Realistic Simulation of Radionuclide Sources in EGSnrc:

A predictive model of the Vinten Ionization Chamber

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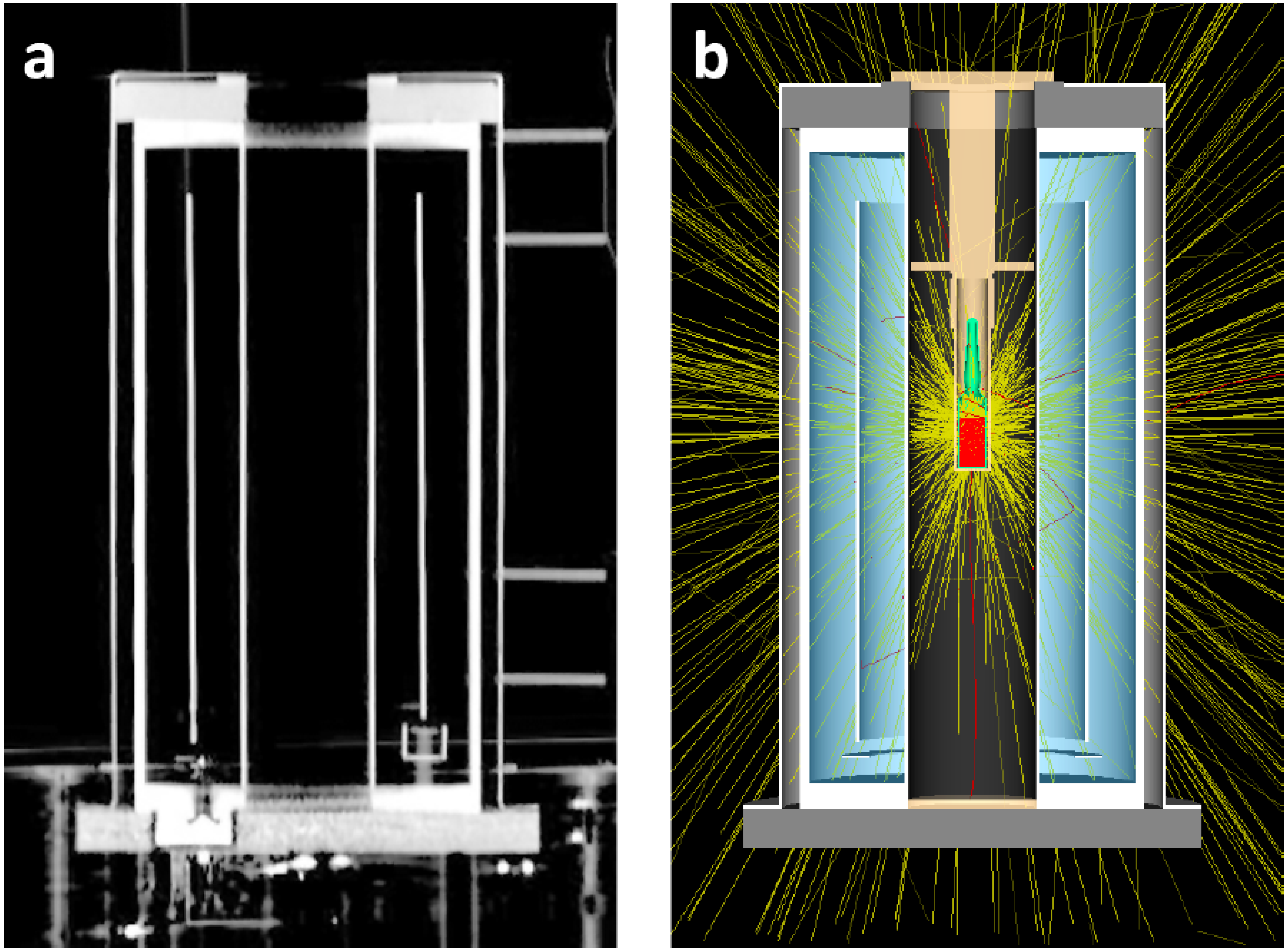
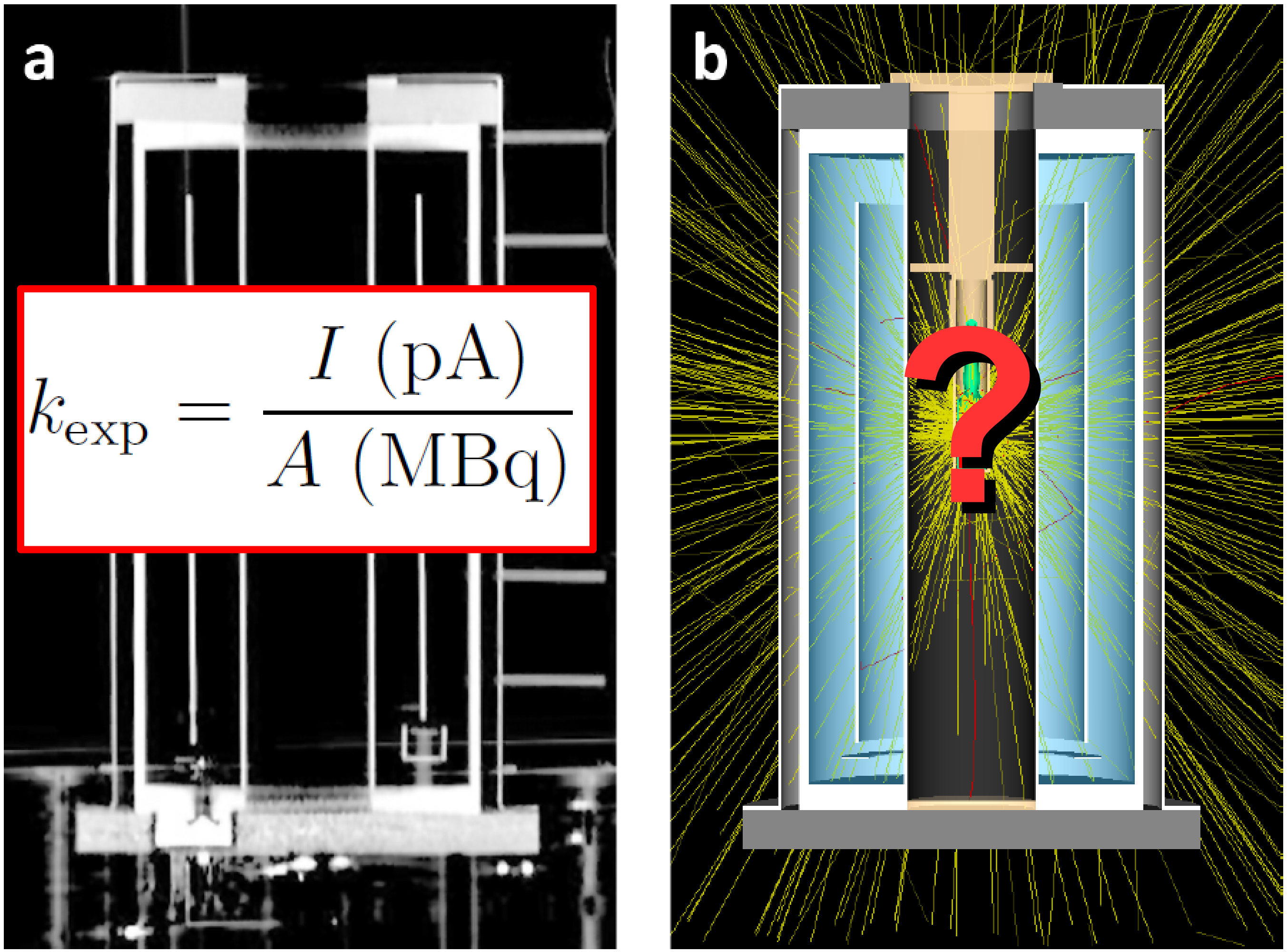
Measurement Science and Standards
National Research Council Canada

Radionuclide detectors convert activity to signal



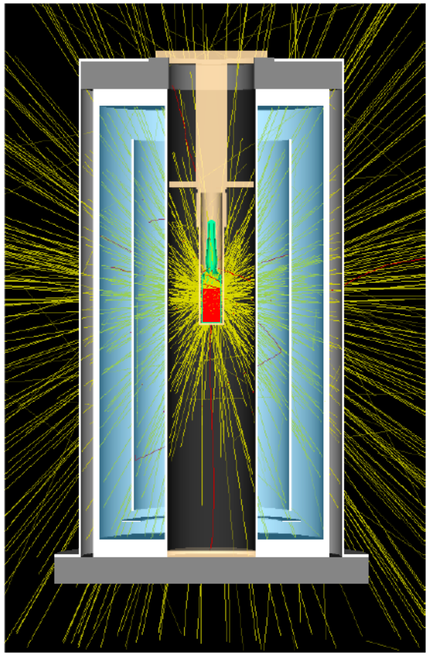
Simulations can produce an absolute result



$$k_{\mathrm{exp}} = \frac{I \ (\mathrm{pA})}{A \ (\mathrm{MBq})}$$

Simulations provide experimental refinement

- An EGSnrc model of your detector allows you to:
  - Validate experiments
  - Predict detector response for unknown isotopes
  - Refine experimental uncertainty budget
    - Test geometrical variations
    - Test manufacturing tolerances
    - Test radioimpurity effects



Electron Gamma Shower

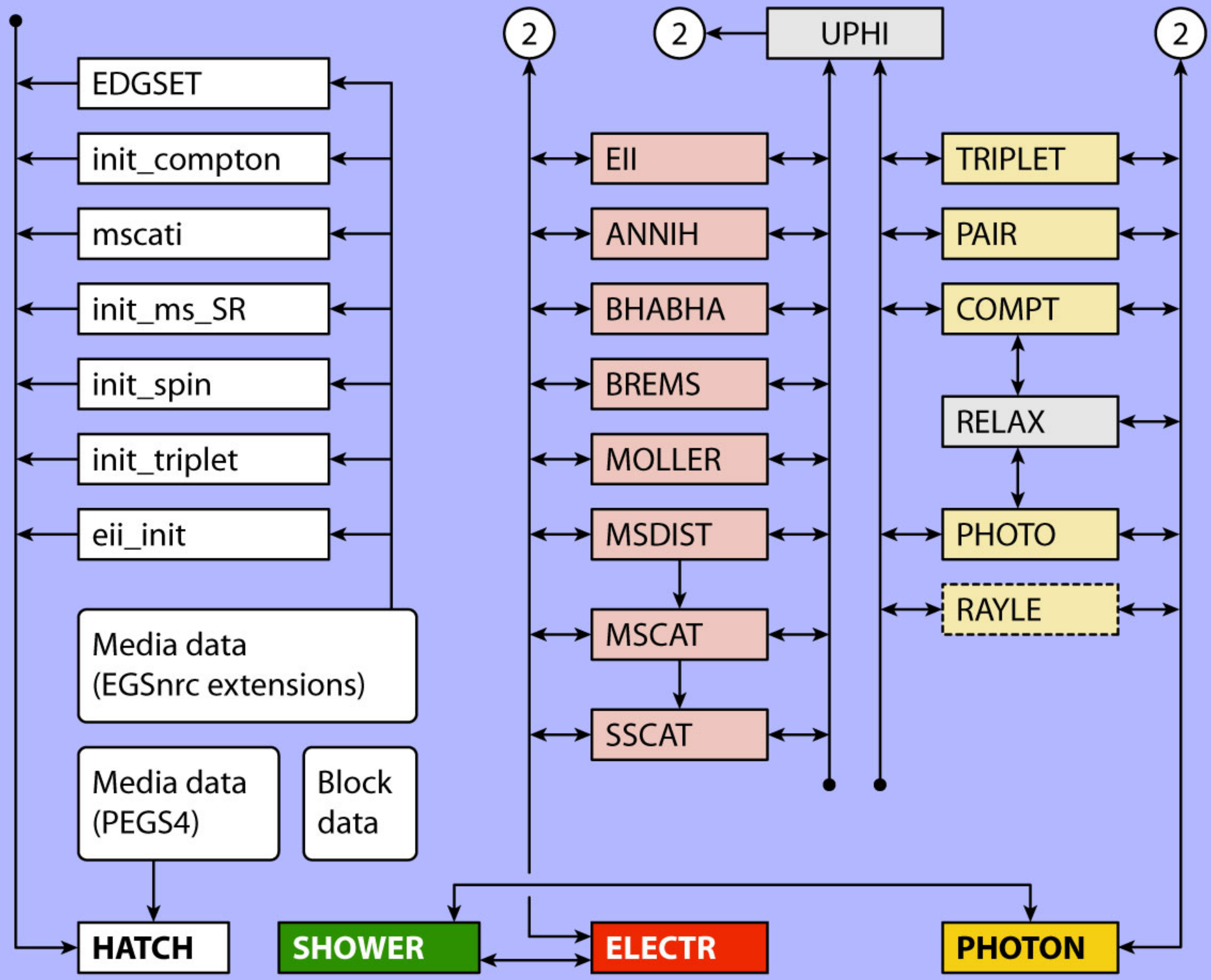
EGSnrc

General purpose: energies from 1 keV to 10 GeV

Efficient: released in 2000 as the new EGS4 version

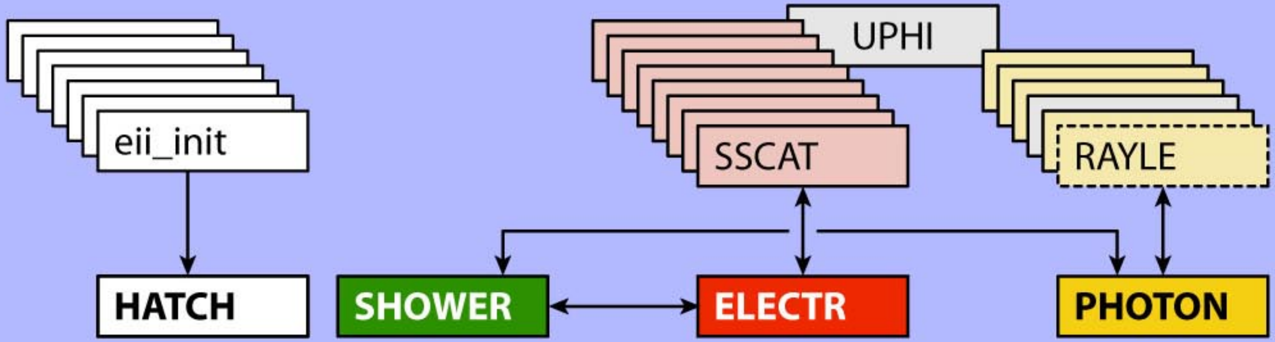
Accurate physics: nominal accuracy at 0.1% level

