

A New Radioactive Decay Code for Geant4



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S. Hauf, M. Kuster, M. Batič, Z. W. Bell, D. H. H. Hoffmann, P. M. Lang, M. G. Pia, G. Weidenspointner, A. Zoglauer

```
class G4RadioactiveDecay : public G4VRestDiscreteProcess {
public:
//G4RadioactiveDecay(const G4String& processName="RadioactiveDecay");
statisticalApproach=true, G4bool
G4RadioactiveDecay(const G4String& processName="RadioactiveDecay", G4bool
taccountForRecoil=true, G4bool statisticalApproach=true, G4bool
tdecayChainAnalysis=false);
~G4RadioactiveDecay();
void SetStatistic
G4VParticleChange * DecayIt(const G4Track& theTrack, const G4Step& theStep);
GetVREmission() {return vrDoEmission;}
void SetVREmission(G4int Z, G4int A) {vrDoEmission[Z][A]=true; vrAll=false;}
G4bool GetVREmission(G4int Z, G4int A) {return vrDoEmission[Z][A];}
std::unordered_map<G4int, std::unordered_map<G4int, G4bool> > GetVREmission()
{return vrDoEmission;}
#include "G4FragmentVect
void SetVRN0ForNucleus( G4int Z, G4int A, G4double N){N0[Z][A]=1.; vr=true;
vrAll=true; ntimesVR=N;}

```

Contents



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- ▶ Radioactive decays in Monte-Carlo Simulations
- ▶ Validation and Verification
- ▶ Decay-Chains & Activation

Radioactive decays in Monte-Carlo Simulations



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- ▶ Radioactive decays play a role in diverse fields: material sciences, astrophysics, nuclear physics, biophysics, nuclear proliferation monitoring, homeland security...
- ▶ Usually: observable and/or background source
- ▶ Problem: as experiments get more complex radiation characteristics and background are not easily predictable
- ▶ Common solution: Monte Carlo simulations

Radioactive decays in Monte-Carlo Simulations



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- ▶ Radioactive decay code implementations exist in popular general purpose Monte-Carlo frameworks:

MCNP

- ▶ Delayed gammas from tabulated data
- ▶ Possibility to integrate specialized tools such as ORIGEN2 or CINDER90, adding activation, processing of decay chains
- ▶ Alpha and beta-particles from tabulated input
- ▶ Summary statistics

FLUKA

- ▶ Generates and transports gamma and beta radiation
- ▶ Alpha decays only added in newest version
- ▶ Decay chains and activation
- ▶ NNDC library based on ENSDF
- ▶ Summary statistics

Geant4

- ▶ Generation of alpha, beta and gamma radiation
- ▶ Three distinct processes involved
- ▶ Decay library based on ENSDF
- ▶ Decay chains
- ▶ Activation present as distinct process
- ▶ Per-decay simulation

Radioactive decays in Monte-Carlo Simulations



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- ▶ Radioactive decay code implementations exist in popular general purpose Monte-Carlo frameworks:

MCNP

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Geant4

- ▶ Generation of alpha, beta and gamma radiation
- ▶ Three distinct processes involved
- ▶ Decay library based on ENSDF
- ▶ Decay chains
- ▶ Activation present as distinct process
- ▶ **Per-decay simulation**

- ▶ **Experimental requirements (per-decay, summary) defines framework**

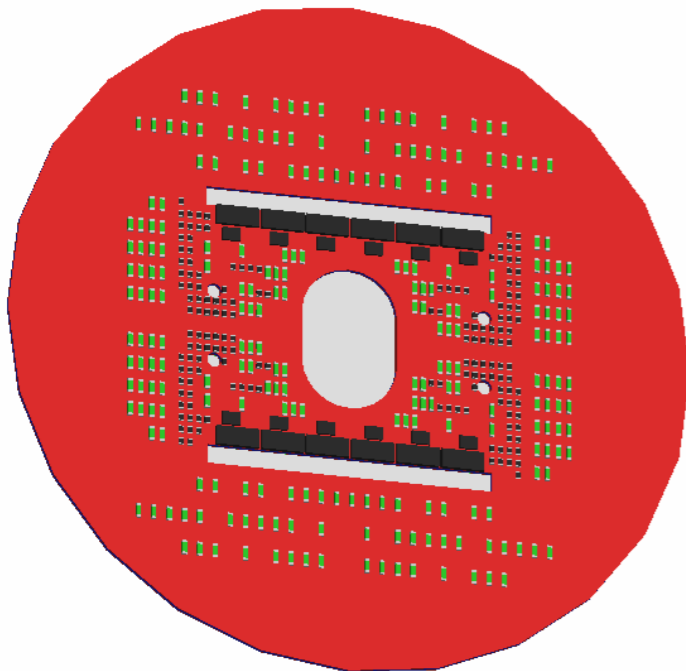
Radioactive decays in Monte-Carlo Simulations



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- ▶ Radioactive decay code implementations exist in popular general purpose Monte-Carlo frameworks
- ▶ Experimental requirements (per-decay, summary) defines framework
- ▶ **What if other requirements favor other frameworks?**

Geometry



Code-Requirements

C++
~~Fortran~~

Necessary Physics

- ✓ PIXE
- ✓ Scattering
- ✓ Fluorescence
- ✓ Annihilation
- ✓ Spallation

Radioactive decays in Monte-Carlo Simulations



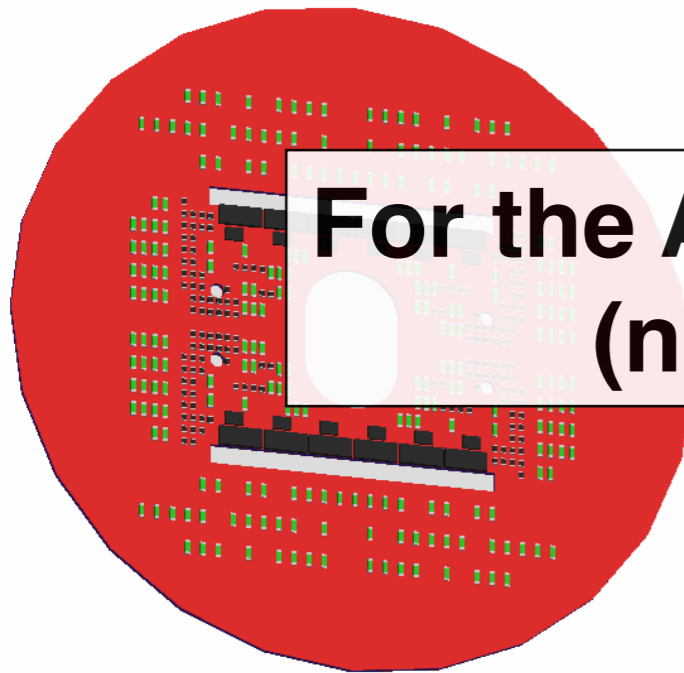
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- ▶ Radioactive decay code implementations exist in popular general purpose Monte-Carlo frame-works
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- ▶ **What if other requirements favor other frame-works?**

Geometry

Code-Requirements

Necessary Physics



For the ATHENA X-ray telescope simulation (next talk) these lead to Geant4

~~Fortran~~

✓ PIXE

✓ Scattering

✓ Fluorescence

✓ Annihilation

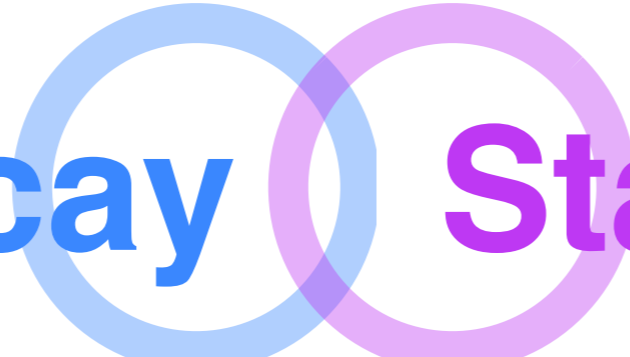
✓ Spallation

Radioactive decays in Monte-Carlo Simulations



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- ▶ Radioactive decay code implementations exist in popular general purpose Monte-Carlo frameworks
- ▶ Experimental requirements (per-decay, summary) defines framework
- ▶ What if other requirements favor other frameworks?
- ▶ **Solution: an implementation which allows for physically accurate per-decay sampling AND statistical sampling when the outcome of many decays is of interest.**

Per-decay  Statistical

Software Requirements for a Radioactive Decay Simulation



- ▶ **Decay an unstable nucleus**
 - ▶ Sample discrete decay emission: alpha, neutrinos (EC)
 - ▶ Sample continuous decay emission: Beta-Fermi-function (e, neutrinos)
 - ▶ Generate daughter nucleus
 - ▶ Take care of kinematics: energy- and momentum conservation
- ▶ **Deexcite daughter nucleus**
 - ▶ Sample gamma, X-rays and conversion electrons resulting from nuclear deexcitation
 - ▶ Sample fluorescence and Auger-electrons due to shell vacancies
- ▶ **Handle Decay chains efficiently**
- ▶ **Handle long term activation**

The per-Decay approach of the *current* Geant4 Radioactive Decay Code



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- ▶ Original implementation: F. Lei & P. Truscott (QinetiC), Geant4.9.4-p04
- ▶ Functional per-decay approach with *a few inconsistencies* and missing features
- ▶ Based on popular ENSDF library

Adapt what is good

Improve where necessary

Add what is missing

- ✓ **Decay an unstable nucleus**
 - ✓ Sample discrete decay emission: alpha, neutrinos (EC)
 - ✓ Sample continuous decay emission: Beta-Fermi-function (e, neutrinos)
 - ✓ Generate daughter nucleus
 - ✓ *Take care of kinematics: energy- and momentum conservation*
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A *new* Radioactive Decay Code for Geant4



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▶ **Novel statistical sampling approach**

- ▶ ENSDF-based library only data source
- ▶ Compatible with NuDAT
- ▶ Efficient sampling of many decays

▶ **Per-decay approach based on adapted F. Lei & P. Truscott implementation.**

- ▶ Corrected fluorescence sampling bug (independently corrected in G4.9.5)
- ▶ Corrected energy conservation problem (present in G4.9.5)
- ▶ Flexible delegation to deexcitation and relaxation processes, i.e. changes can easily be included

▶ **Flexible Beta-Fermi function implementation**

▶ **Efficient handling of decay chains sampling only isotopes of interest**

▶ **Radioactive background sources**

▶ **Provision of bookkeeping classes for long term activation**



✓ **Decay an unstable nucleus**

- ✓ Sample discrete decay emission: alpha, neutrinos (EC)
- ✓ Sample continuous decay emission: Beta-Fermi-function (e, neutrinos)
- ✓ Generate daughter nucleus
- ✓ Take care of kinematics: energy- and momentum conservation

✓ **Deexcite daughter nucleus**

- ✓ Sample gamma, X-rays and conversion electrons resulting from atomic deexcitation
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✓ **Handle Decay chains efficiently**

