Activation

Radiation Protection Topical Course

25-27 November 2024, CERN

Outline

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- Estimation of nuclide yields/activities with event-based methods
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  - The use of **AUXSCORE**
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- Estimation of nuclide yields/activities with fluence-based methods
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Introduction

Introduction

- The estimation of induced radioactivity, total and/or specific activity for the various radionuclides, is an integral part of many RP assessments, for instance:
  - Comparison to regulatory limits for clearance of materials, establishing appropriate transport conditions, establishing appropriate disposal pathways
  - Estimation of committed effective dose due to inhalation or ingestion

- Several built-in scoring options are available in FLUKA:
  - These are **event-based methods**, that is methods for which the estimation of induced radioactivity is based on the radionuclide creation events:
    - `RESNUCLE`: scoring on a region basis, provides the full inventory (including isomers)
    - `USRBIN` (`ACTIVITY` or `ACTOMASS`): scoring on mesh basis, provides one value per bin, but filtering/weighting is also possible with `AUXSCORE` and `comscw.f`
- Various user routines allow for more flexibility if needed:
  - With these, the User can typically also implement **fluence-based methods**, that is methods for which the estimation of induced radioactivity is based first on the estimation of particle fluences followed by their folding with radionuclide production cross sections or derived coefficients.

Covered in the FLUKA Beginner Course, will be recalled today

Typically, only mentioned in the FLUKA Advanced Course

Recalls on settings for activation calculations 1/4

- **Evaporation** of heavy fragments and **coalescence** must be requested with the `PHYSICS` card.
  - Remember to run with `flukadpm` or use `ldpmqmd` to compile your executable to link RQMD and DPMJET.
  - Since FLUKA4-2.0, a model for deuteron nuclear reactions below 150 MeV/n has been implemented: the `IONSPLIT` card recommended in the past is no longer appropriate.

PHYSICS	Type: EVAPORAT ▾	Model: New Evap with heavy frag ▾
	Zmax: 0	Amax: 0
PHYSICS	Type: COALESCE ▾	Activate: On ▾

- Note that, **if appropriate**:
  - Full transport of heavy ions can be activated with `IONTRANS`: this is relevant for cases in which the produced isotopes can have sufficient kinetic energy to escape a region (i.e. gas regions)
  - For ultra-relativistic heavy ions, **electromagnetic dissociation** has to be explicitly requested

PHYSICS	Type: EM-DISSO ▾	EM Disso: Proj&Target EM-Disso ▾

  - **Photonuclear interactions** (not on by default) can be enabled via the `PHOTONUC` card at selected/all energy ranges on a per-material basis. Since inelastic scattering lengths for photonuclear interactions can be very long, one may also resort to biasing photonuclear interactions (see `LAM-BIAS`)

PHOTONUC		Type: ▾		All E: On ▾
	E>0.7GeV: off ▾	Δ resonance: off ▾	Quasi D: off ▾	Giant Dipole: off ▾
		Mat: COPPER ▾	to Mat: COPPER ▾	Step:

Recalls on settings for activation calculations 2/4

- Note that, **if appropriate**:
  - A e^+/e^- can interact with a target nucleus via the exchange of a virtual photon. **Electronuclear interactions** (off by default) can be enabled via the **PHOTONUC** card. Note that:
    - These nuclear reactions can be important for energies above 10 MeV and for thin targets ($\ll X_0$).
    - As for photonuclear reactions, one may also resort to biasing electronuclear interactions (see **LAM-BIAS**).
    - Enabling electronuclear reactions automatically enables photonuclear reactions if not yet enabled.

PHOTONUC Type: ELECTNUC ▾ All E: On ▾
E>0.7GeV: off ▾ Δ resonance: off ▾ Quasi D: off ▾ Giant Dipole: off ▾
Mat: COPPER ▾ to Mat: COPPER ▾ Step:

  - A μ^+/μ^- can interact with a target nucleus via the exchange of a virtual photon. **Muon photonuclear interactions** (off by default) can be enabled via the **MUPHOTON** card on a per-material basis. Note that:
    - This may be relevant for both high-energy electron machines (bremsstrahlung $\gamma \rightarrow \mu^+\mu^-$) and for high-energy hadron machines (0.999877 branching in pion decay $\pi^+ \rightarrow \mu^+ + \nu_\mu$, $\pi^- \rightarrow \mu^- + \overline{\nu_\mu}$)
    - Muon pair production by photons should be activated (see **PHOTONUC** with **SDUM MUMUPAIR** or **MUMUPRIM**): the biasing is requested in the same card. This may be relevant for both high-energy electron machines (bremsstrahlung $\gamma \rightarrow \mu^+\mu^-$) and for high-energy hadron machines ($\pi^0 \rightarrow \gamma\ \gamma$).