Gold standard for electron-photon transport

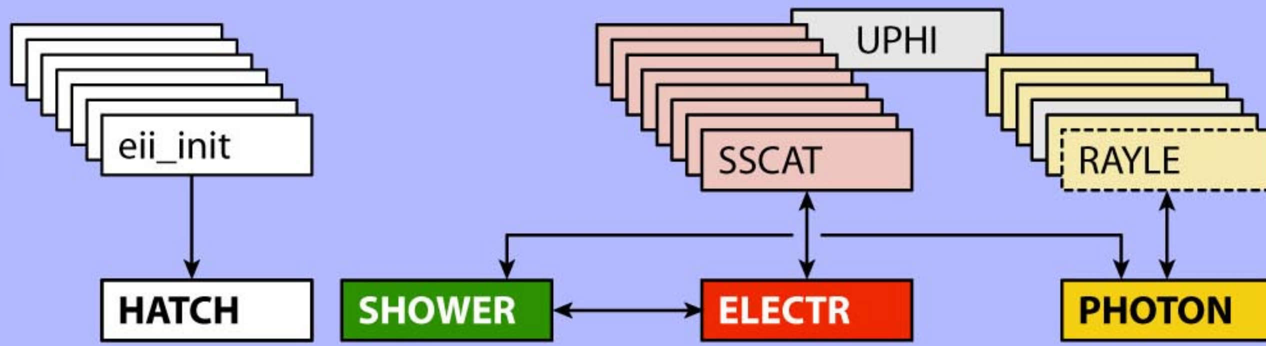


EDGSET
init_compton
mscati
init_ms_SR
init_spin
init_triplet
eii_init
Media data (EGSnrc extensions)
Media data (PEGS4)
Block data
2
2
UPHI
2
EII
ANNIH
BHABHA
BREMS
MOLLER
MSDIST
MSCAT
SSCAT
TRIPLET
PAIR
COMPT
RELAX
PHOTO
RAYLE
HATCH
SHOWER
ELECTR
PHOTON

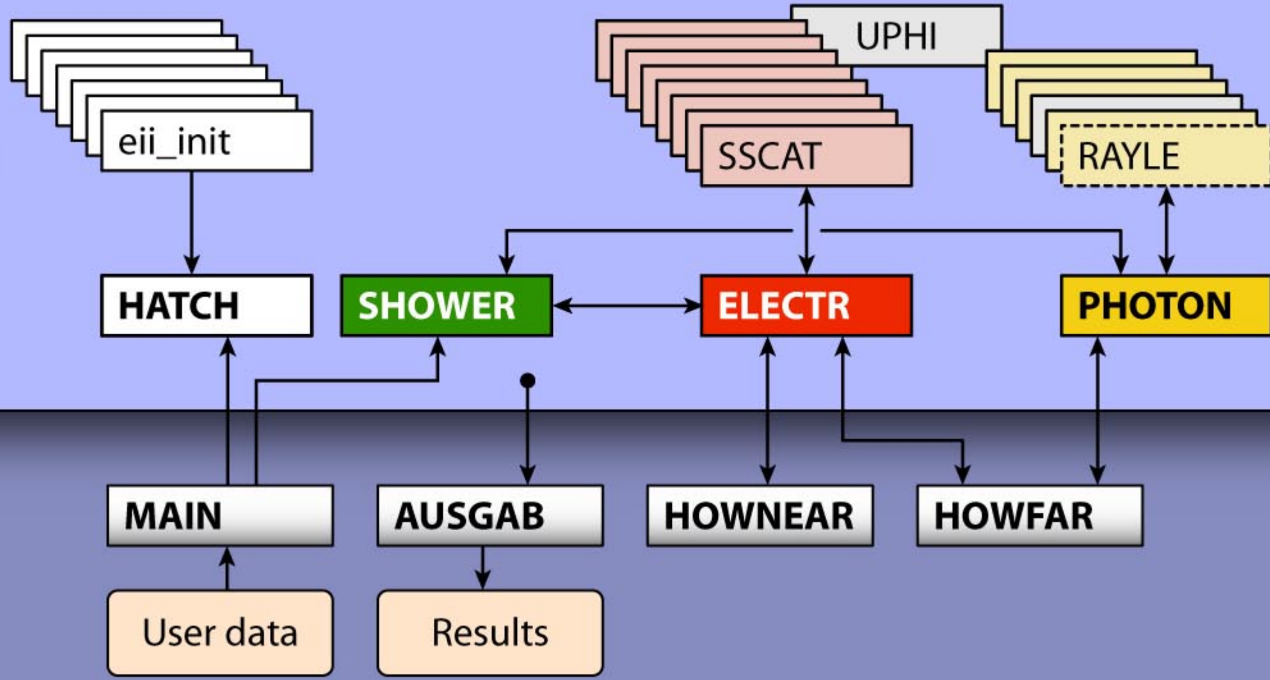
EGSnrc



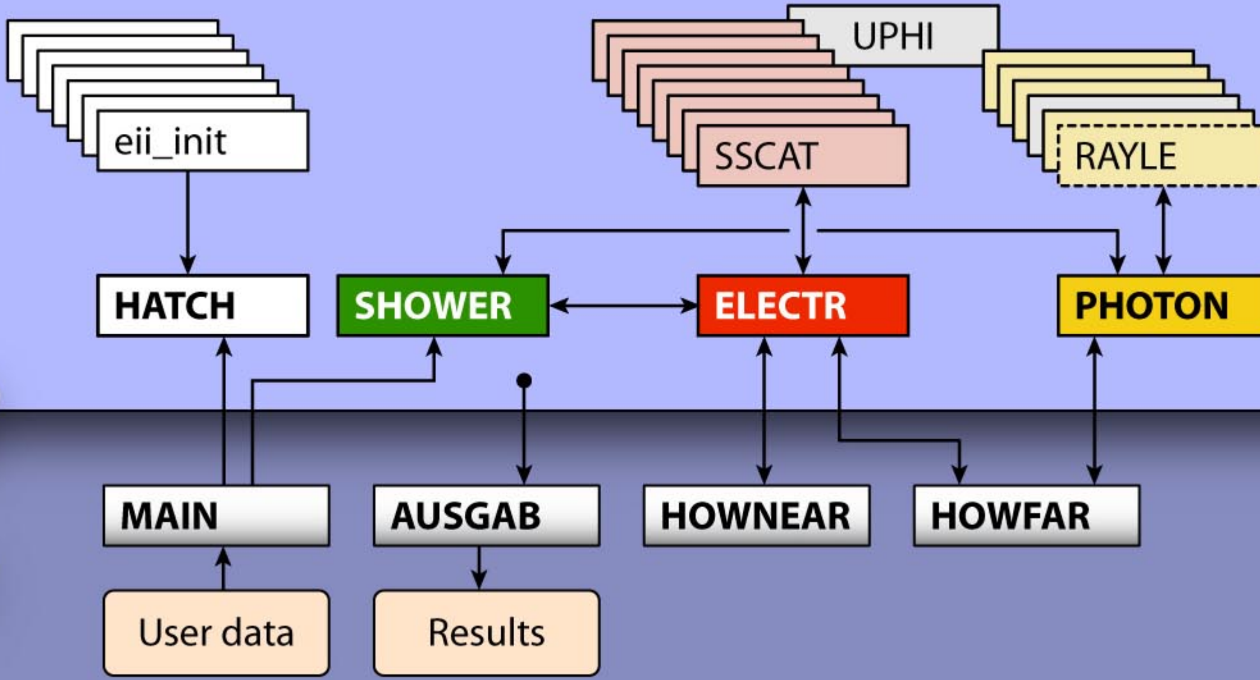
EGSnrc



EGSnrc


eii_init
UPHI
SSCAT
RAYLE
HATCH
SHOWER
ELECTR
PHOTON
MAIN
AUSGAB
HOWNEAR
HOWFAR
User data
Results

EGSnrc



eii_init
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AUSGAB
HOWNEAR
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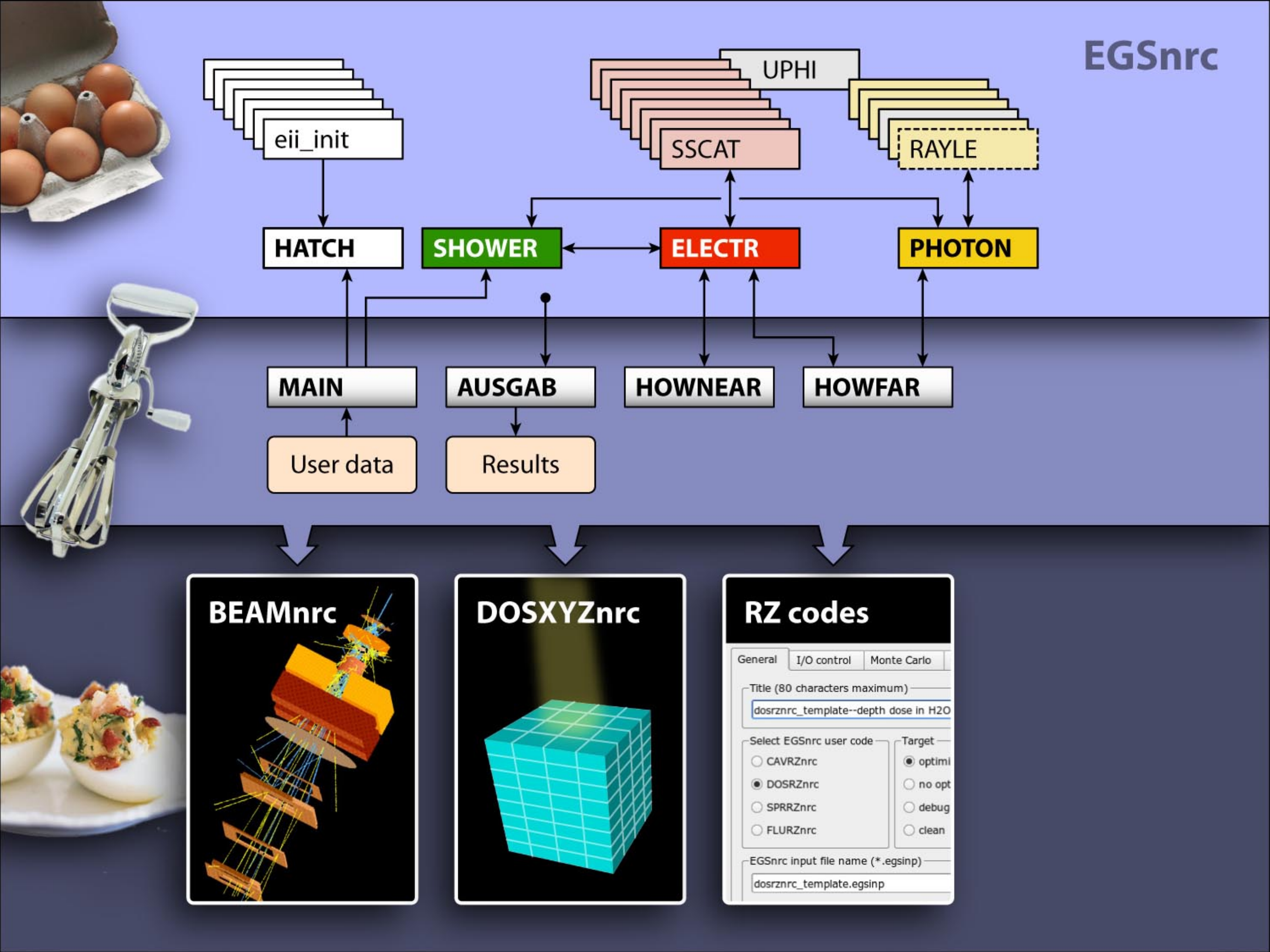
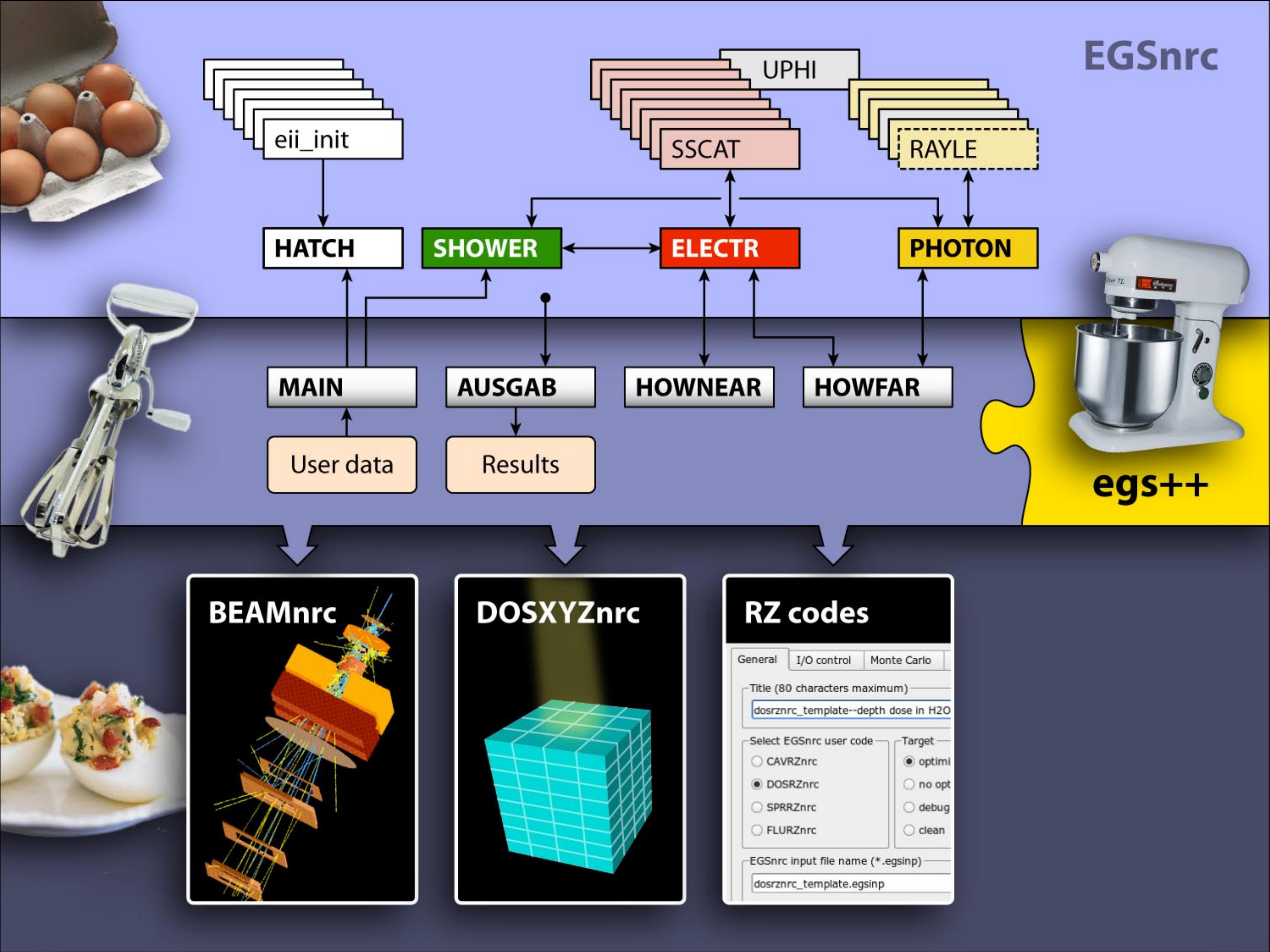
User data
Results