✓ **Handle long term activation**

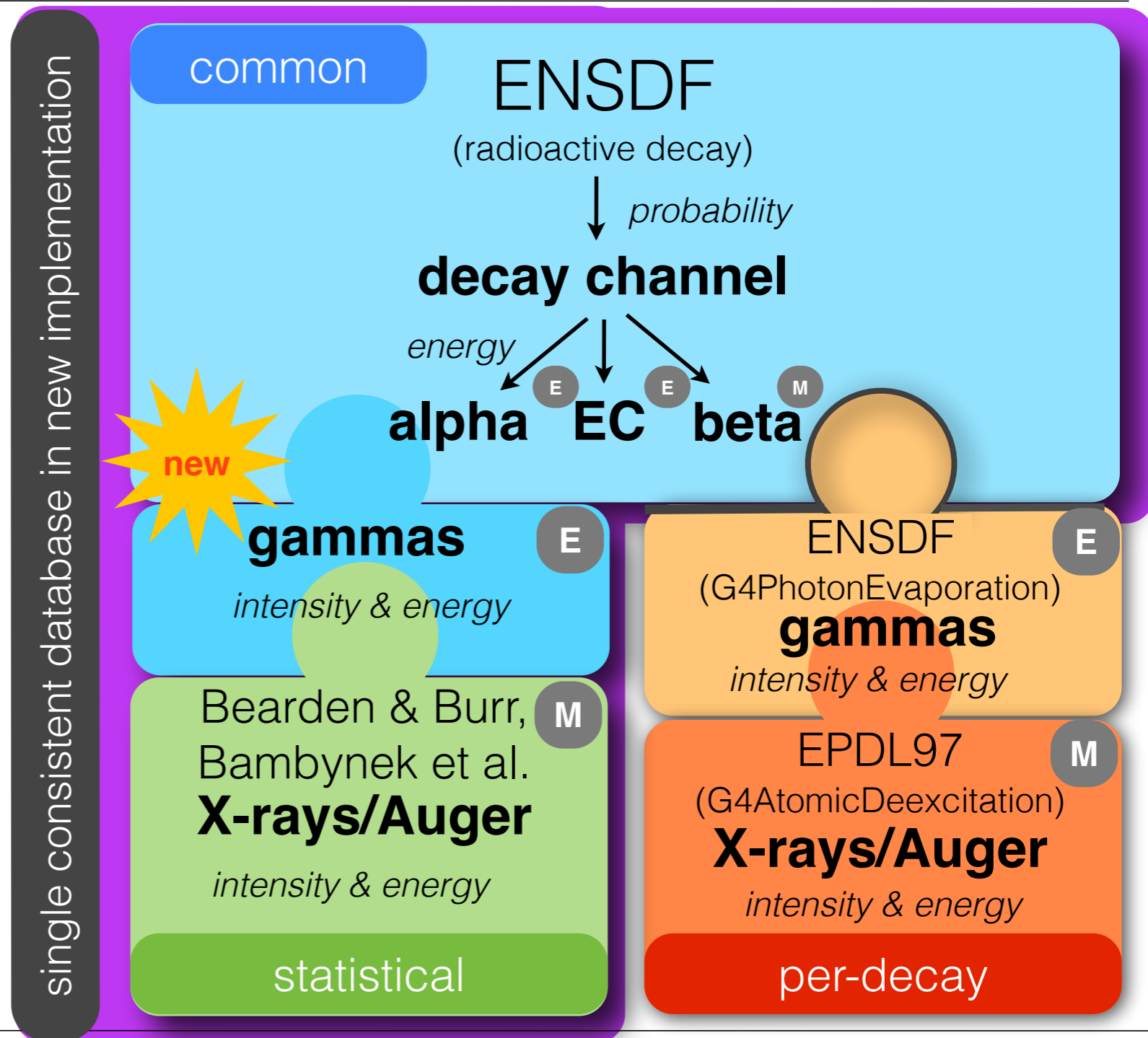
✓ **New statistical sampling approach**

Verification of both Codes with ENSDF



- ▶ Both codes use a library based on the Evaluated Nuclear Structure Data File (ENSDF)
- ▶ Verification/Validation data from NNDC supplied program *RADLST*
- ▶ **~3000 isotopes&levels, broader than any previous verification**
- ▶ **Additionally validation against own data from HPGe detector measurements**

- E** Experimental data
- M** Derived from models



Intensity Verification Gamma Rays (>30 keV)



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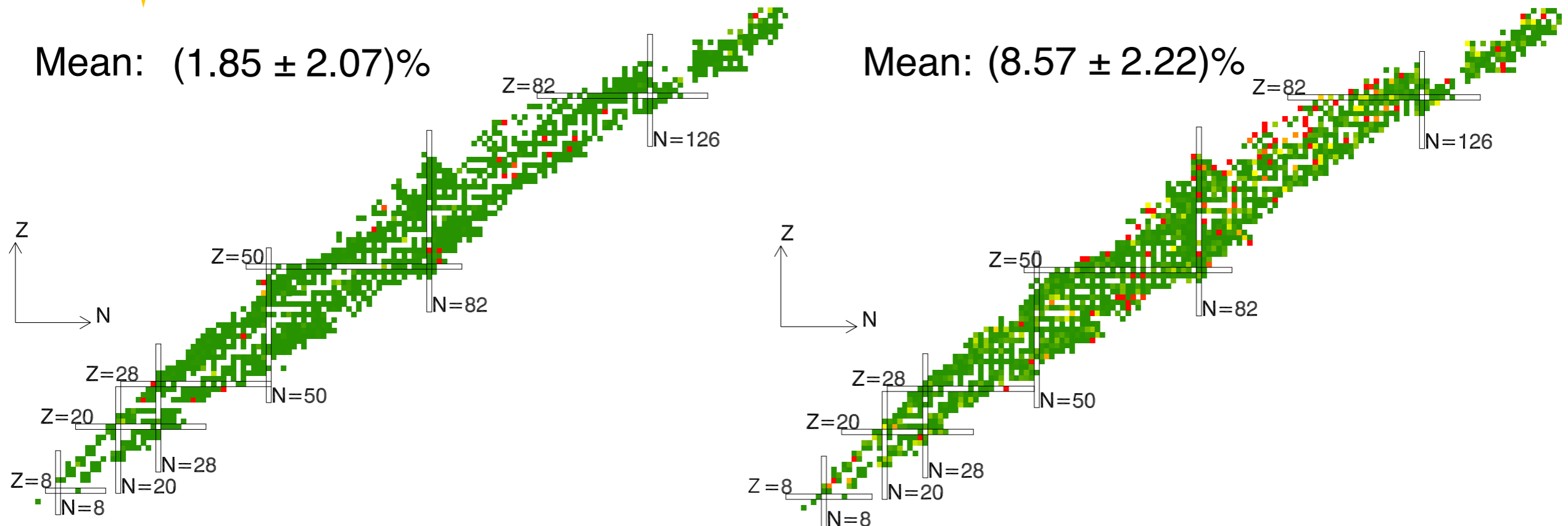
Statistical approach

Per-decay approach

E

Mean: $(1.85 \pm 2.07)\%$

Mean: $(8.57 \pm 2.22)\%$



Relative median intensity deviation



0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50

Intensity Verification Electrons (<30 keV)



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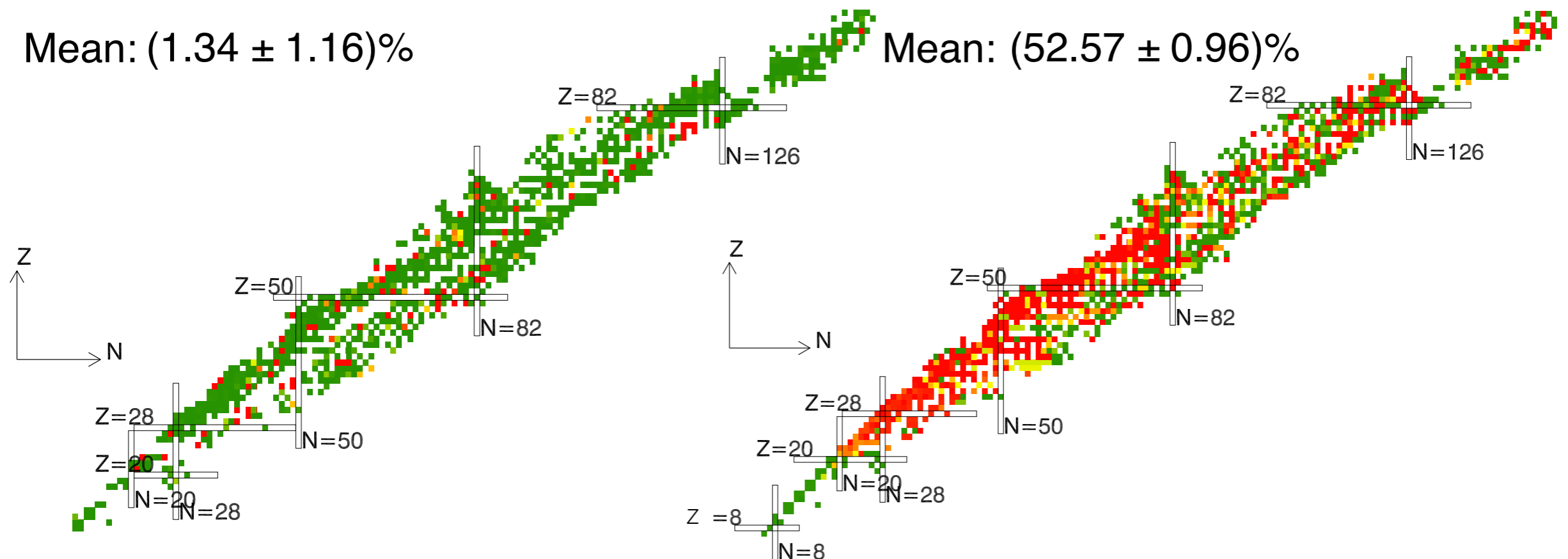
Statistical approach

Per-decay approach

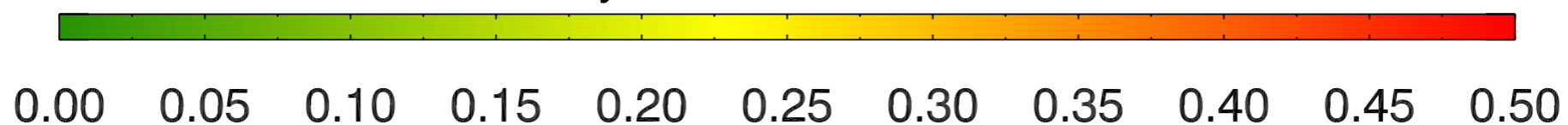
M

Mean: $(1.34 \pm 1.16)\%$

Mean: $(52.57 \pm 0.96)\%$



Relative median intensity deviation



Energy Verification

All radiation types (>30 keV)

