaline earth metals
- transitional metals
- other metals
- nonmetals
- noble gases

1 1.01 H Hydrogen																	2 4.003 He Helium
3 6.94 Li Lithium	4 9.01 Be Beryllium											5 10.81 B Boron	6 12.01 C Carbon	7 14.01 N Nitrogen	8 15.999 O Oxygen	9 18.998 F Fluorine	10 20.18 Ne Neon
11 22.99 Na Sodium	12 24.31 Mg Magnesium											13 26.98 Al Aluminum	14 28.09 Si Silicon	15 30.97 P Phosphorus	16 32.06 S Sulfur	17 35.45 Cl Chlorine	18 39.95 Ar Argon
19 39.10 K Potassium	20 40.08 Ca Calcium	21 44.96 Sc Scandium	22 47.90 Ti Titanium	23 50.94 V Vanadium	24 51.996 Cr Chromium	25 54.94 Mn Manganese	26 55.85 Fe Iron	27 58.93 Co Cobalt	28 58.70 Ni Nickel	29 63.55 Cu Copper	30 65.37 Zn Zinc	31 69.72 Ga Gallium	32 72.59 Ge Germanium	33 74.92 As Arsenic	34 78.96 Se Selenium	35 79.90 Br Bromine	36 83.80 Kr Krypton
37 85.47 Rb Rubidium	38 87.62 Sr Strontium	39 88.91 Y Yttrium	40 91.22 Zr Zirconium	41 92.91 Nb Niobium	42 95.94 Mo Molybdenum	43 (98) Tc Technetium	44 101.07 Ru Ruthenium	45 102.91 Rh Rhodium	46 106.42 Pd Palladium	47 107.87 Ag Silver	48 112.41 Cd Cadmium	49 114.82 In Indium	50 118.69 Sn Tin	51 121.75 Sb Antimony	52 127.60 Te Tellurium	53 126.90 I Iodine	54 131.30 Xe Xenon
55 132.91 Cs Cesium	56 137.33 Ba Barium	57 138.91 La ▸ Lanthanum	72 178.49 Hf Hafnium	73 180.95 Ta Tantalum	74 183.84 W Tungsten	75 186.21 Re Rhenium	76 190.23 Os Osmium	77 192.22 Ir Iridium	78 195.09 Pt Platinum	79 196.97 Au Gold	80 200.59 Hg Mercury	81 204.37 Tl Thallium	82 207.19 Pb Lead	83 208.98 Bi Bismuth	84 (209) Po Polonium	85 (210) At Astatine	86 (222) Rn Radon
87 (223) Fr Francium	88 (226) Ra Radium	89 227.03 Ac ▸ Actinium	104 (261) Rf Rutherfordium	105 (262) Db Dubnium	106 (266) Sg Seaborgium	107 (262) Bh Bohrium	108 (265) Hs Hassium	109 (266) Mt Meitnerium	110 (271)	111 (272)	112 (277)		114 (285)		116 (289)		118 (293)

Lanthanide series ▸	58 140.12 Ce Cerium	59 140.91 Pr Praseodymium	60 144.24 Nd Neodymium	61 (145) Pm Promethium	62 150.36 Sm Samarium	63 151.96 Eu Europium	64 157.25 Gd Gadolinium	65 158.93 Tb Terbium	66 162.50 Dy Dysprosium	67 164.93 Ho Holmium	68 167.26 Er Erbium	69 168.93 Tm Thulium	70 173.04 Yb Ytterbium	71 174.97 Lu Lutetium
Actinide series ▸	90 232.04 Th Thorium	91 231.04 Pa Protactinium	92 238.03 U Uranium	93 237.05 Np Neptunium	94 (244) Pu Plutonium	95 (243) Am Americium	96 (247) Cm Curium	97 (247) Bk Berkelium	98 (251) Cf Californium	99 (252) Es Einsteinium	100 (257) Fm Fermium	101 (258) Md Mendelevium	102 (259) No Nobelium	103 (262) Lr Lawrencium

2. X-ray properties of the elements - a useful link

NIST Database and web application for the retrieval of elements and compounds attenuation coefficient: http://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html

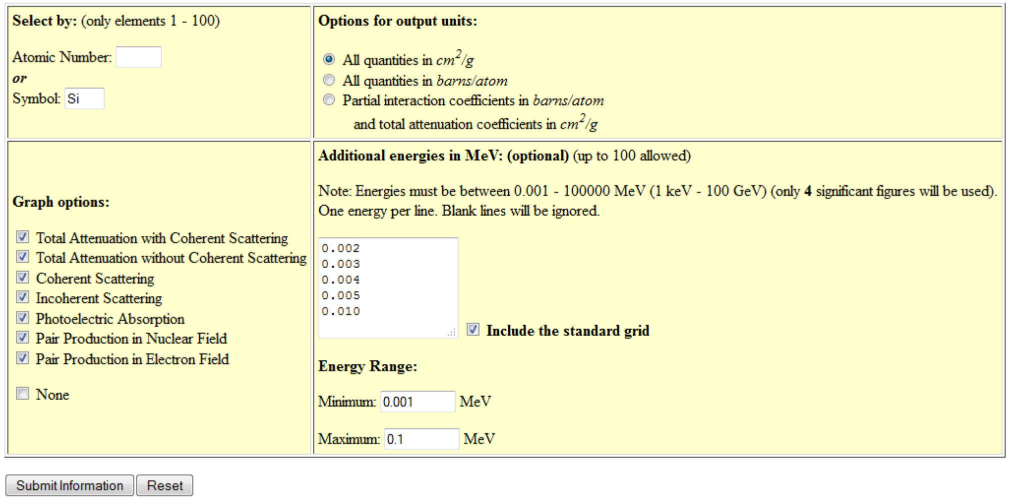


Identify material by:

- ● Element
- ○ Compound
- ○ Mixture

Method of entering additional energies: (optional)

- ● Enter additional energies by hand
- ○ Additional energies from file (*Note: Your browser must be file-upload compatible*)



Select by: (only elements 1 - 100)

Atomic Number:

or

Symbol: Si

Options for output units:

- ● All quantities in *cm²/g*
- ○ All quantities in *barns/atom*
- ○ Partial interaction coefficients in *barns/atom* and total attenuation coefficients in *cm²/g*

Graph options:

- ☑ Total Attenuation with Coherent Scattering
- ☑ Total Attenuation without Coherent Scattering
- ☑ Coherent Scattering
- ☑ Incoherent Scattering
- ☑ Photoelectric Absorption
- ☑ Pair Production in Nuclear Field
- ☑ Pair Production in Electron Field
- ☐ None

Additional energies in MeV: (optional) (up to 100 allowed)

Note: Energies must be between 0.001 - 100000 MeV (1 keV - 100 GeV) (only **4** significant figures will be used). One energy per line. Blank lines will be ignored.

```
0.002
0.003
0.004
0.005
0.010
```

☑ **Include the standard grid**

Energy Range:

Minimum: 0.001 MeV

Maximum: 0.1 MeV