EGSnrc
eii_init
UPHI
SSCAT
RAYLE
HATCH
SHOWER
ELECTR
PHOTON
MAIN
AUSGAB
HOWNEAR
HOWFAR
User data
Results
BEAMnrc
DOSXYZnrc
RZ codes
General
I/O control
Monte Carlo
Title (80 characters maximum)
dosrznrc_template--depth dose in H2O
Select EGSnrc user code
Target
CAVRZnrc
DOSRZnrc
SPRRZnrc
FLURZnrc
optimi
no opt
debug
clean
EGSnrc input file name (*.egsinp)
dosrznrc_template.egsinp



EGSnrc
eii_init
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RAYLE
HATCH
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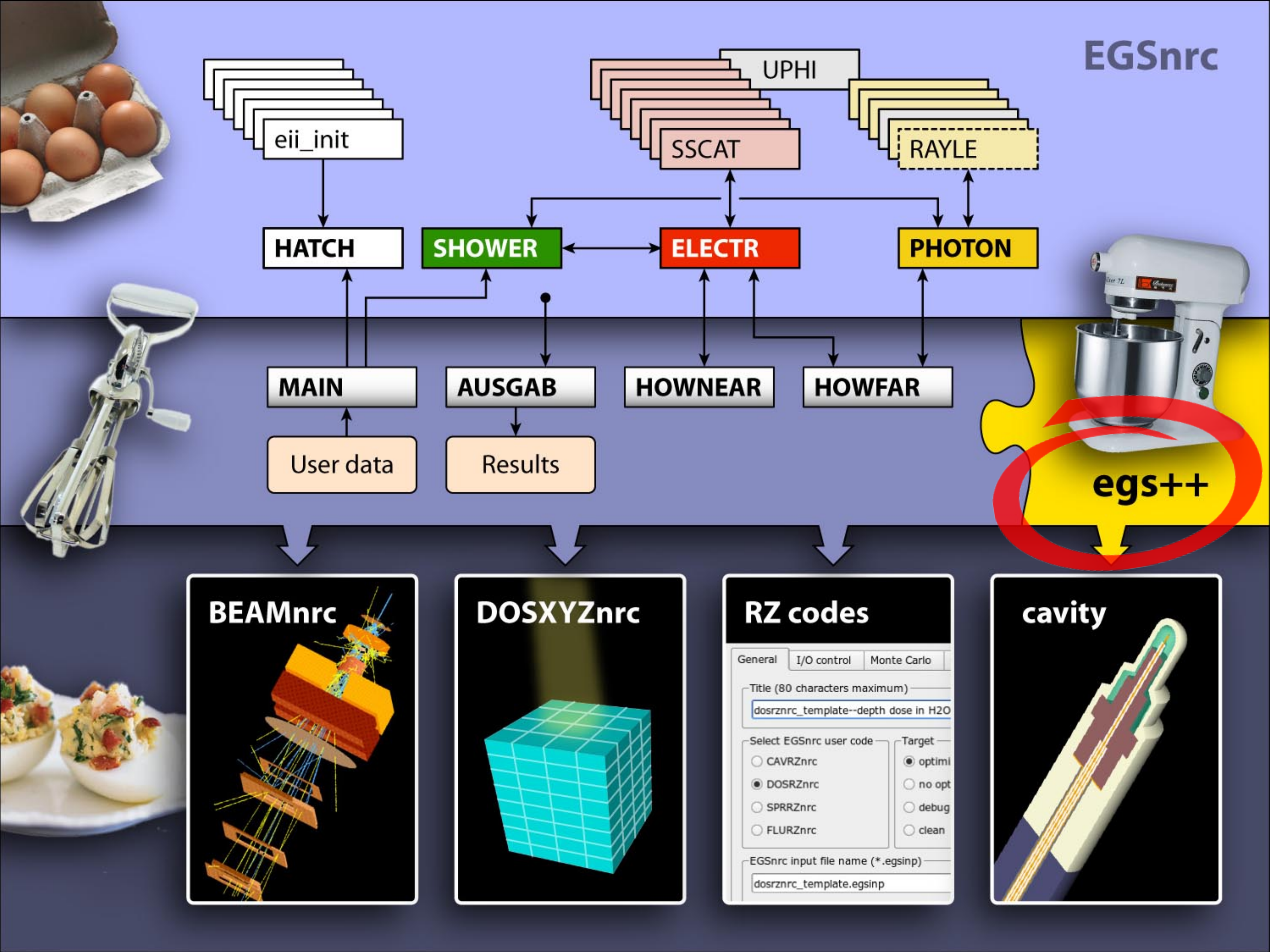
EGSnrc
eii_init
UPHI
SSCAT
RAYLE
HATCH
SHOWER
ELECTR
PHOTON
MAIN
AUSGAB
HOWNEAR
HOWFAR
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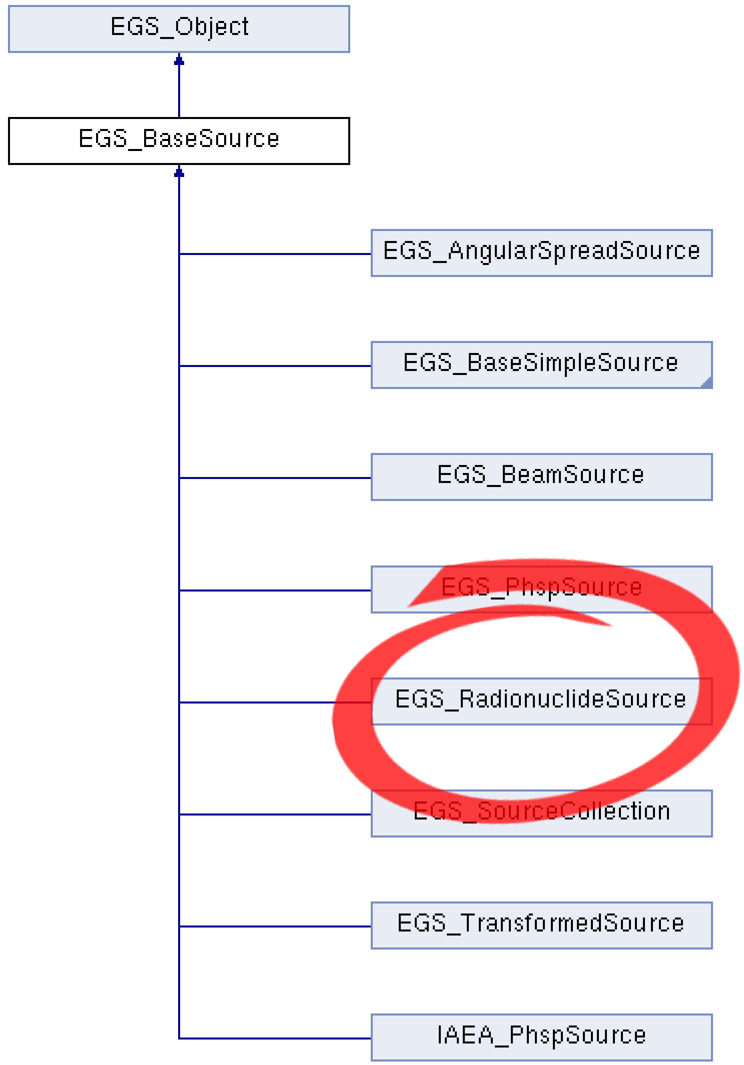
FLURZnrc
optimi
no opt
debug
clean
EGSnrc input file name (*.egsinp)
dosrznrc_template.egsinp
cavity

We are discussing a new source model

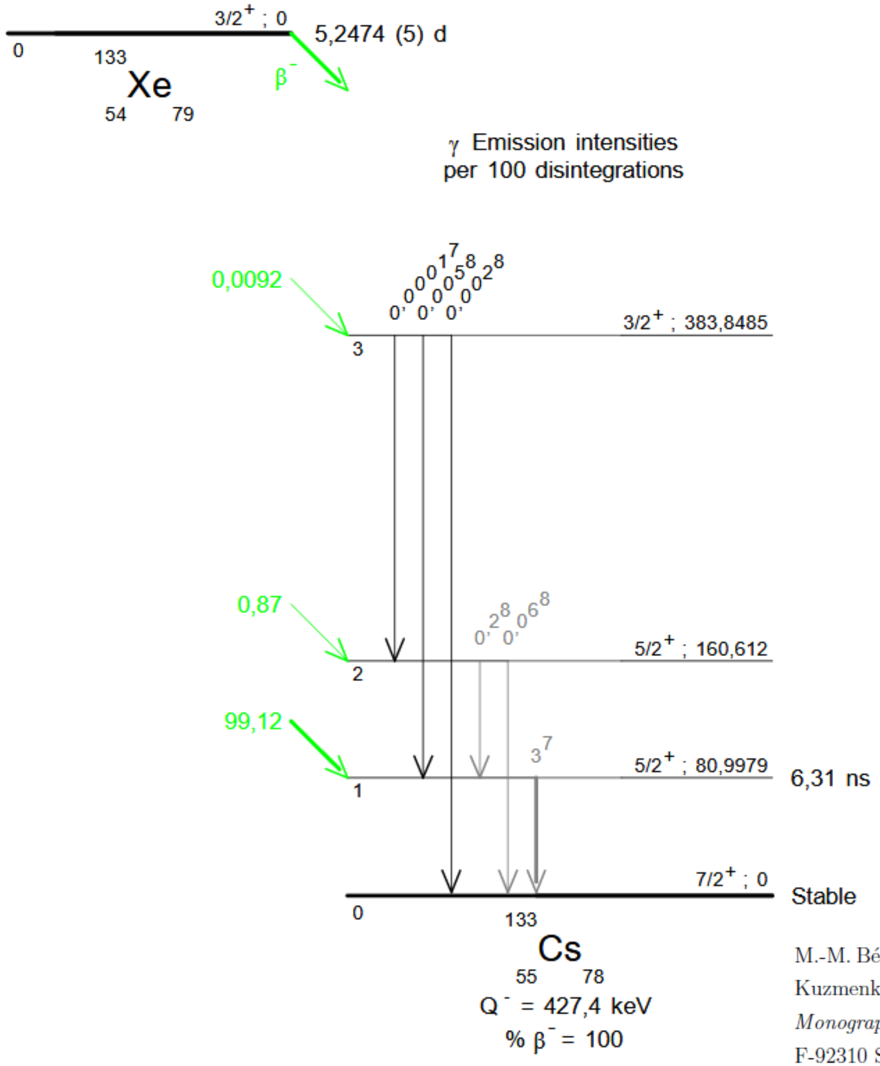
A Monte Carlo simulation for radiation transport requires that you provide the:

1. **geometry** (divide space into regions)
2. **material properties** (elements, density)
3. **source of particles** (distribution in space, energy, direction)
4. **physical parameters** (e.g., cutoff energy)
5. **simulation parameters** (histories, random numbers)
6. **application** (mostly EGSnrc's responsibility)
7. **computer resources** (entirely your responsibility!)
8. **data analysis tools** (mostly your responsibility)

Introducing: EGS_RadionuclideSource



Radionuclide decays are complex to model



M.-M. Bé, V. Chisté, C. Dulieu, M.A. Kellett, X. Mougeot, A. Arinc, V.P. Chechev, N.K. Kuzmenko, T. Kibédi, A. Luca, and A.L. Nichols. *Table of Radionuclides*, volume 8 of *Monographie BIPM-5*. Bureau International des Poids et Mesures, Pavillon de Breteuil, F-92310 Sèvres, France, 2016.

Radionuclide production branches

- Disintegration modes
  - β^- decay
  - β^+ decay
  - Electron capture decay
  - α decay → Decay is modelled but α's are discarded
- Gamma transitions
  - ϒ photon emission
  - Conversion electron emission
  - Electron-positron pair emission → currently neglected

Radionuclide production branches

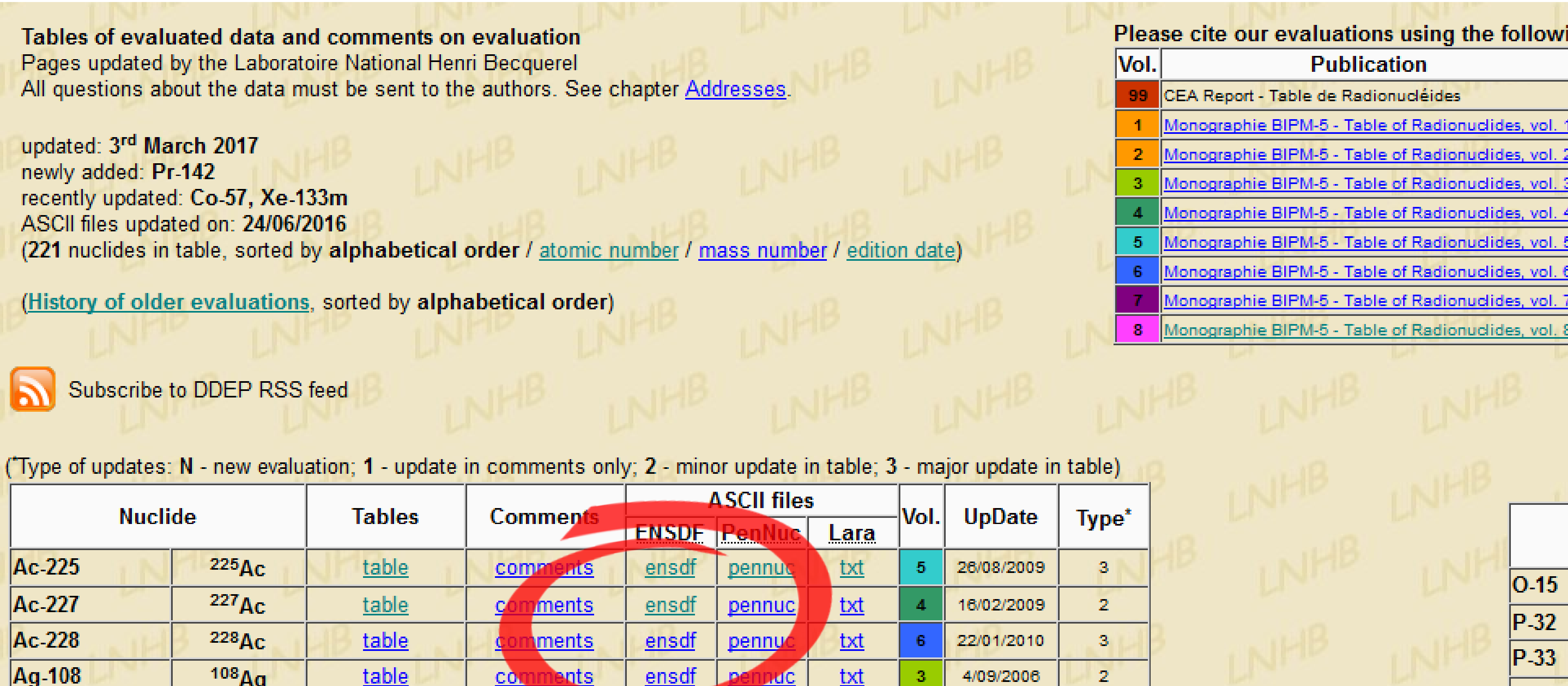
- Electron rearrangement
    - Cascade of X-rays or Auger electrons to fill shell vacancies

→ Currently uncorrelated with decays

- Secondary phenomena accompanying nuclear transformations
    - Internal bremsstrahlung/ionization/excitation

Radionuclide data from LNHB

- Data from Laboratoire National Henri Becquerel (LNHB)
  - http://www.nucleide.org/DDEP_WG/DDEPdata.htm



Tables of evaluated data and comments on evaluation
Pages updated by the Laboratoire National Henri Becquerel
All questions about the data must be sent to the authors. See chapter Addresses.

updated: **3rd March 2017**
newly added: **Pr-142**
recently updated: **Co-57, Xe-133m**
ASCII files updated on: **24/06/2016**
(**221** nuclides in table, sorted by **alphabetical order** / atomic number / mass number / edition date)

(History of older evaluations, sorted by **alphabetical order**)

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Vol.	Publication
99	CEA Report - Table de Radionucléides
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3	Monographie BIPM-5 - Table of Radionuclides, vol. 3
4	Monographie BIPM-5 - Table of Radionuclides, vol. 4
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8	Monographie BIPM-5 - Table of Radionuclides, vol. 8

(*Type of updates: **N** - new evaluation; **1** - update in comments only; **2** - minor update in table; **3** - major update in table)

Nuclide		Tables	Comments	ASCII files			Vol.	UpDate	Type*
				ENSDF	PenNuc	Lara			
Ac-225	^{225}Ac	table	comments	ensdf	pennuc	txt	5	26/08/2009	3
Ac-227	^{227}Ac	table	comments	ensdf	pennuc	txt	4	16/02/2009	2
Ac-228	^{228}Ac	table	comments	ensdf	pennuc	txt	6	22/01/2010	3
Ag-108	^{108}Ag	table	comments	ensdf	pennuc	txt	3	4/09/2006	2

O-15
P-32
P-33

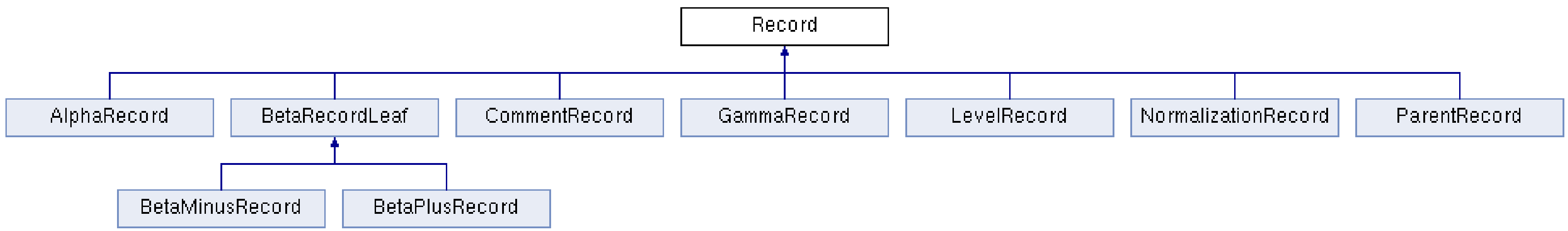
The ENSDF format is widely used

- Evaluated Nuclear Structure Data File (ENSDF)

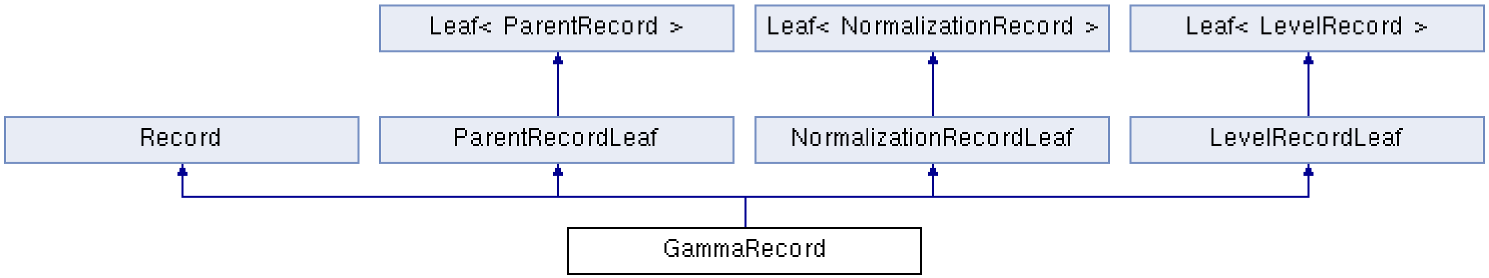
```
67ZN    67GA EC DECAY (3.2613 D)
...
 67ZN T  Auger electrons and X ray energies and emission intensities:
 67ZN T       {U Energy (keV)}   {U Intensity}  {U Line}
 67ZN T
 67ZN T        8.61587            17.0      6      XKA2
 67ZN T        8.63896            33.0     12      XKA1
...
 67ZN T
 67ZN T        7.21-7.55      |]                   KLL AUGER
 67ZN T        8.31-8.63      |]  60.4     21      KLX AUGER
 67ZN T        9.39-9.65      |]                   KXY AUGER
 67ZN T        0.732-0.997        167.5    21      L AUGER
 67GA  P 0.0         3/2-              3.2613 D  5               1000.8    12
 67ZN  N 1.0         1.0        1        1.0
 67ZN  L 0           5/2-               STABLE
 67ZN  E                      3.3     326.532
 67ZN2 E CK=0.8836   15$CL=0.0989   12$CM=0.0164    4$CN=0.0011     1
 67ZN  L 93.31       1/2-              9.00 US   4
 67ZN  E                      50.5    175.261
 67ZN2 E CK=0.8834   15$CL=0.0991   12$CM=0.0164    4$CN=0.0011     1
 67ZN  G 93.307    1238.1     7E2                         0.854  12
 67ZN2 G KC=0.748    11$LC=0.0922   13$MC=0.01300  19$NC=0.000388  6
 67ZN  L 184.58      3/2-              1.028 NS  14
 67ZN  E                      22.3    275.523
 67ZN2 E CK=0.8832   15$CL=0.0993   12$CM=0.0164    4$CN=0.0011     1
 67ZN  G 91.263    153.09     7M1+E2     0.123   25     0.091   6
```

ENSDF records converted to c++ objects

- egs++ design is object-oriented



It's a tree-like structure



Public Member Functions

	GammaRecord (vector< string > ensdf, ParentRecord *myParent, NormalizationRecord *myNormalization, LevelRecord *myLevel)
	GammaRecord (GammaRecord *gamma)
double	**getDecayEnergy** () const
double	**getTransitionIntensity** () const
void	**setTransitionIntensity** (double newIntensity)
int	**getCharge** () const
LevelRecord *	**getFinalLevel** () const
void	**setFinalLevel** (LevelRecord *newLevel)
void	**incrNumSampled** ()
EGS_I64	**getNumSampled** () const

Beta decay energies from Fermi distribution

- "Recall" beta- decay:

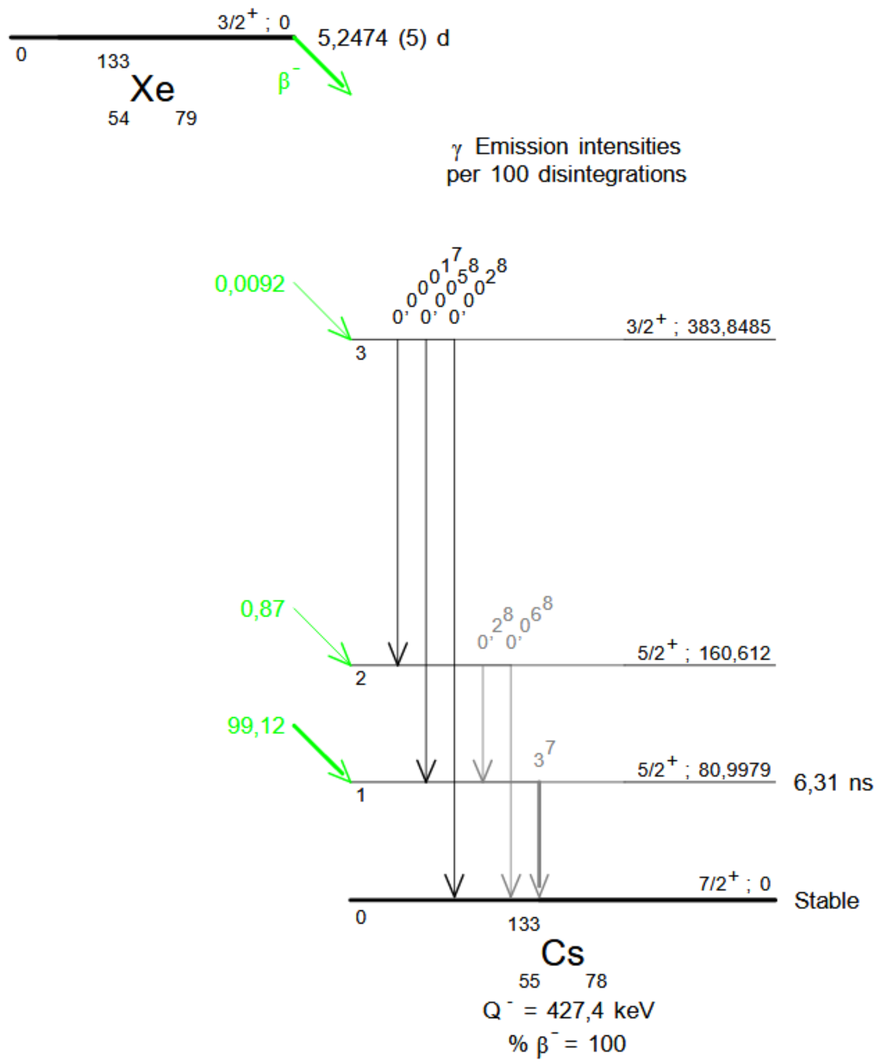
$$ {}^{A}_{Z}\mathrm{X} \rightarrow {}^{A}_{Z+1}\mathrm{Y} + \beta^{-} + \bar{\nu} $$

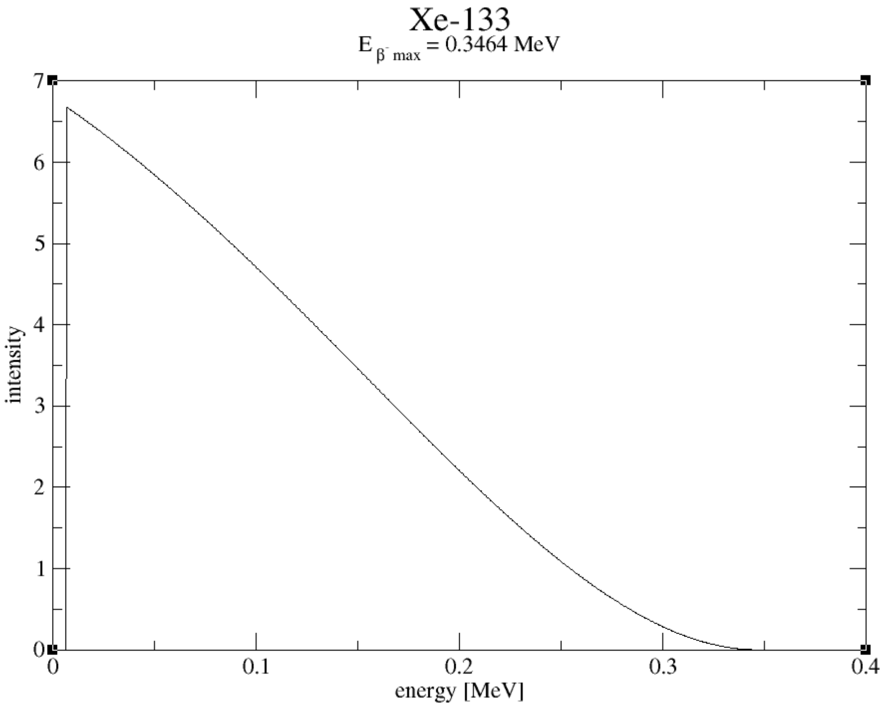
- Beta- energy is a spectrum, with maximum:

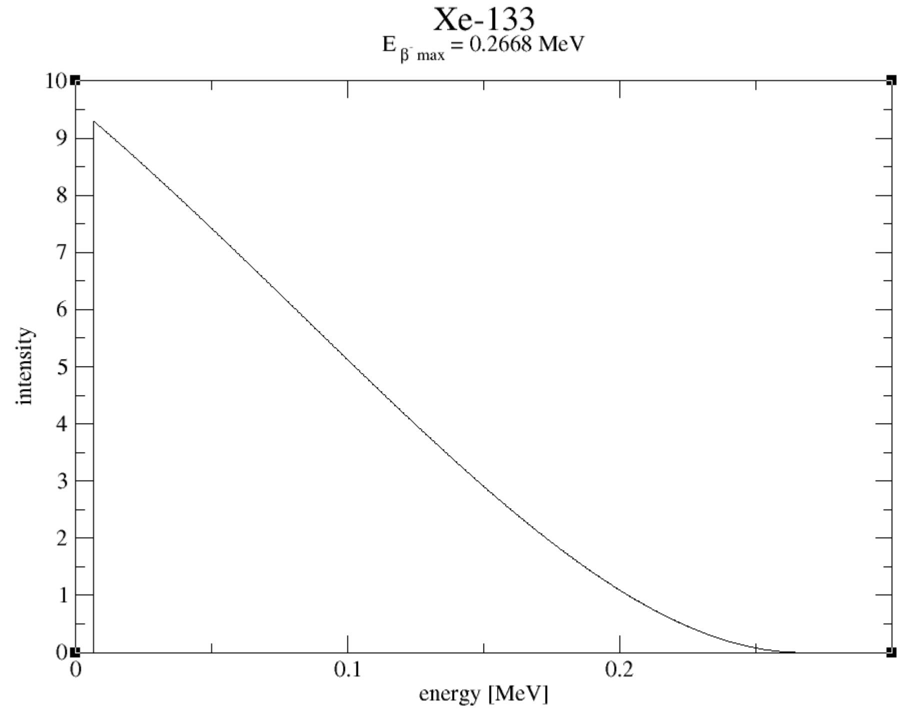
$$ E_{\beta^{-}max} = Q^{-} - E_i $$

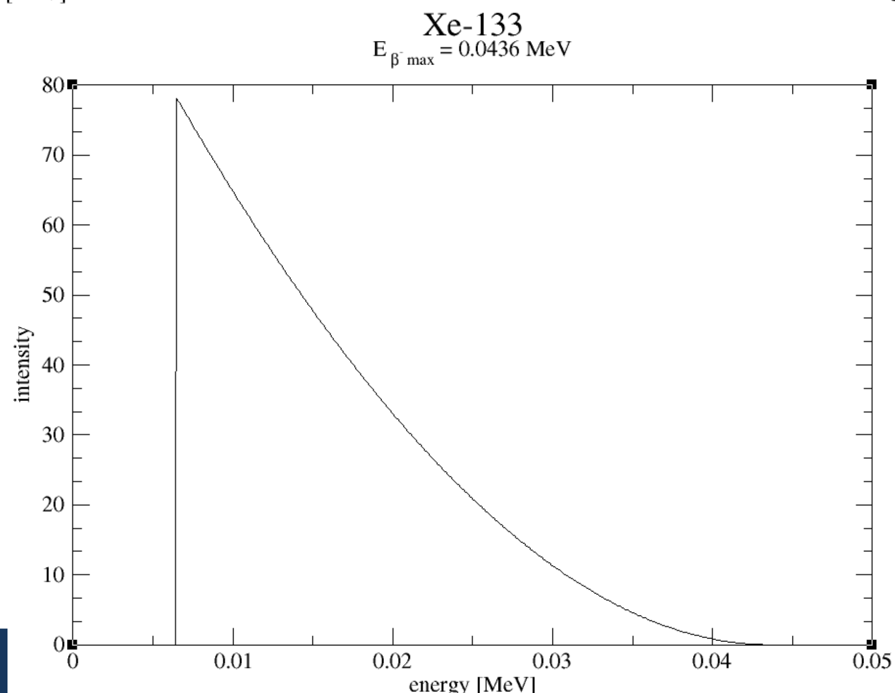
  - Where Q^{-} is the energy of disintegration and E_i is the energy of the level to which decay occurs.

Example: Xe-133 has 3 beta- decays




Xe-133
$E_{\beta^- max}$ = 0.3464 MeV
intensity
energy [MeV]
0
1
2
3
4
5
6
7
0.1
0.2
0.3
0.4


Xe-133
$E_{\beta^- max}$ = 0.2668 MeV
intensity
energy [MeV]
0
1
2
3
4
5
6
7
8
9
10
0.1
0.2


Xe-133
$E_{\beta^- max}$ = 0.0436 MeV
intensity
energy [MeV]
0
10
20
30
40
50
60
70
80
0.01
0.02
0.03
0.04
0.05

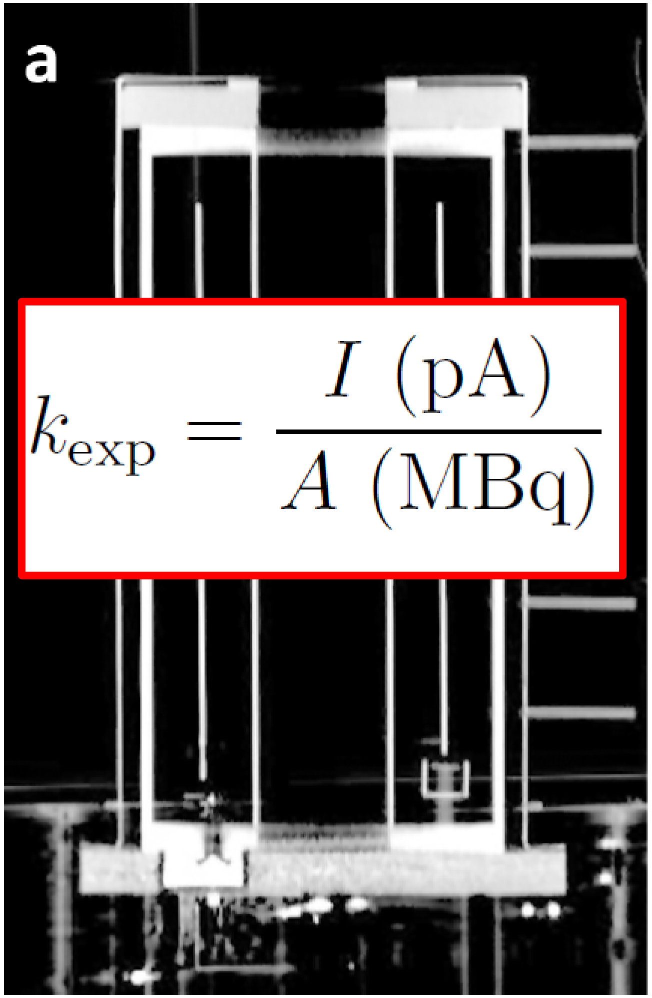
The input file is easy

```
:start source:
    name                    = my_mixture

    library                 = egs_radionuclide_source
    activity                = total activity of mixture, assumed constant

    ... optional arguments ...

    :start shape:
        definition of the source shape
    :stop shape:

    :start spectrum:
        Next slide...
    :stop spectrum:
:stop source:
```