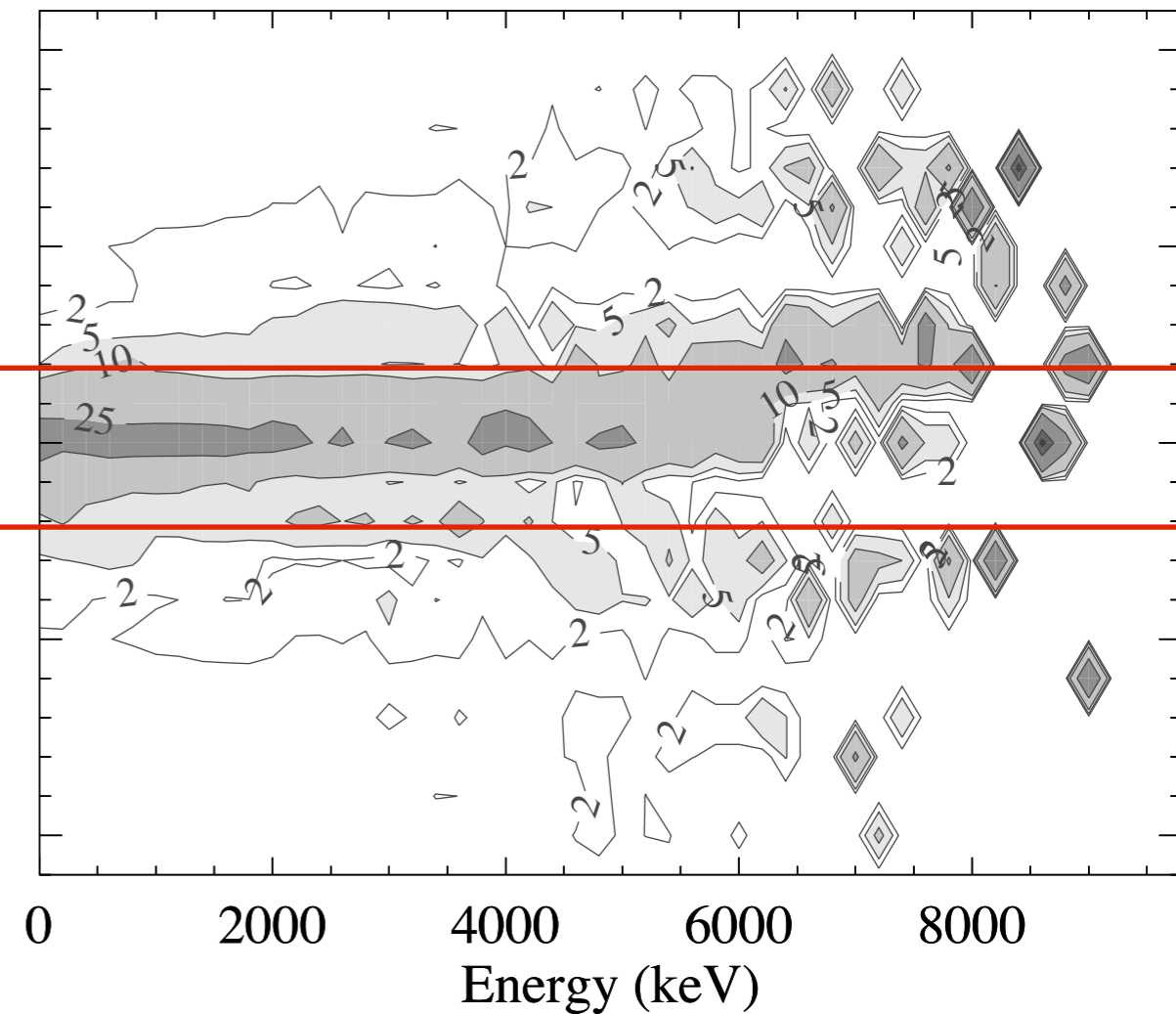
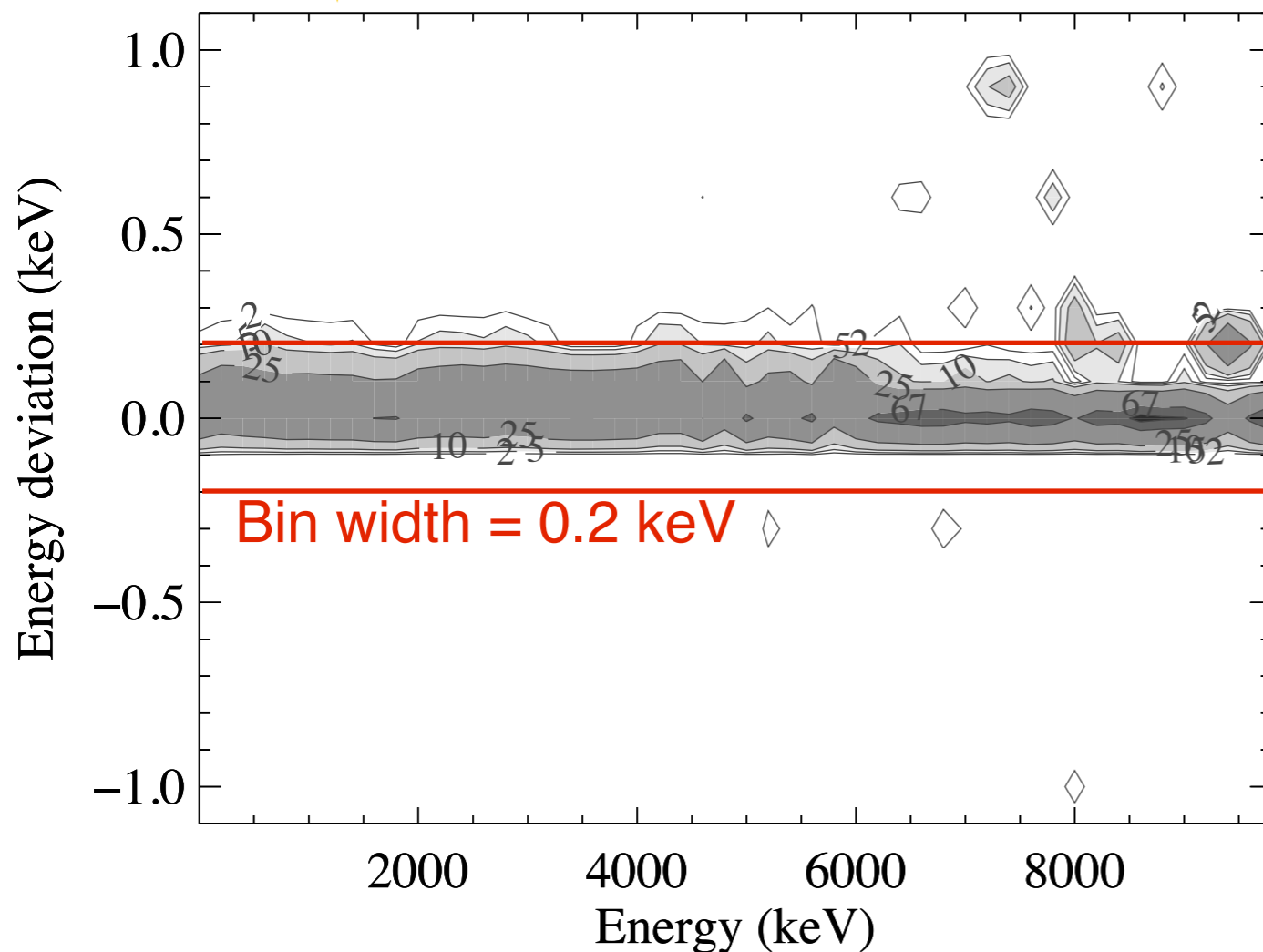


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new

Statistical approach

Per-decay approach

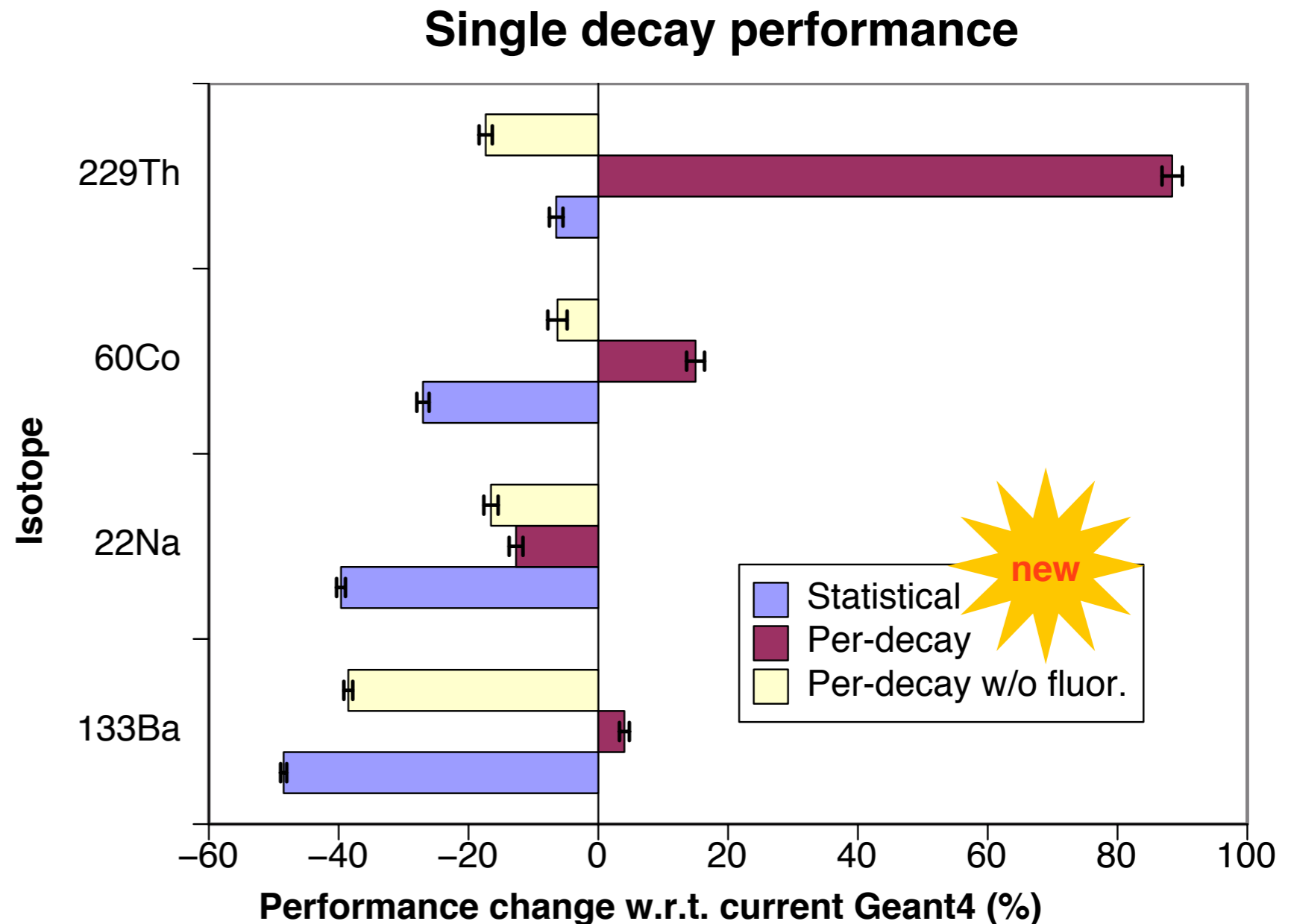


Computational Performance

Single decays



- ▶ Mean of 200 repetitive simulations with 10,000 decays:
 - ▶ ^{133}Ba : Electron Capture
 - ▶ ^{22}Na : Beta+
 - ▶ ^{60}Co : Beta-
 - ▶ ^{229}Th : Alpha
 - ▶ Empty geometry
- ▶ 12-core XEON system, Ubuntu 10.04
- ▶ Fixed bug concerning atomic deexcitation (also fixed in G4.9.5)



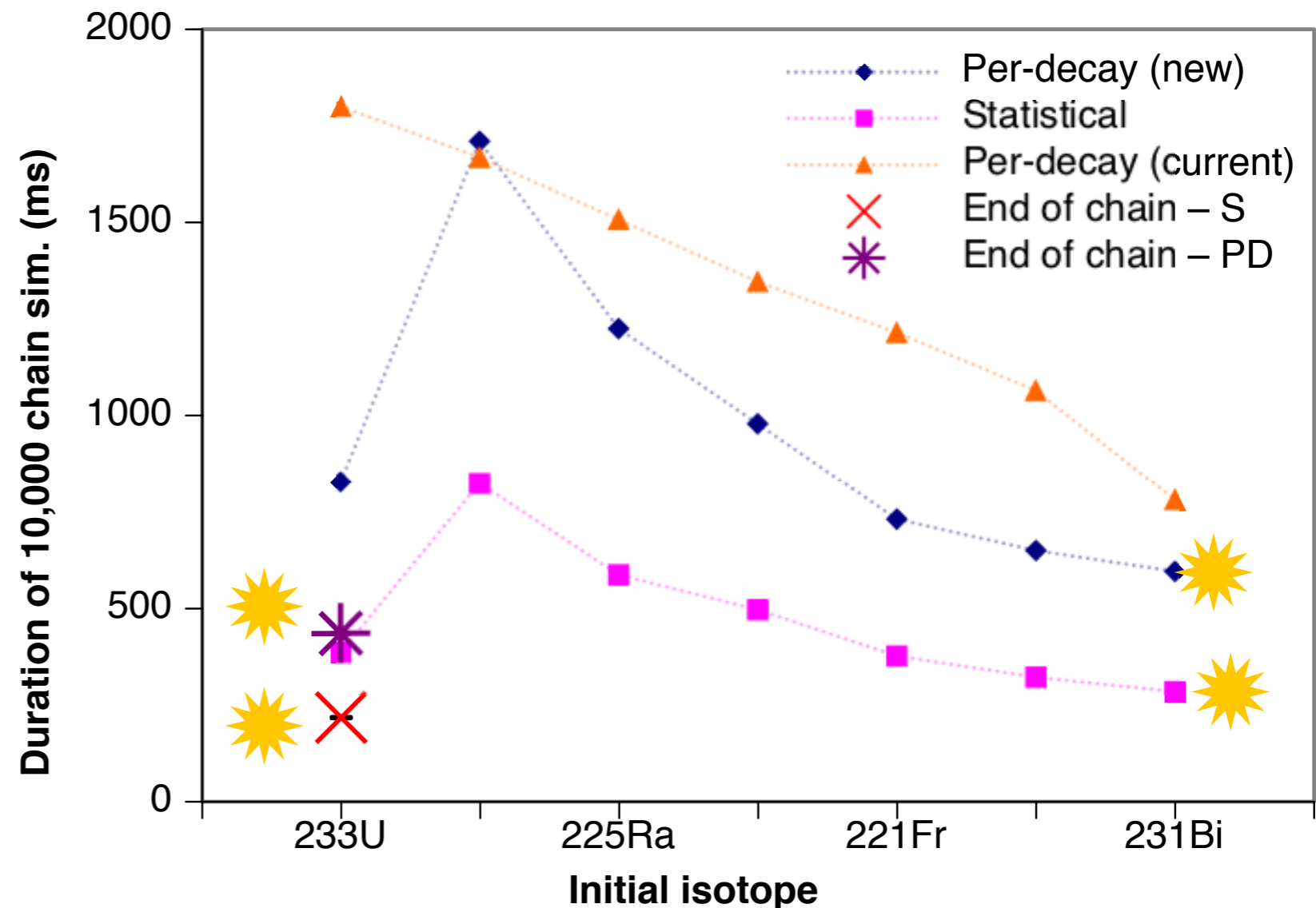
Efficient treatment of Decay Chains



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- ▶ Usual procedure: extended Bateman solution with branching and recursive implementation
- ▶ New approach: algebraic solution developed by M. Amaku *et al.*
- ▶ Advantage: only need to retrieve decay properties once, reuse for any initial isotope number
- ▶ More details in next talk on long-term activation

Decay chain performance - ^{233}U , $\Delta t=95$ kyr



Summary up to now...