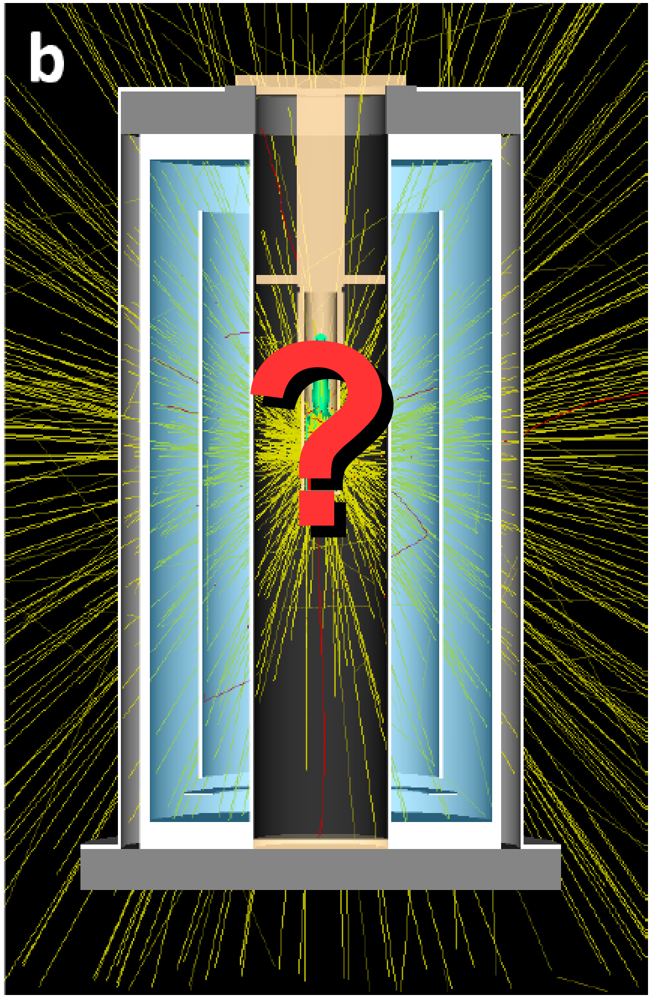
The input file is easy

```
:start source:
    ... source definition (previous) ...

    :start spectrum:

        type              = radionuclide
        isotope           = name of the isotope (e.g. Sr-90)

        relative activity = [optional] the relative activity (sampling
                            probability) for this isotope in a mixture

    :stop spectrum:

    :start spectrum:
        type                  = radionuclide
        isotope               = name of next isotope in mixture (e.g. Y-90)
        relative activity     = ...
    :stop spectrum:

:stop source:
```

Simulations can produce an absolute result



$$k_{\text{exp}} = \frac{I\ (\text{pA})}{A\ (\text{MBq})}$$



EGSnrc cumulates energy depositions

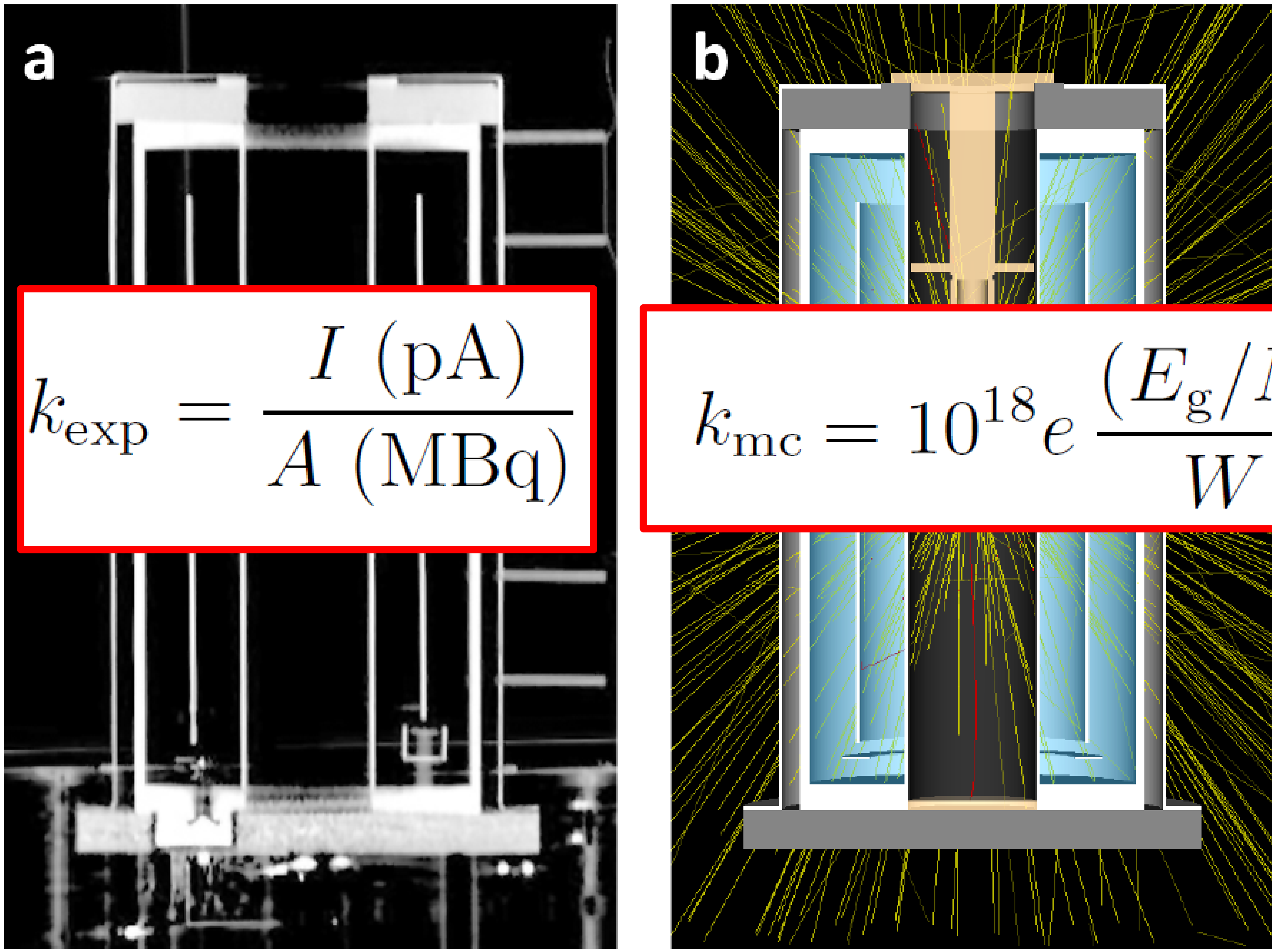
- EGSnrc reports energy deposited in nitrogen [eV]: E_g
- Convert to total charge [C]: $Q = \left(\frac{E_\mathrm{g}}{W}\right) e$

$W = 34.8 \pm 0.2\ \mathrm{eV}$ (average energy to create ion pair in nitrogen)

- The charge is deposited for exactly N decays

$$k_\mathrm{mc} = \frac{I\ (\mathrm{pA})}{A\ (\mathrm{MBq})} = 10^{18} \cdot \frac{Q}{N} = 10^{18} e \frac{(E_\mathrm{g}/N)}{W}$$

Simulations can produce an absolute result



$$k_{\mathrm{exp}} = \frac{I\ (\mathrm{pA})}{A\ (\mathrm{MBq})}$$

$$k_{\mathrm{mc}} = 10^{18} e \frac{(E_{\mathrm{g}}/N)}{W}$$

There was a problem with the detector model

- Initially, the modelled detector response was systematically low
    - An energy-dependent difference (~7%)

- This indicates a physical discrepancy:
    - Material properties (density, composition)?
    - Geometrical (wall thicknesses)?

We increased the gas pressure

- Varying within manufacturer tolerances could not account
- There was no tolerance on the nitrogen pressure (nominal 1MPa)
  - Increasing the pressure ~7% worked (chi-squared optimized)

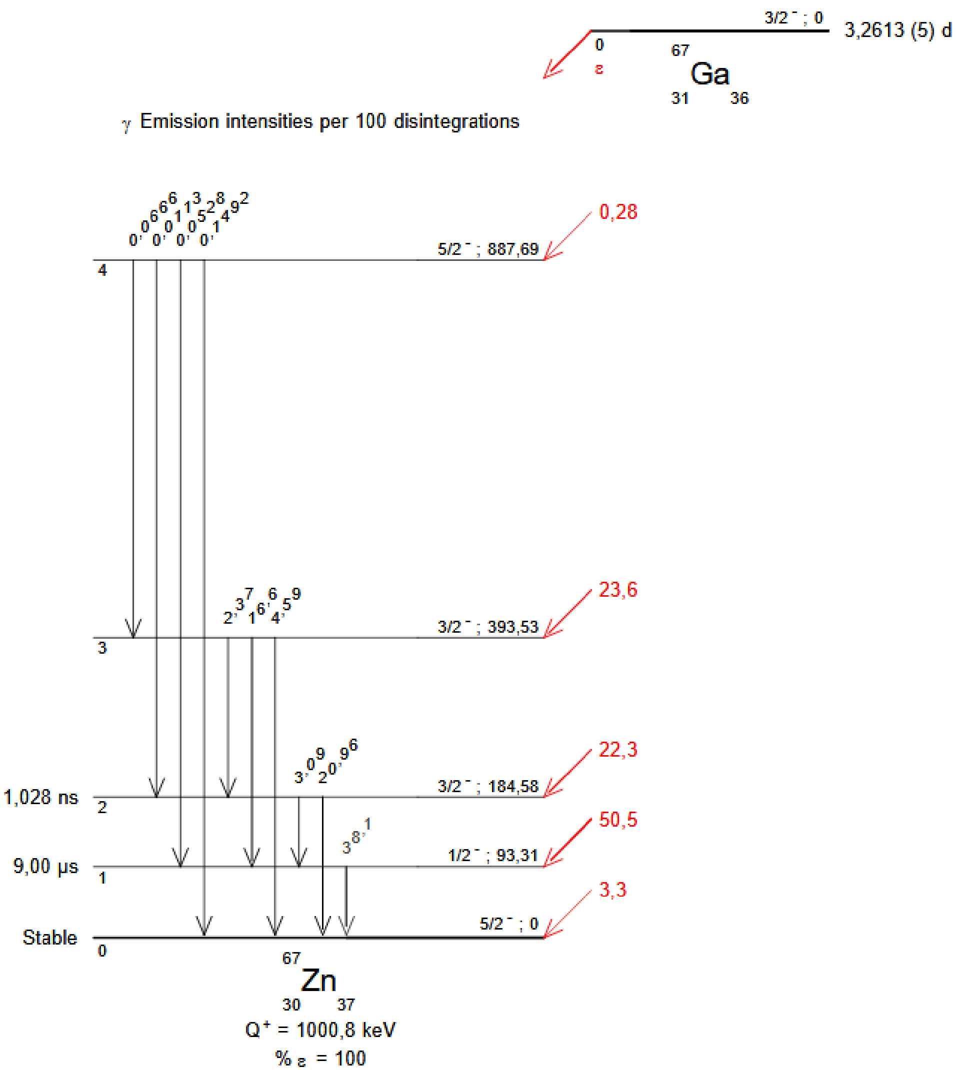
- Therefore, our model **predicts** a 7% higher pressure

Turns out it's corroborated

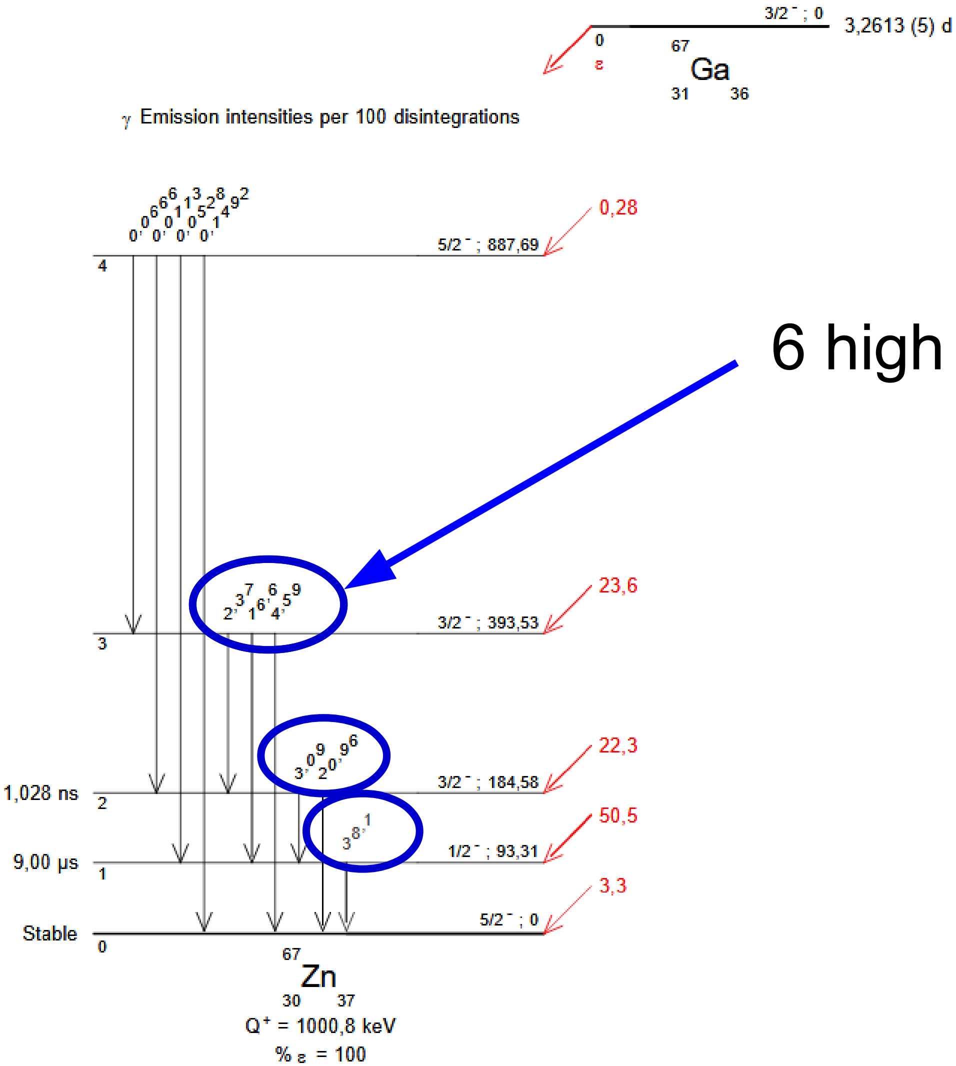
- Strikingly, a previous group also found a 7.2% higher pressure by simulations of a similar chamber using PENELOPE

A De Vismes and MN Amiot. Towards absolute activity measurements by ionisation chambers using the penelope monte-carlo code. *Applied radiation and isotopes*, 59(4):267–272, 2003.