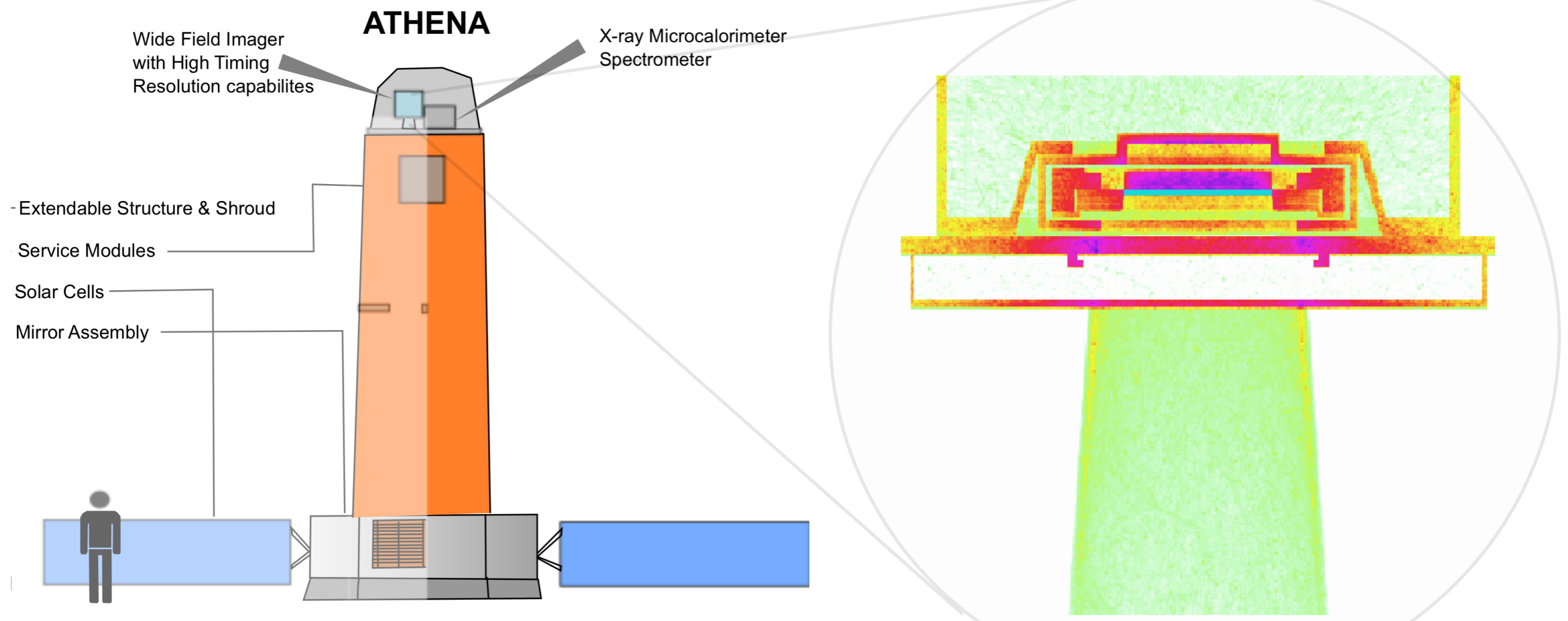
- ▶ Radioactive decay in Monte-Carlo simulations follows two flavors:
 - ▶ Per-decay simulation
 - ▶ Statistical summary of many decays
- ▶ Experimental requirements for both approaches exists
- ▶ Currently, no general purpose Monte-Carlo framework offers both
- ▶ **Newly developed radioactive decay code allows for both approaches**
 - ▶ Verification shows: it is **more accurate with respect to ENSDF** library
 - ▶ Computational performance tests show: it is **faster than current Geant4** code concerning single decays and especially decay chains
 - ▶ Additional bonus: **modern code design**, i.e. more maintainable
 - ▶ Additional bonus: **useful long term activation implementation** (see next talk)
 - ▶ And: bug fixes concerning energy/momentum conservation, decay emission production
 - ▶ **Additional validation with measurements from HPGe detector (N14-240)**

The Influence of In-Orbit Activation Buildup on the of the ATHENA Wide Field Imager



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Contents



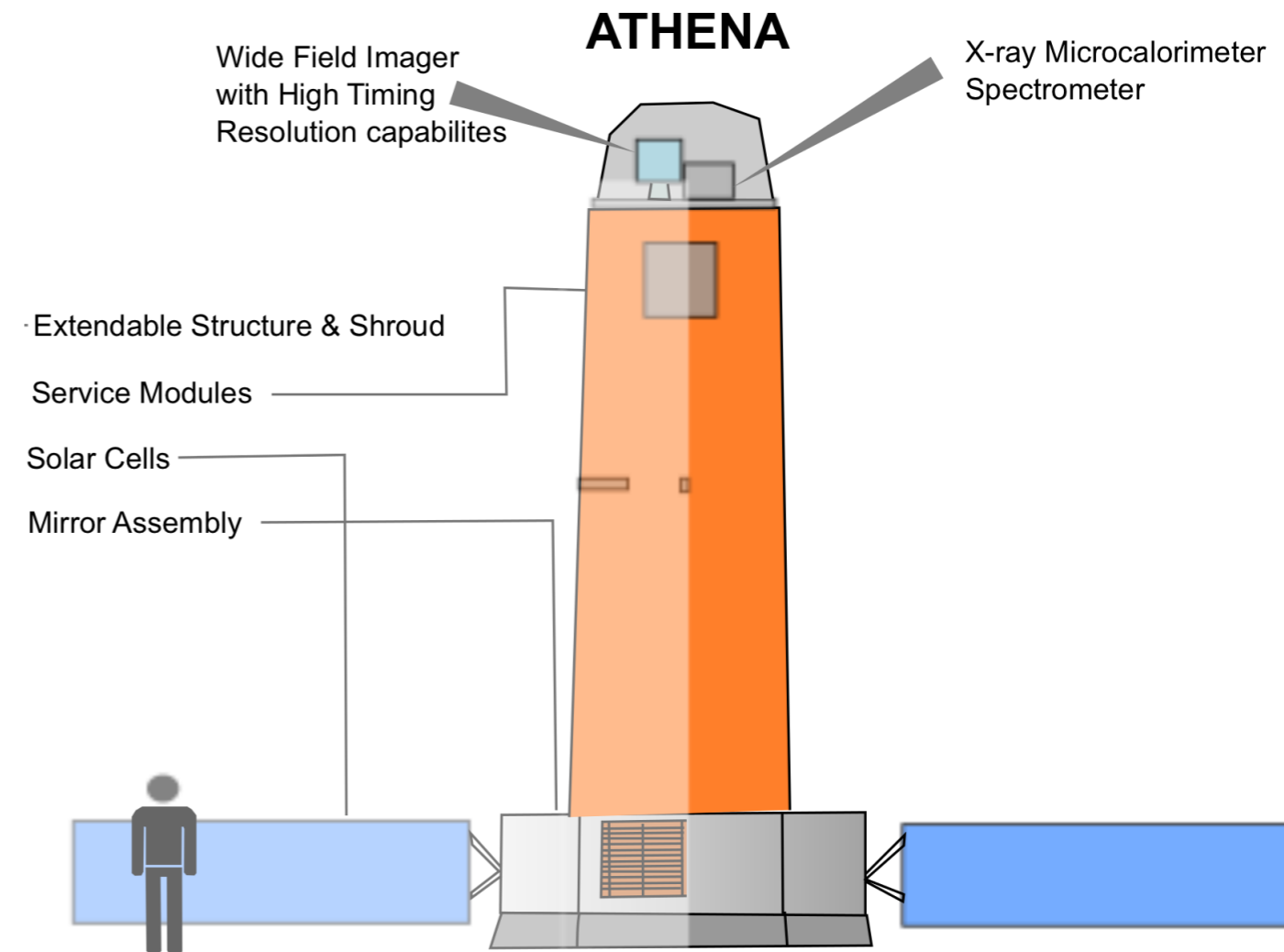
- ▶ A short introduction to ATHENA and the Wide Field Imager
- ▶ In-orbit background sources
- ▶ The prompt background
- ▶ Handling long-term activation in the new Geant4 Decay Code
- ▶ Results of the delayed background simulation

A Telescope for High ENergy Astrophysics - ATHENA

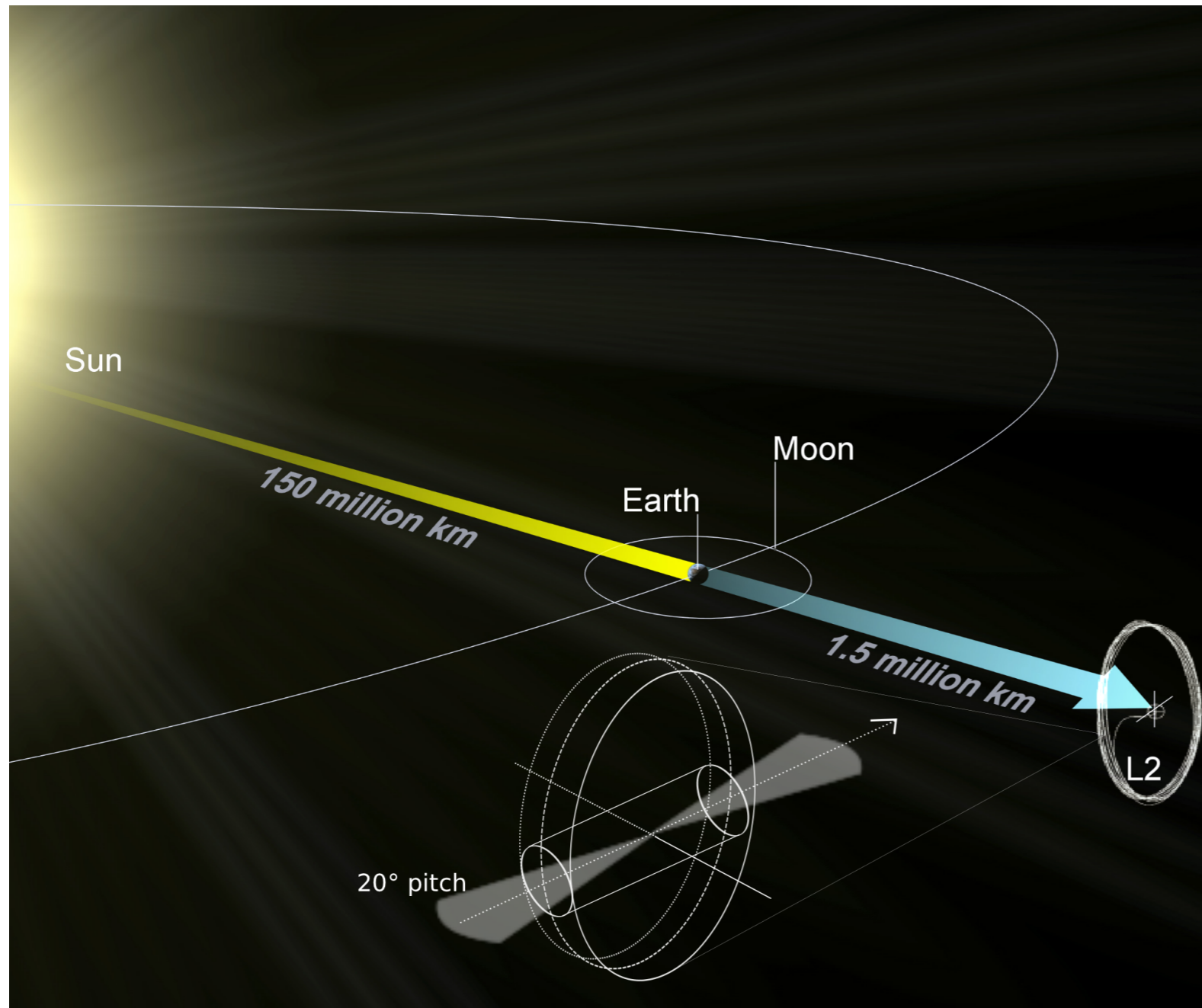


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- ▶ Planned next generation X-ray telescope
- ▶ Designated successor for XMM Newton (max. until 2018) and Chandra (max. until 2015)
- ▶ High sensitivity
→ max. background: $10^{-3} \text{ cts keV}^{-1} \text{ cm}^{-2} \text{ s}^{-1}$
- ▶ Good spatial resolution $< 10''$
- ▶ Good temporal resolution $\sim 10 \mu\text{s}$
- ▶ Good spectral resolution $\sim 3\text{eV @ } 1\text{keV}$
- ▶ DePFET-based **Wide Field Imager** imaging spectroscopy at energies between 0.1-15 keV on 640x640 pixel



The ATHENA Background Environment



- ▶ Position: 2nd Lagrangian
- ▶ Benefit: allows continuous observations not affected by passes through Earth's shadow and radiation belts
- ▶ Downside: unprotected by geomagnetic field. Harsh cosmic ray environment, solar protons and X-ray @ energies in the keV-TeV range
- ▶ **Satellite and detector components will get activated**
- ▶ **What background is to be expected?**
- ▶ **Can't replicate environment on Earth – need Monte-Carlo Simulations**

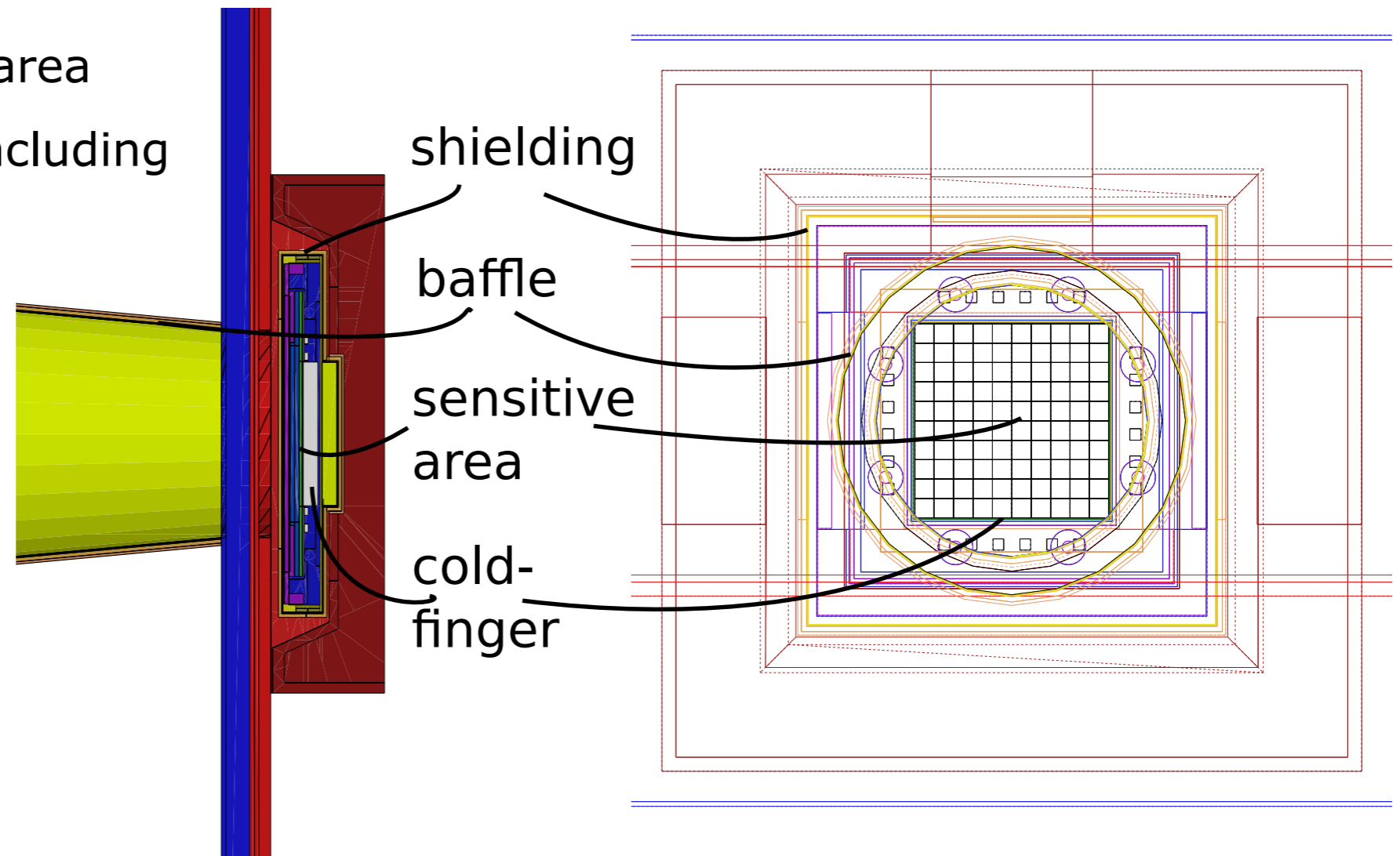
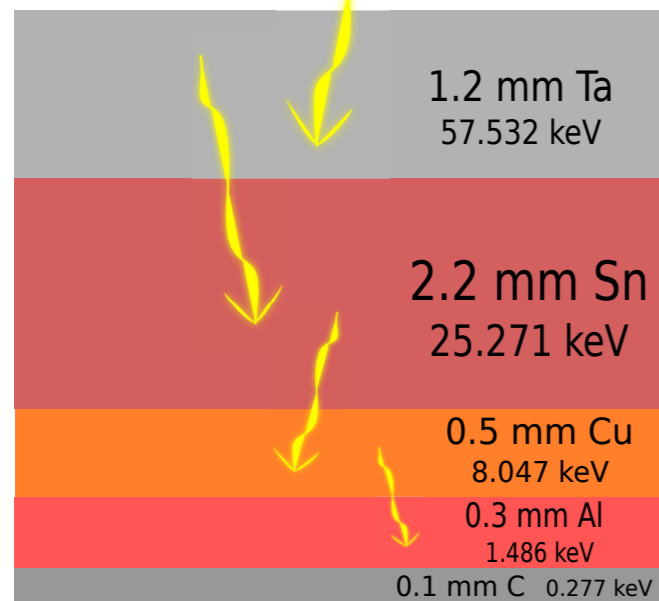
Background-Image: Wikipedia, Orbit-Plot: Bacons et Al, 20

ATHENA Simulation Geometry in Geant4



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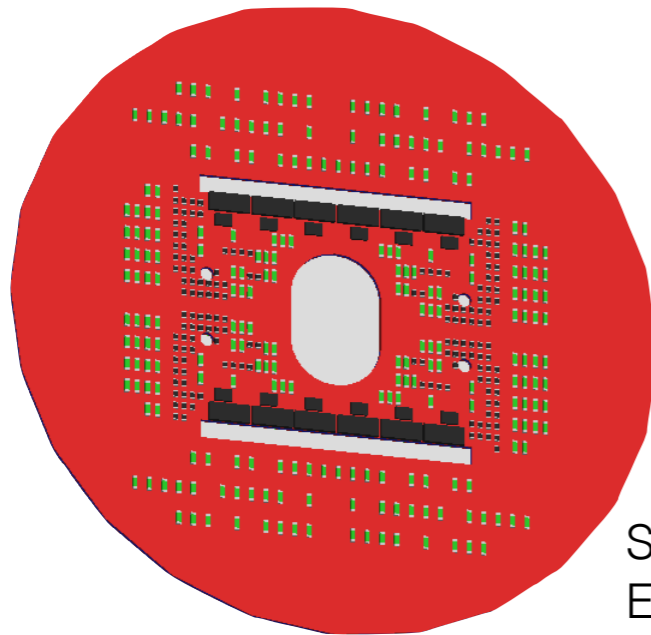
- ▶ Detailed detector geometry consisting of
 - ▶ Fully pixelized sensitive area
 - ▶ Detailed entry window including filter layers
 - ▶ Graded-Z shielding



DePFET

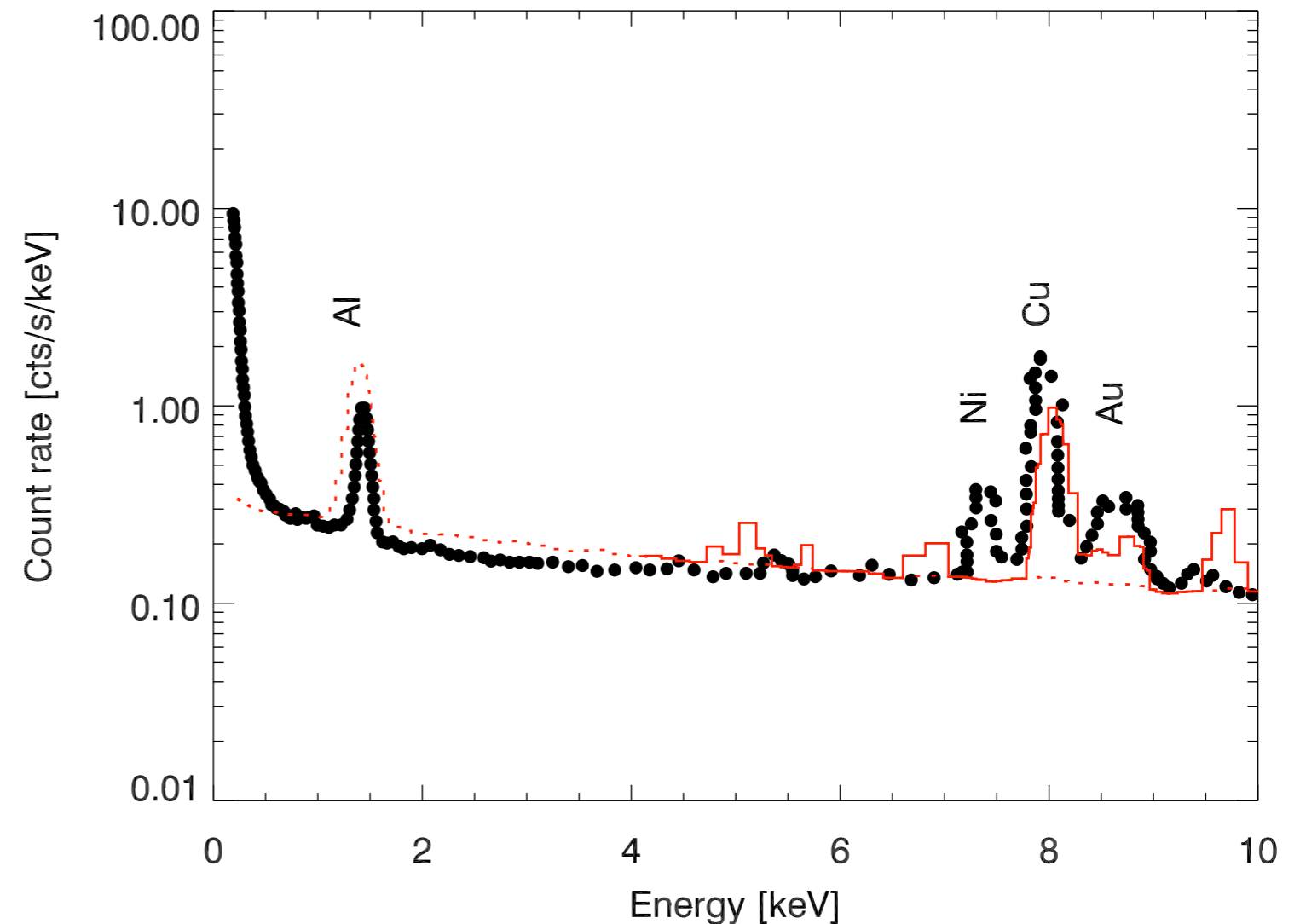
Validation of the Simulation Environment with XMM Newton EPIC-pn Data