Calculating calibration factors: an example

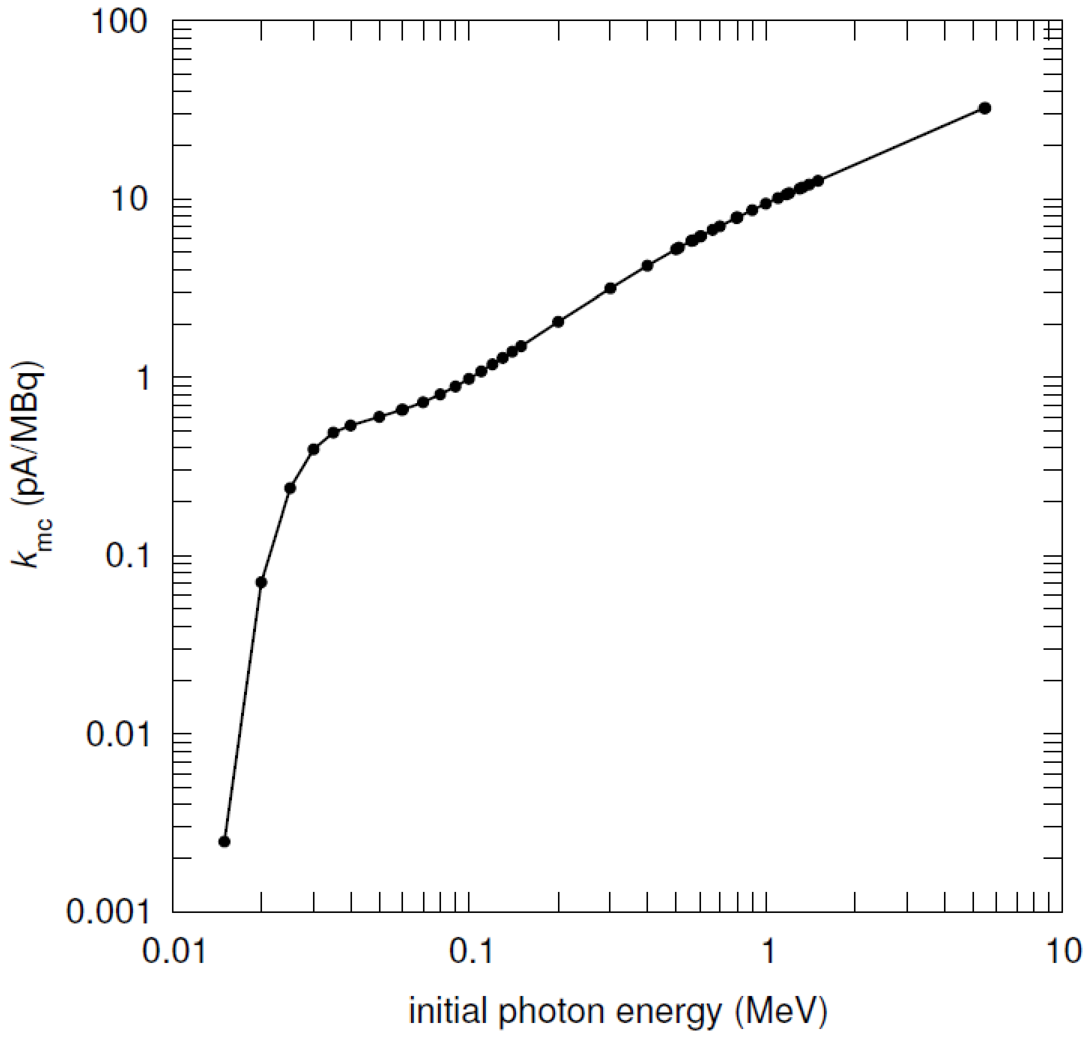


Let's try this the “old way”