- ▶ Simulation of EPIC-pn recorded filter-wheel closed data, i.e. only cosmic rays and secondaries hit sensitive area
- ▶ Details only for PCB, everything else was an aluminum box
- ▶ Magnitude and shape of background in general agreement except for Ni-line



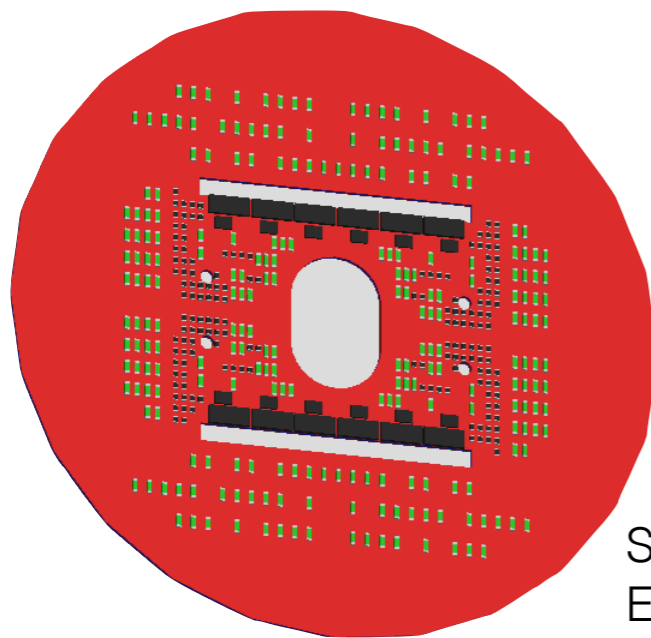
Simulation model of the EPIC-pn PCB (backside shown)

Comparison **simulation** - measurement



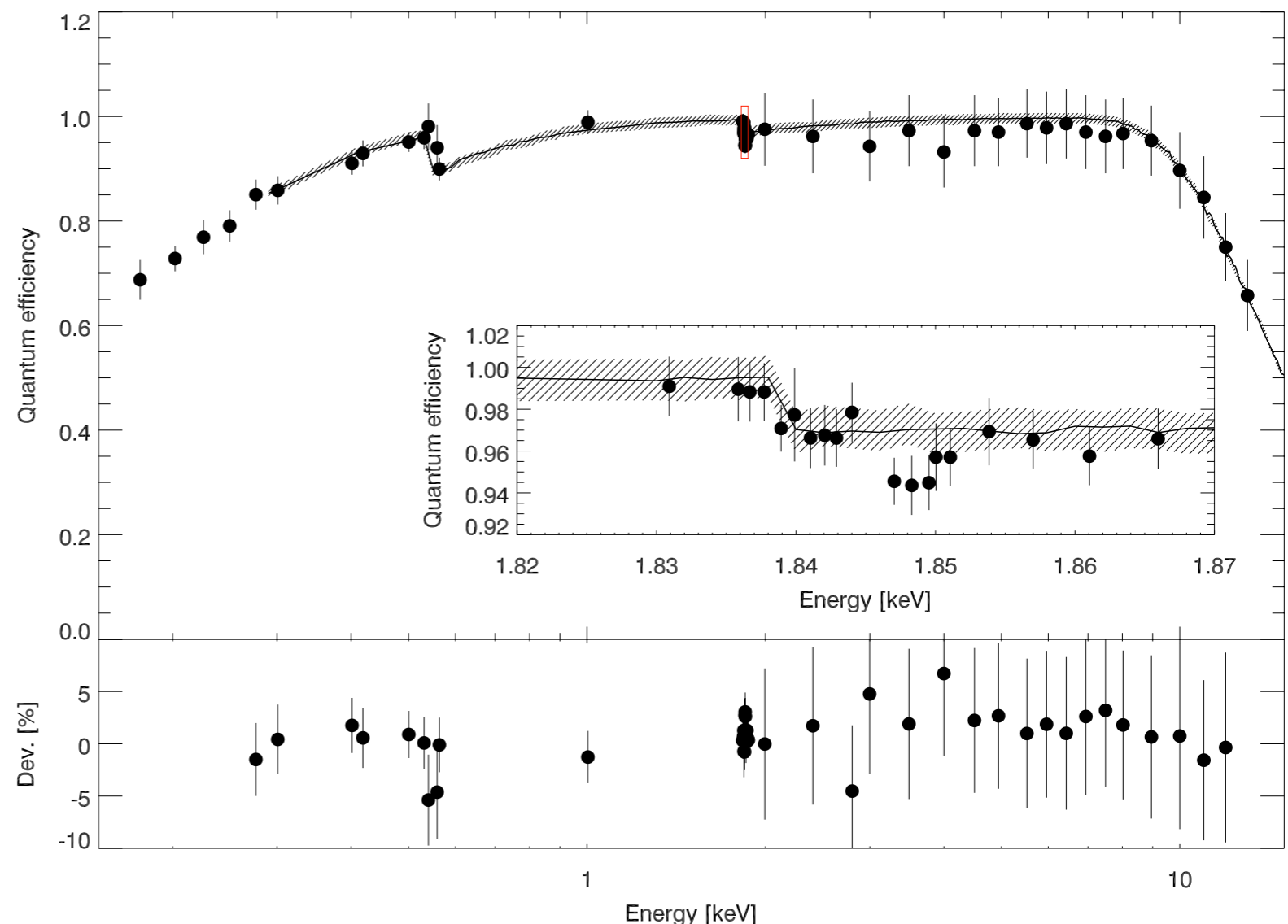
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Simulation model of the EPIC-pn PCB (backside shown)

EPIC-pn quantum efficiency

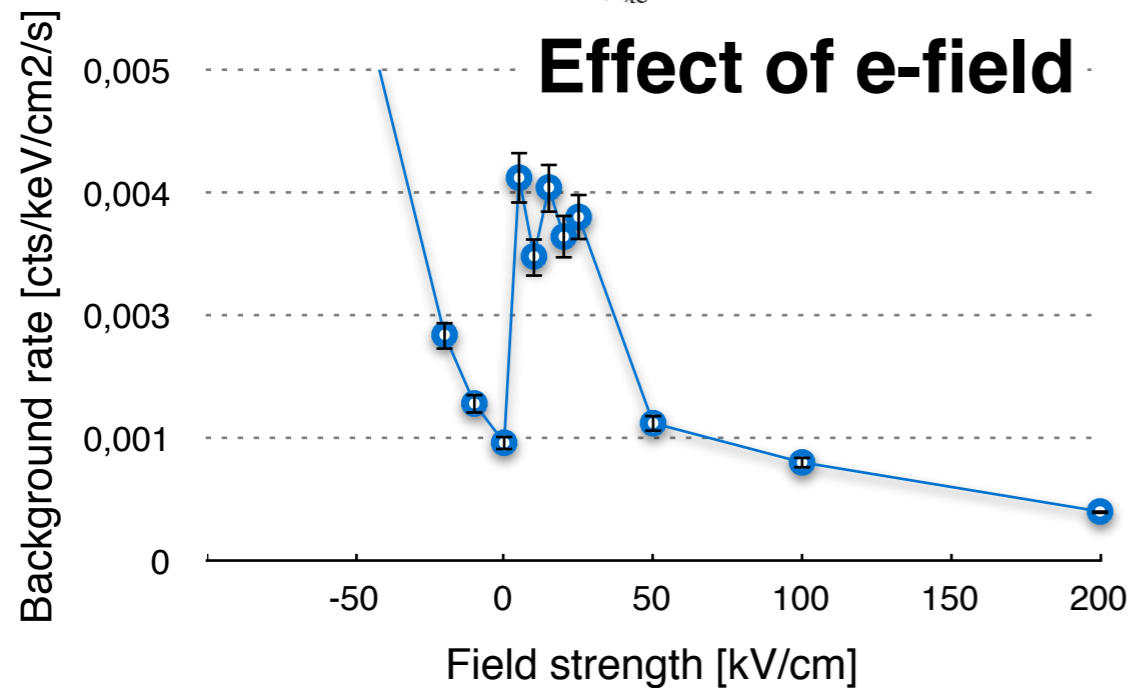
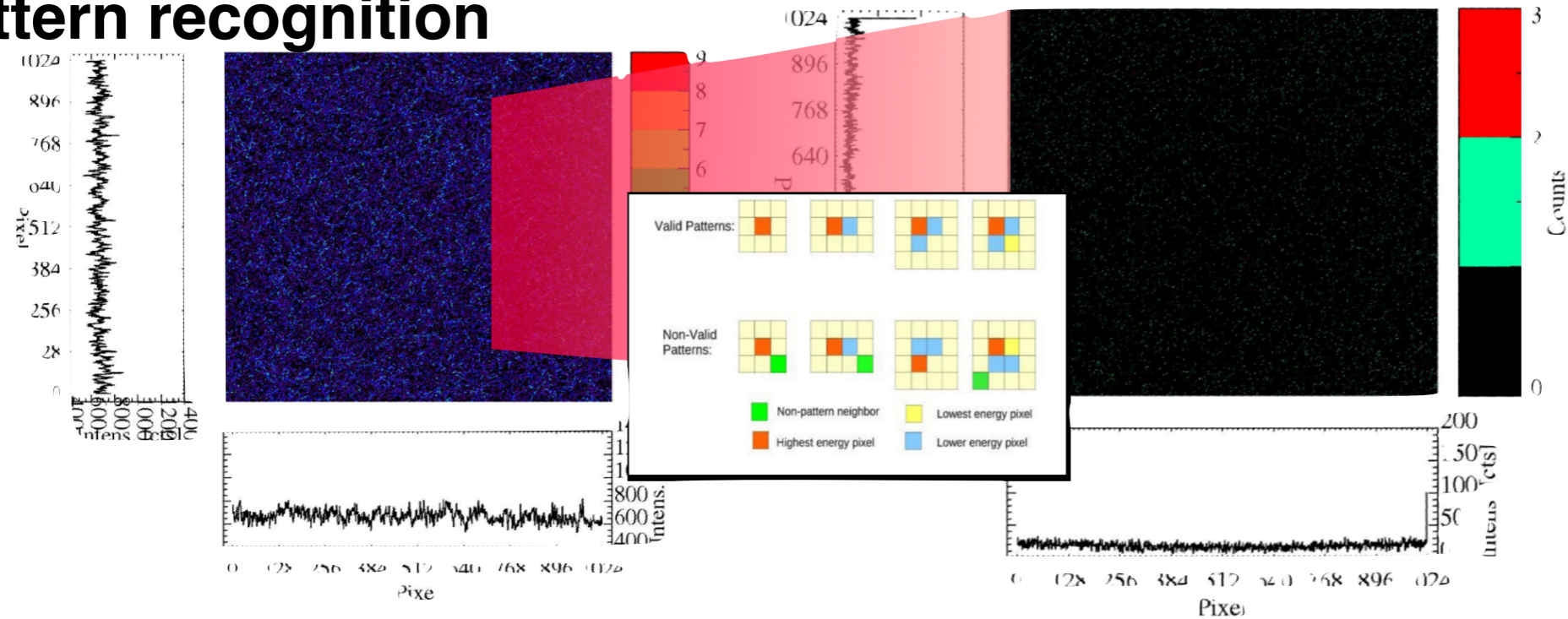


Lessons learned from the prompt Background of the ATHENA WFI



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Pattern recognition



- ▶ Pattern recognition reduces background by >99.6%
- ▶ Variable exclusion radii
- ▶ Further reduction possible if electrical field accelerates secondary electrons
- ▶ Background rate $\approx 10^{-3}$ cts/s/keV/cm² feasible
- ▶ **What effect will the delayed background have?**