6 high intensity photon lines

Use a series of monoenergetic simulations



Interpolate response

$k_1=0.899$

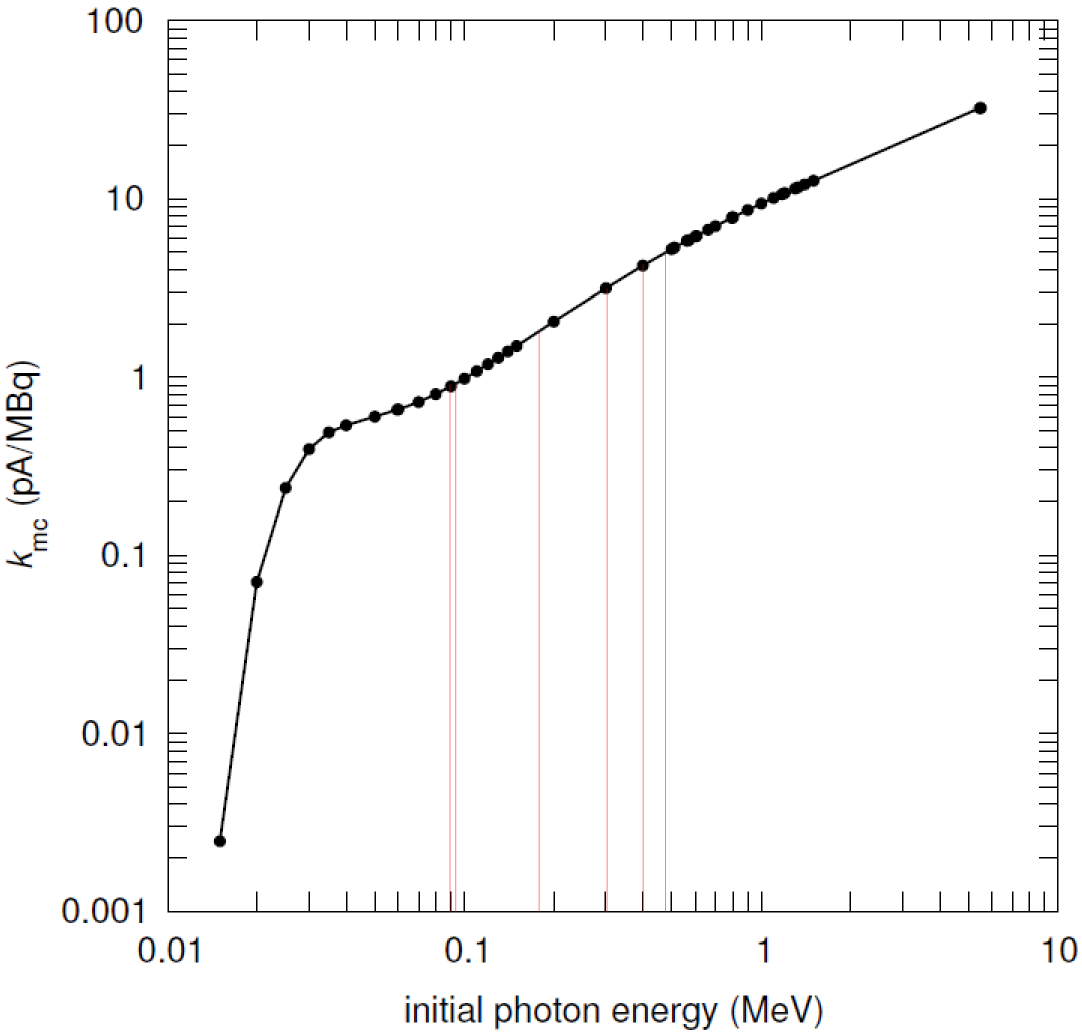
$k_2=0.917$

$k_3=1.877$

$k_4=2.146$

$k_5=3.142$

$k_6=4.140$



Perform weighted sum using relative intensities

$k_1=0.899$ $P_1=3.09$

$k_2=0.917$ $P_2=38.1$

$k_3=1.877$ $P_3=20.96$

$k_4=2.146$ $P_4=2.37$

$k_5=3.142$ $P_5=16.6$

$k_6=4.140$ $P_6=4.59$

$\rightarrow$ $k_{hand} = 1.533$

Perform weighted sum using relative intensities

$k_1 = 0.899$ $P_1 = 3.09$

$k_2 = 0.917$ $P_2 = 38.1$

$k_3 = 1.877$ $P_3 = 20.96$

$k_4 = 2.146$ $P_4 = 2.37$

$k_5 = 3.142$ $P_5 = 16.6$

$k_6 = 4.140$ $P_6 = 4.59$

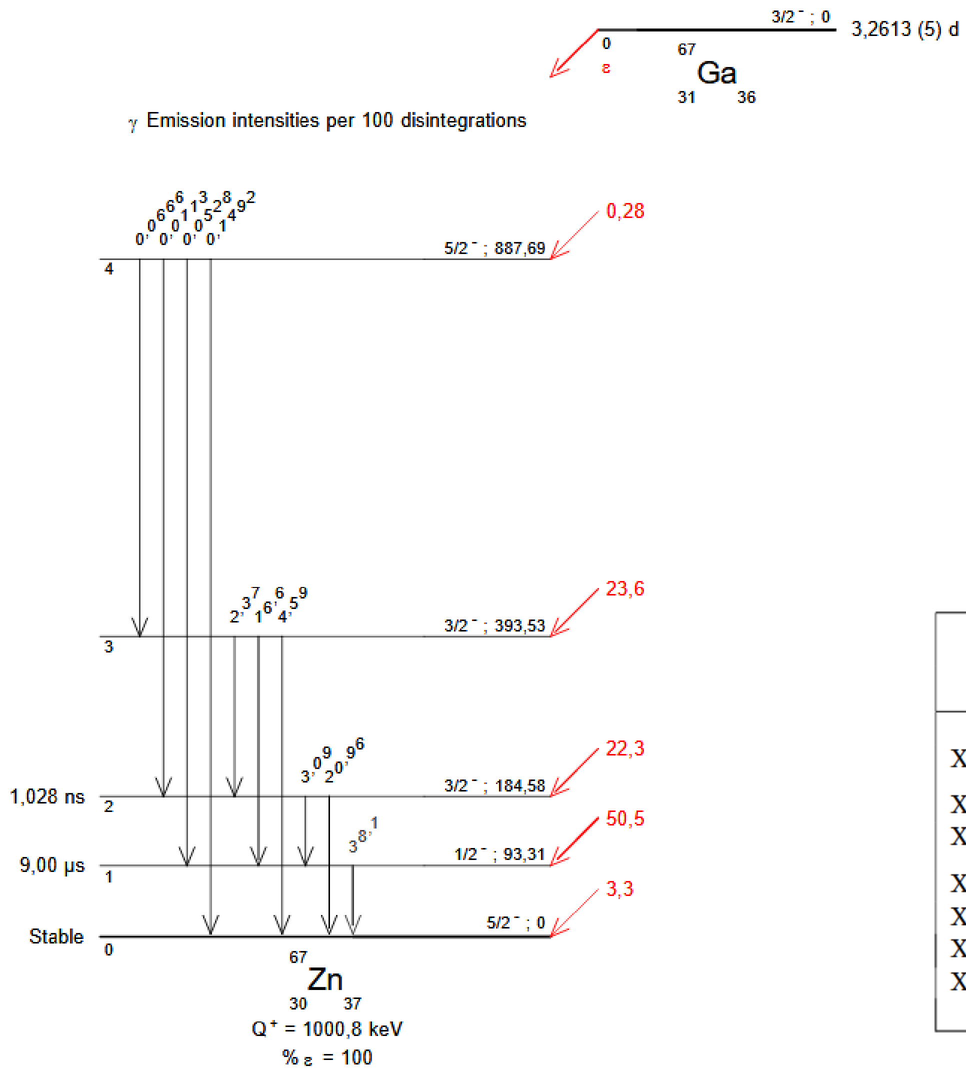
→

$k_{hand} = 1.533$

$k_{exp} = 1.583$

-3.1%

The radionuclide source models a bit more

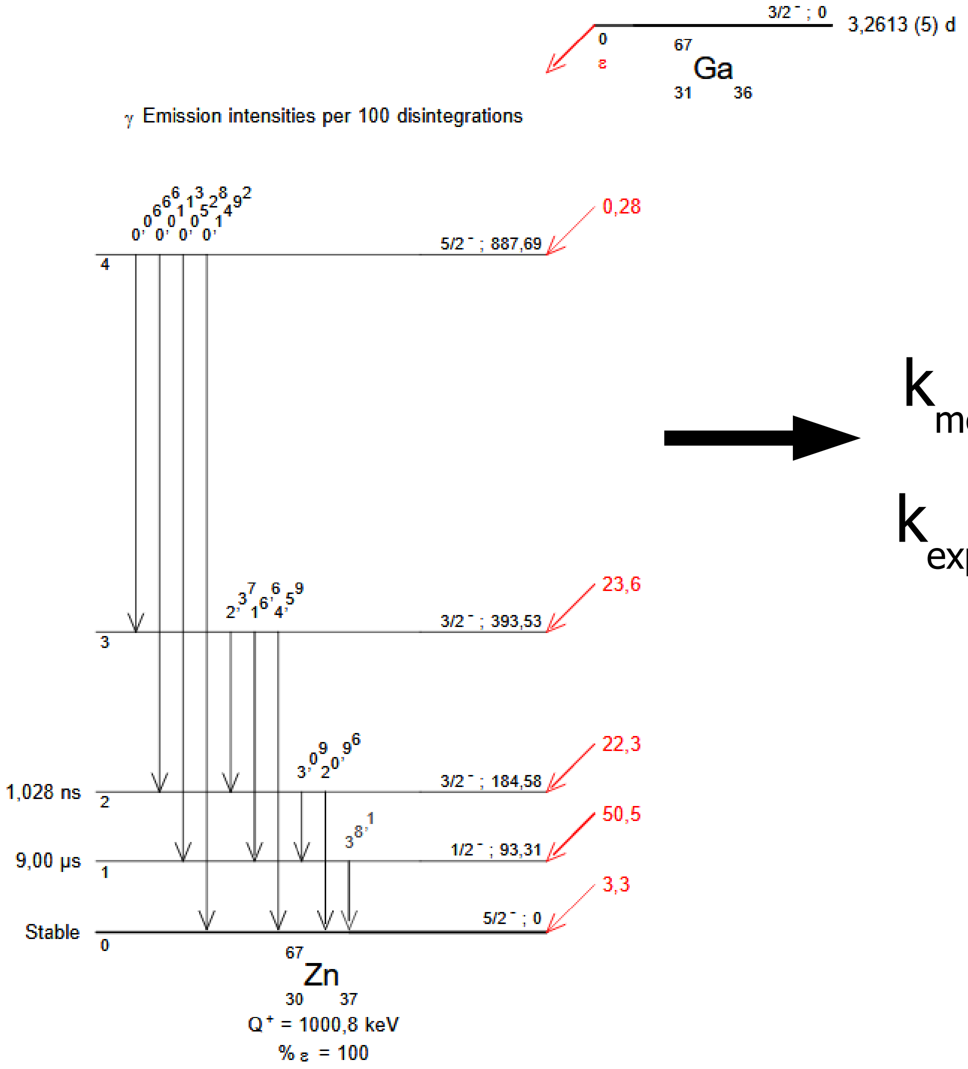


		Energy keV			Electrons per 100 disint.
e_{AL}	(Zn)	0,732	-	0,997	167,5 (21)
e_{AK}	(Zn)				60,4 (21)
	KLL	7,21	-	7,55	}
	KLX	8,31	-	8,63	}
	KXY	9,39	-	9,65	}
$ec_{2,1\ K}$	(Zn)	81,604		(15)	0,250 (16)
$ec_{1,0\ K}$	(Zn)	83,651		(5)	28,4 (7)
$ec_{1,0\ L}$	(Zn)	92,116	-	93,290	3,55 (9)
$ec_{1,0\ M}$	(Zn)	93,174	-	93,302	0,522 (13)
$ec_{2,0\ K}$	(Zn)	174,918		(17)	0,316 (40)
$ec_{3,1\ K}$	(Zn)	290,558		(10)	0,060 (3)

		Energy keV		Photons per 100 disint.	
XL	(Zn)	0,8836 — 1,1861		1,75 (5)	
$XK\alpha_2$	(Zn)	8,61587		17,0 (6)	} $K\alpha$
$XK\alpha_1$	(Zn)	8,63896		33,0 (12)	}
$XK\beta_1$	(Zn)	9,5721	}	7,08 (26)	$K\beta_1'$
$XK\beta_5''$	(Zn)	9,6499	}		
$XK\beta_2$	(Zn)	9,6581	}		
$XK\beta_4$	(Zn)		}		$K\beta_2'$

M.-M. Bé, V. Chisté, C. Dulieu, M.A. Kellett, X. Mougeot, A. Arinc, V.P. Chechev, N.K. Kuzmenko, T. Kibédi, A. Luca, and A.L. Nichols. *Table of Radionuclides*, volume 8 of *Monographie BIPM-5*. Bureau International des Poids et Mesures, Pavillon de Breteuil, F-92310 Sèvres, France, 2016.

Closer agreement!



$k_{mc} = 1.5547$

$k_{exp} = 1.583$

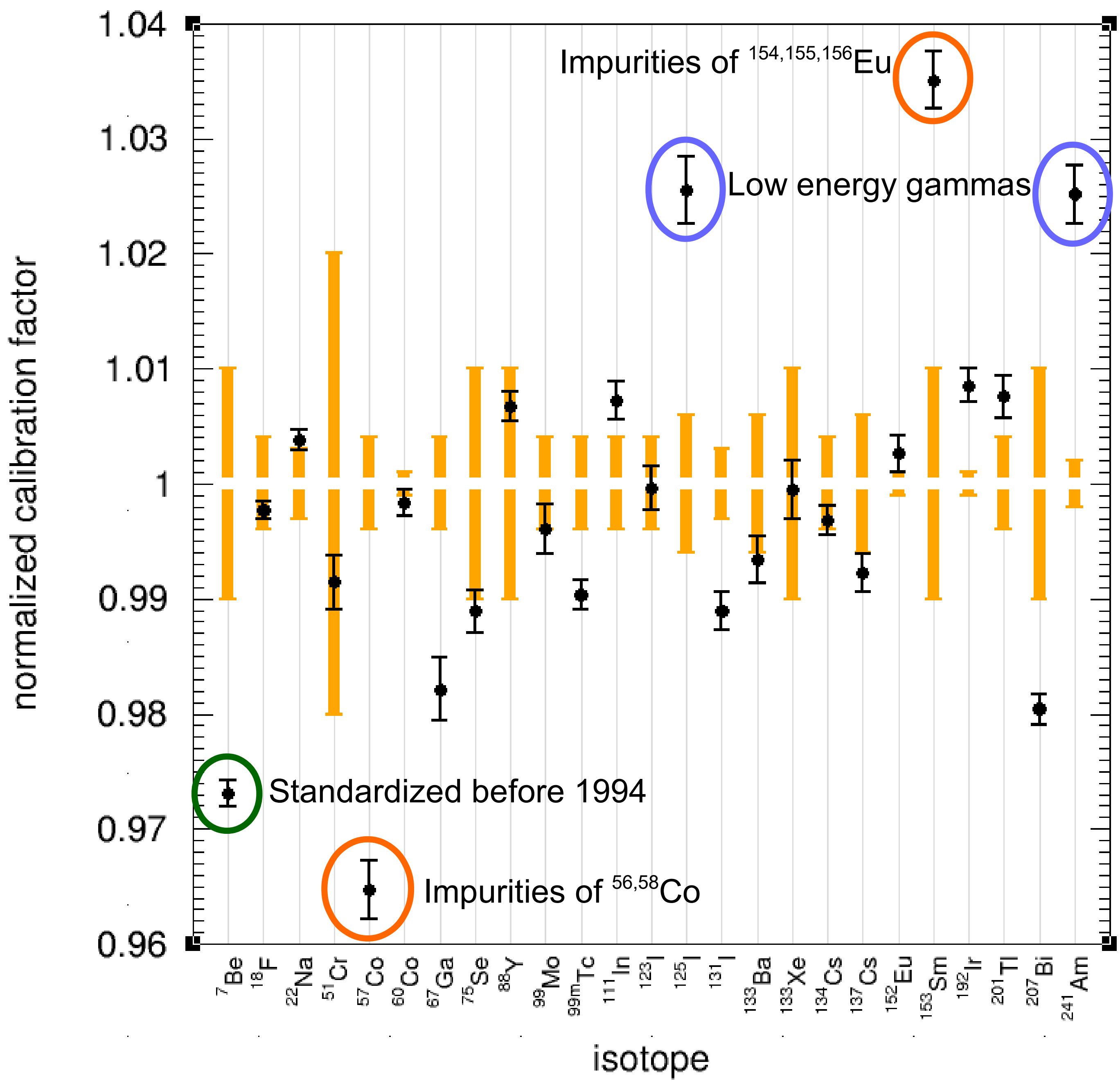
-1.8%

(factor of 1.7 closer)

After a few minutes on the cluster...

Isotope	k_{mc} (pA/MBq)	Statistical uncertainty	k_{exp} (pA/MBq)	Measurement uncertainty	Percent difference
^{7}Be	0.5206	0.1%	0.535	1%[a]	−2.69%
^{18}F	10.3163	0.1%	10.34	0.3%	−0.23%
^{22}Na	20.8490	0.1%	20.77	0.3%	0.38%
^{51}Cr	0.3324	0.2%	0.3353	2%	−0.85%
^{57}Co	1.1818	0.3%	1.225	0.4%	−3.53%
^{60}Co	22.2038	0.1%	22.24	0.1%	−0.16%
^{67}Ga	1.5547	0.3%	1.583	0.4%	−1.79%
^{75}Se	3.9437	0.2%	3.988	1%[b]	−1.11%
^{88}Y	22.6812	0.1%	22.53	1%	0.67%
^{99}Mo*	2.6784	0.2%	2.689	0.4%	−0.39%
^{99m}Tc	1.2389	0.1%	1.251	0.4%	−0.97%
^{111}In	4.1335	0.2%	4.104	0.4%	0.72%
^{123}I	1.7733	0.2%	1.774	0.4%	−0.04%
^{125}I	0.4974	0.3%	0.485	0.6%	2.56%
^{131}I	3.9884	0.2%	4.033	0.3%	−1.11%
^{133}Ba	4.2695	0.2%	4.298	0.6%	−0.66%
^{133}Xe	0.5052	0.3%	0.5055	1%[c]	−0.05%
^{134}Cs	15.5403	0.1%	15.59	0.4%	−0.32%
^{137}Cs	5.6963	0.2%	5.741	0.6%	−0.78%

Isotope	k_{mc} (pA/MBq)	Statistical uncertainty	k_{exp} (pA/MBq)	Measurement uncertainty	Percent difference
^{152}Eu	11.0289	0.2%	11.00	0.1%	0.26%
^{153}Sm	0.6785	0.2%	0.6555	1%[b]	3.51%
^{192}Ir	8.5532	0.2%	8.481	0.1%	0.85%
^{201}Tl	0.9053	0.2%	0.8985	0.4%	0.76%
^{207}Bi	14.6473	0.1%	14.94	1%[b]	−1.96%
^{241}Am	0.2515	0.3%	0.2453	0.2%	2.52%



normalized calibration factor
1.04
1.03
1.02
1.01
1
0.99
0.98
0.97
0.96
Impurities of 154,155,156Eu
Low energy gammas
Standardized before 1994
Impurities of 56,58Co
7Be
18F
22Na
51Cr
57Co
60Co
67Ga
75Se
88Y
99Mo
99mTc
111In
123I
125I
131I
133Ba
133Xe
134Cs
137Cs
152Eu
153Sm
192Ir
201Tl
207Bi
241Am
isotope

Now we know where to focus

- The discrepancies highlight isotopes inviting a closer look

- In the experiment:
    - Radio-impurities?
    - Re-standardization by primary method?
    - Sharpen uncertainties by testing different conditions
- In the model:
    - Pure water used as the source solution (even for gases!)
    - Lead shielding around detector
    - Materials, geometries, source modelling etc.

Simulations provide answers

- With an accurate EGSnrc model at our disposal, we can now look at the questions:
  - How does the uncertainty on a parameter affect measurement?
  - What is the calibration factor for a radionuclide not previously measured?
  - What is the calibration factor for a non-standard geometry?
  - What is the effect of radioimpurities?

https://nrc-cnrc.github.io/EGSnrc/

View on GitHub

EGSnrc

Toolkit for Monte Carlo simulation of ionizing radiation transport

tar.gz .zip

Documentation

- EGSnrc core manual (PIRS-701)
- BEAMnrc accelerators (PIRS-509a)
- DOSXYZnrc voxel dose (PIRS-794)
- egs++ class library (PIRS-898)
- Applications for RZ geometries (PIRS-702)
- egs_inprz RZ user interface (PIRS-801)
- BEAMDP phase-space processor (PIRS-509c)
- STATDOSE 3D dose processor (PIRS-509f)

Installation

EGSnrc can be installed on computers running Linux, macOS or Windows. Please read the installation instructions for details on how to download and properly configure EGSnrc on your operating system.

What is EGSnrc?

EGSnrc is a software toolkit to perform Monte Carlo simulation of ionizing radiation transport through matter. It models the propagation of photons, electrons and positrons with kinetic energies between 1 keV and 10 GeV, in homogeneous materials. EGSnrc is an extended and improved version of the Electron Gamma Shower (EGS) software package originally developed at the Stanford Linear Accelerator Center (SLAC) in the 1970s. Most notably, it incorporates significant refinements in charged particle transport, better low energy cross sections, and the egs++ class library to model elaborate geometries and particle sources.

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Reid Townson, Frédéric Tessier, Raphael Galea

Measurement Science and Standards
National Research Council Canada