Back to the new Decay Code: how decay chains and activation are handled



- ▶ Usual procedure: extended Bateman solution with branching and recursive implementation
- ▶ New approach: algebraic solution developed by M. Amaku *et al.*
(building upon work by R. J. Onega, D. Pressyanov, L. Moral and A. F. Pacheco, T. M. Senkov and D. Yuan and W. Kernan)
- ▶ Advantage: only need to retrieve decay properties once, reuse for any initial isotope number
- ▶ By defining chain members of interest and taking into account time spans only necessary isotopes are actually decayed

$$\begin{aligned}\frac{dN_1(t)}{dt} &= -k_1 N_1(t) \\ \frac{dN_2(t)}{dt} &= \lambda_1 N_1(t) - k_2 N_2(t) \\ &\vdots \\ \frac{dN_n(t)}{dt} &= \lambda_{n-1} N_{n-1}(t) - k_n N_n(t)\end{aligned}$$

$$k_i = \lambda_i + \alpha_i.$$

Decay Activation
constant parameter

Isotopes in chain after time t

$$\mathbf{N}(t) = e^{\Lambda t} \mathbf{N}(0)$$

- [1] M. Amaku, P. R. Pascholati, and V. R. Vanin, "Decay chain differential equations: Solution through matrix algebra," *Computer Physics Communications*, vol. 181, pp. 21–23, 2010.
- [2] R. J. Onega, "Radioactivity calculations," *American Journal of Physics*, vol. 37, no. 10, pp. 1019–1022, 1969. [Online]. Available: <http://link.aip.org/link/?AJP/37/1019/1>
- [3] D. S. Pressyanov, "Short solution of the radioactive decay chain equations," *American Journal of Physics*, vol. 70, pp. 444–445, 2002.
- [4] L. Moral and A. F. Pacheco, "Algebraic approach to the radioactive decay equations," *American Journal of Physics*, vol. 71, pp. 684–686, 2003.
- [5] T. M. Semkow, "Comment on "algebraic approach to the radioactive decay equations," by I. Moral and A.F. Pacheco" *American Journal of Physics*, vol. 72, pp. 410–411, 2004.
- [6] D. Yuan and W. Kernan, "Explicit solutions for exit-only radioactive decay chains," *Journal of Applied Physics*, vol. 101, no. 9, p. 094907, 2007.

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Decay matrix

$$\Lambda = \begin{bmatrix} -k_1 & 0 & 0 & 0 \\ k_1 & -k_2 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & k_{n-1} & k_n \end{bmatrix}$$

$$k_i = \lambda_i + \alpha_i$$

Decay constant Activation parameter

Activation is treated here

Isotopes in chain after time t

$$\mathbf{N}(t) = e^{\Lambda t} \mathbf{N}(0)$$

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Back to the new Decay Code: how decay chains and activation are handled



- ▶ α_i needs to be known for each isotope in each volume
- ▶ Code provides a book-keeping class to automatically keep track of these activations resulting from appropriate G4-processes
- ▶ After initial activation simulation activities are calculated
- ▶ Result is saved in XML file
- ▶ Automatic redefinition of geometry including volumes acting as radioactive background sources

Decay matrix

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$$k_i = \lambda_i + \alpha_i$$

Decay constant Activation parameter

Activation is treated here

Isotopes in chain after time t

$$\mathbf{N}(t) = e^{\Lambda t} \mathbf{N}(0)$$

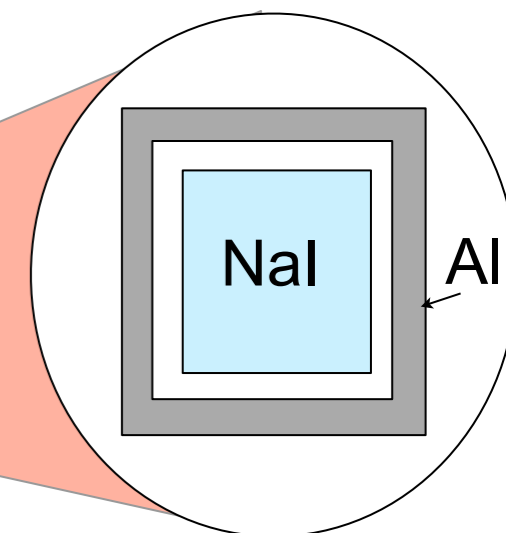
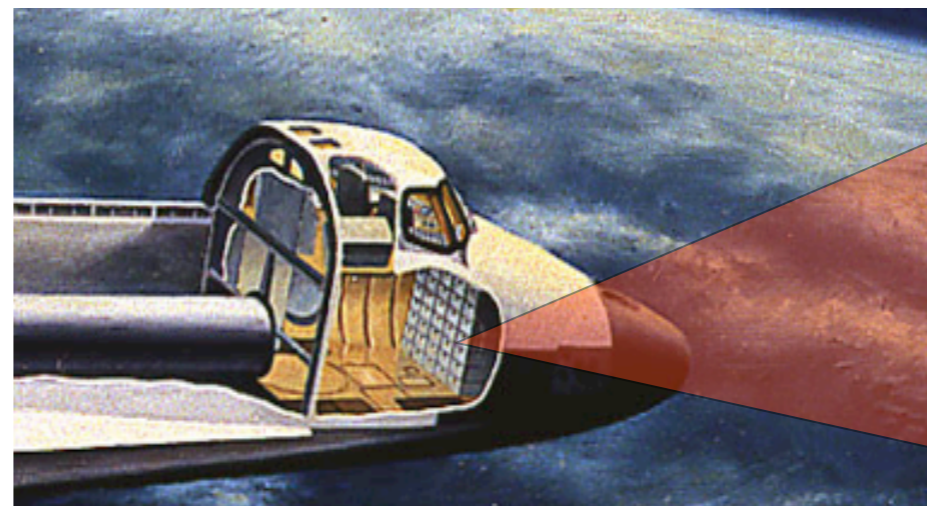
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Validation of long term activation code with Space Shuttle Data



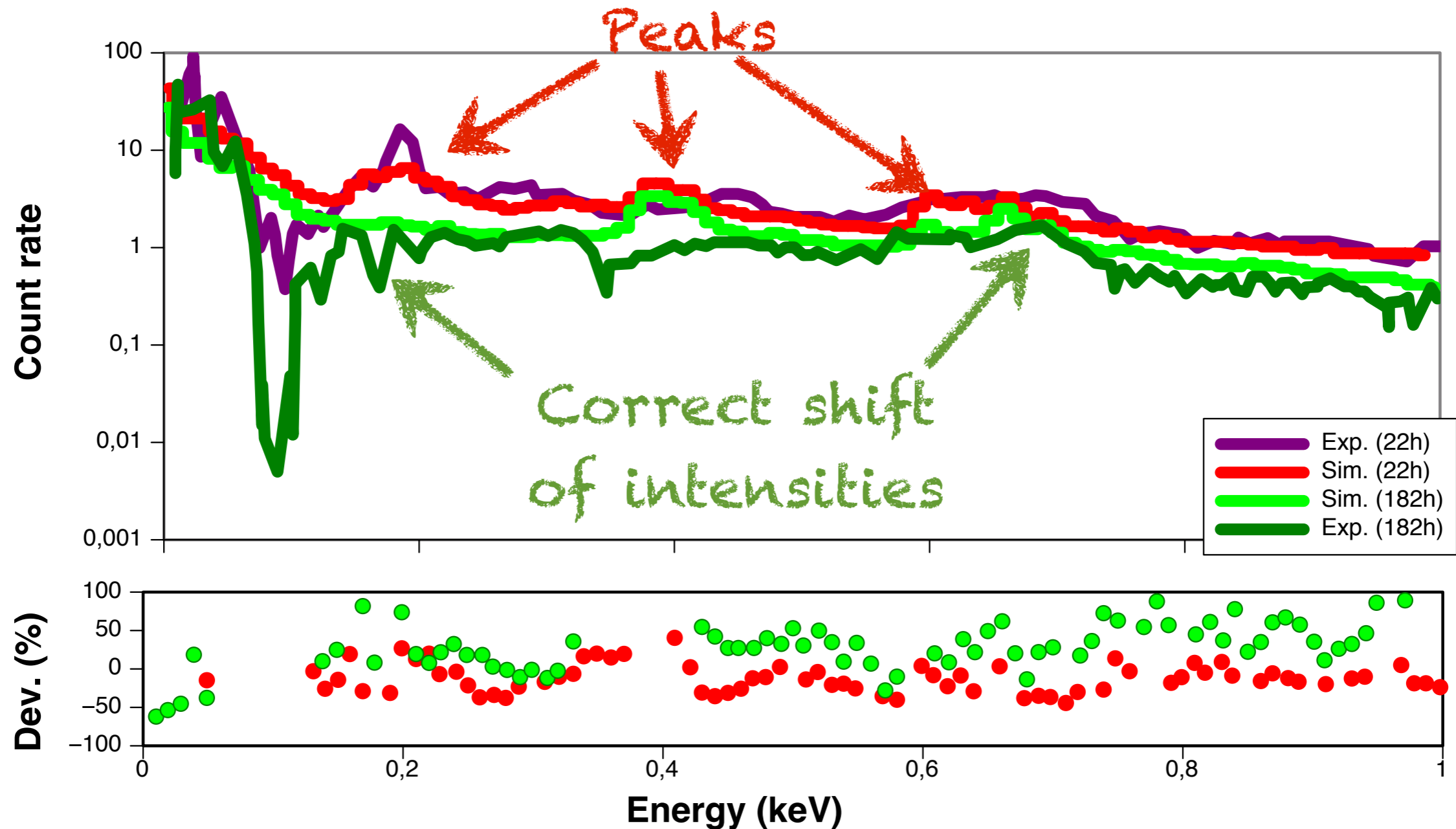
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- ▶ NaI-scintillator crystal stored in locker aboard STS-53 mission
- ▶ Irradiation and activation by cosmic rays during mission
- ▶ After touchdown: mating with PMT and in-situ measurement of gamma-radiation resulting from decaying isotopes (Truscott and Dyer, 1992+94)
- ▶ Much simplified Geant4 simulation: cubic homogeneous crystal in hollow aluminium box



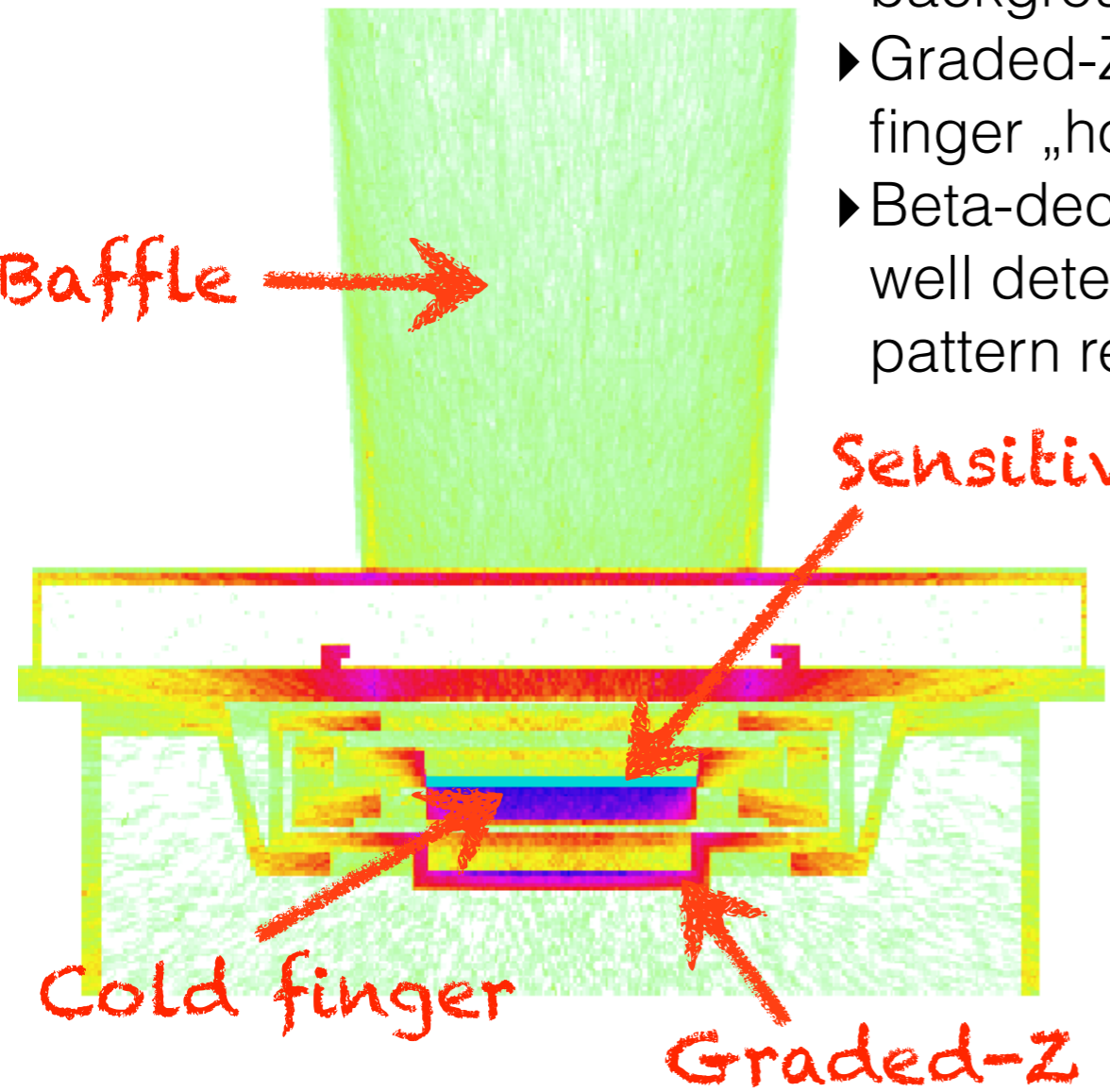
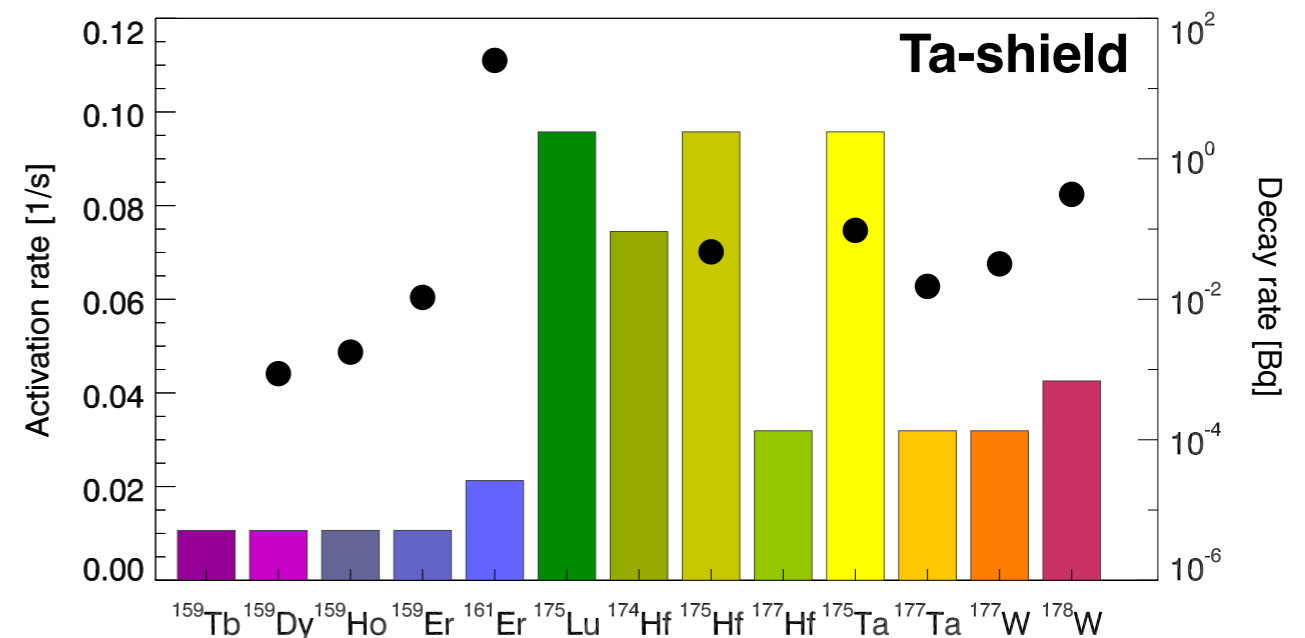
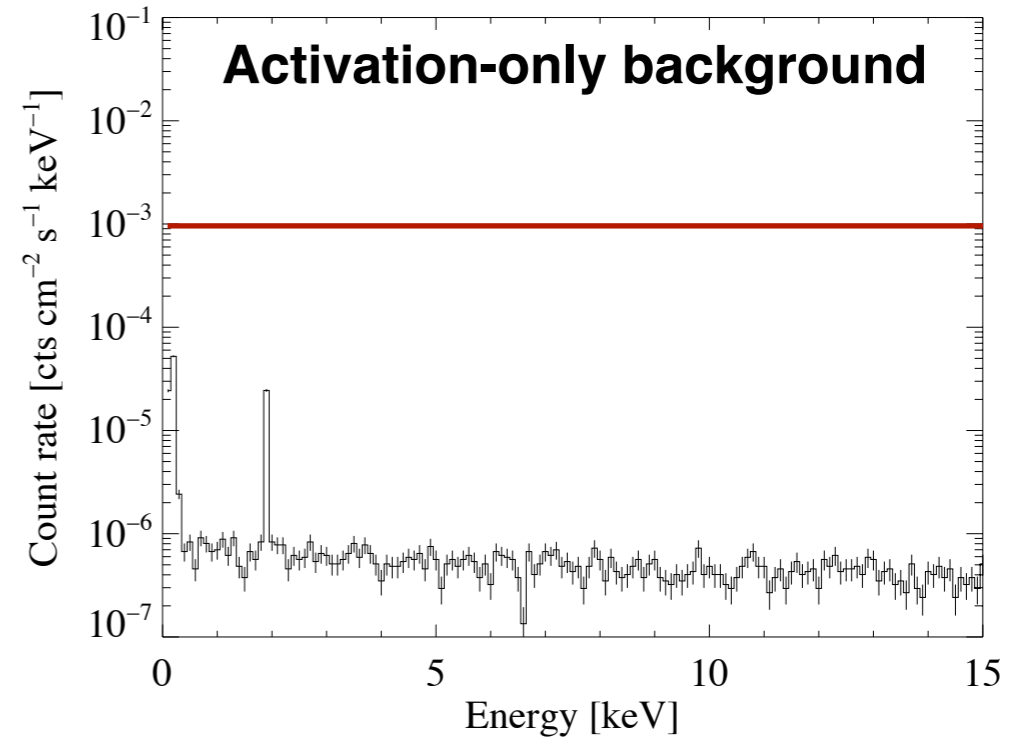
Shuttle image: nasa.gov

Validation of long term activation code with Space Shuttle Data



Long Term Activation of the ATHENA WFI (after 10yr)

- ▶ Activation well below background limit
- ▶ Graded-Z and cold finger „hottest“
- ▶ Beta-decays in CF well detected by pattern rejection



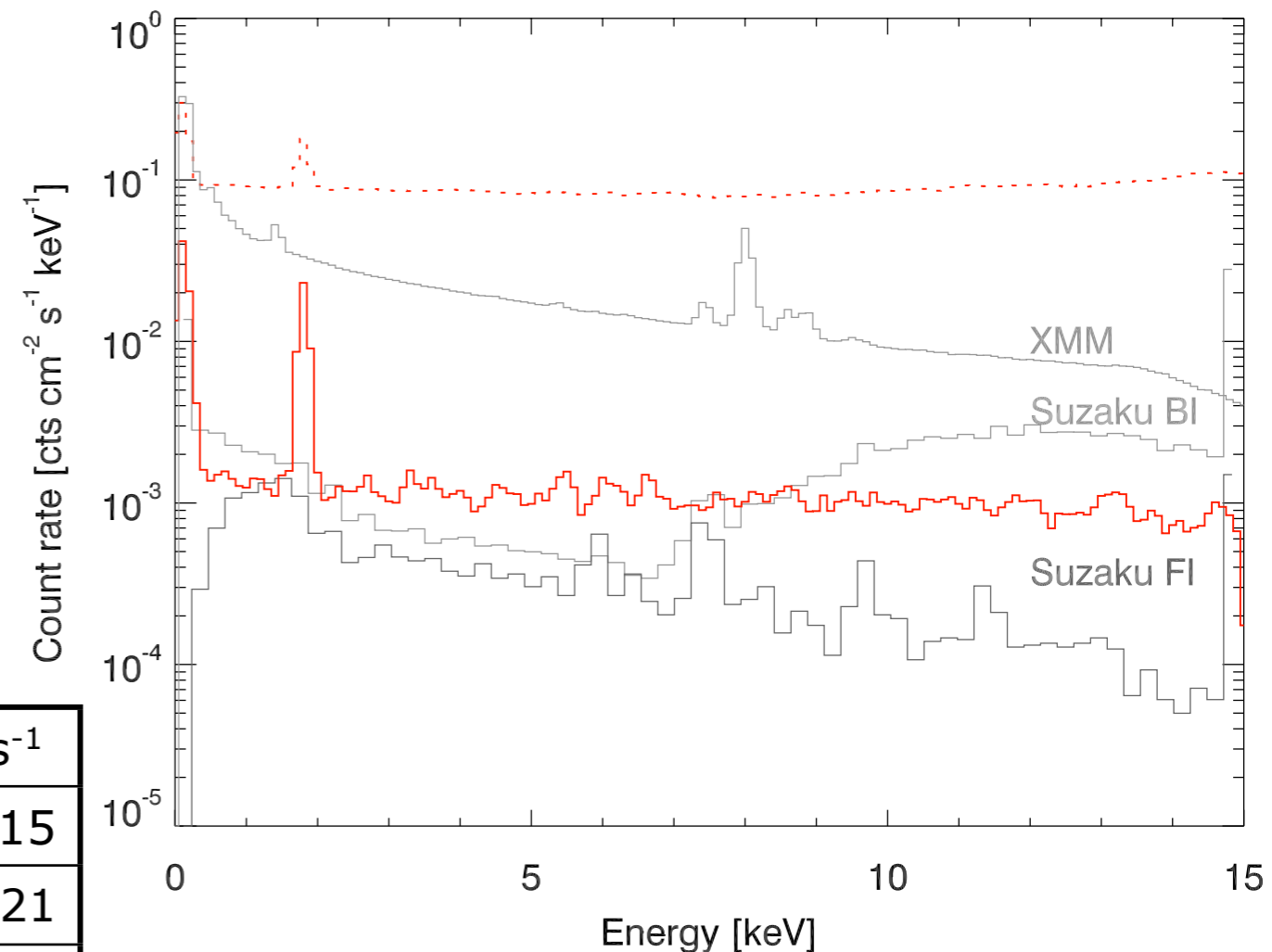
Final Estimates for the ATHENA Wide Field Imager Background



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- ▶ATHENA background is lower or equal to existing missions
- ▶Long term activation plays a negligible role.
- ▶ATHENA background goals are feasible

ATHENA compared with other missions



Selected ATHENA background rates

Scenario	10^{-4} cts keV $^{-1}$ cm $^{-2}$ s $^{-1}$
with frame-dropping	6.42 ± 0.15
with 200px exklusion	12.43 ± 0.21
with e-field (+200kV/cm)	2.70 ± 2.67
Long time activation	0.21 ± 0.05

Conclusion



- ▶ The magnitude of the ATHENA Wide Field Imager background has been estimated using a new radioactive decay code for Geant4
- ▶ At $(0.21 \pm 0.05) \times 10^{-4} \text{cts keV}^{-1} \text{cm}^{-2} \text{s}^{-1}$ it is well below the prompt background rate which has been estimated at $(2.7 - 6.42) \times 10^{-4} \text{cts keV}^{-1} \text{cm}^{-2} \text{s}^{-1}$
- ▶ The high-Z layer of the graded-Z shielding and the cold finger have been identified as the most activated parts. The graded-Z layers are themselves well shielded from the detector, the emission from the cold finger is detected by pattern rejection