MUPHOTON μ Inter: Full ▾ σ long/trans: ρ inter:
Mat: COPPER ▾ to Mat: COPPER ▾ Step:

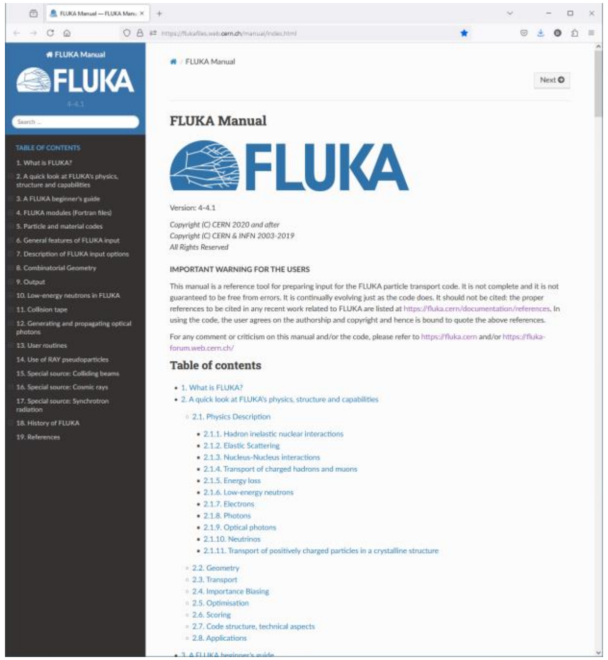
Recalls on settings for activation calculations 3/4

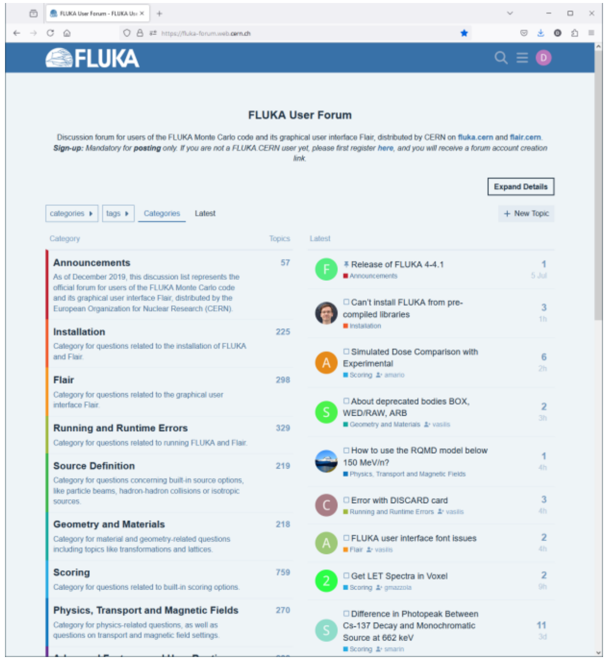
- Transport thresholds can be optimized if one is interested in prompt/activation calculations only.
  - Typical threshold energies for nuclear reactions from charged hadrons are of the order of a couple of MeV
  - Typical threshold energies for photonuclear reactions are of the order of 5-8 MeV, with the exceptions of $^{2}_{1}H$ (2.22 MeV) and $^{9}_{4}Be$ (1.67 MeV)
- For example, for typical hadron machines and for estimation of prompt quantities or radionuclide inventories only:
  - Neutrons should be transported down to thermal energies (1E-14 GeV) (see **PART-THR**).
  - Charged hadrons can be transported down to a couple of MeV (see **PART-THR**).
  - Muons can be transported down to a couple of tens MeV (see **PART-THR**).
  - Photons can be transported down to a few MeV, or the electromagnetic cascade can even be switched off in first approximation (see **EMF**, **EMFCUT**, **RADDECAY**).
- These considerations, specifically the ones concerning electrons, positrons, and photons, are not valid for residual dose rate estimates (see Lecture on Residual radiation exposure)

Recalls on settings for activation calculations 4/4

- The User should be aware that most Monte Carlo codes have, among others, the following assumptions:
  - Media and geometry are static, homogeneous, and isotropic
  - **Material properties are not affected by particle reactions**, e.g. no simulation of transmutation/burnup

- **Key message**: Question if the chosen simulation settings are appropriate for the specific application. When in doubt, the FLUKA Manual and previous posts on the FLUKA User Forum should be among the first resources to be consulted.





Recalls on FLUKA cards from the Beginner's lectures 1/3

- **RADDECAY** activates the production and simulation of the decay of the radioactive nuclides produced and allows to modify biasing and transport thresholds for the transport of decay radiation

RADDECAY		Decays: Activation ▾	Patch Isom: On ▾	Replicas: 3.0
	h/µ Int: ignore ▾	h/µ LPB: ignore ▾	h/µ WW: ignore ▾	e-e+ Int: ignore ▾
	e-e+ LPB: ignore ▾	e-e+ WW: ignore ▾	Low-n Bias: ignore ▾	Low-n WW: ignore ▾
		decay cut: 10.0	prompt cut: 99999.0	Coulomb corr: ▾

Decays	Activation	Radioactive **decays are activated for requested cooling times**: the time evolution is calculated analytically for fixed cooling times. Daughter nuclei and associated radiation(s) are considered at these cooling times (see Lecture on Radioactive Sources for the other use case).
Patch Isom	On	Activate a rough **isomer production model**, assuming equal production rate among ground state and isomer states.
Replicas	#	Number of replicas of the decay of each individual residual (see the Lecture on Residual Radiation).
h/µ Int .. Low-n WW		Flag for applying biasing features only to prompt radiation, decay radiation, or both.
decay cut	xxxxx	Apply the factor $xxxxx * 0.1$ to $e^+/e^-/\gamma$ transport energy cutoffs (**EMFCUT**) for decay radiation.
prompt cut	yyyyy	Apply the factor $yyyyy * 0.1$ to $e^+/e^-/\gamma$ transport energy cutoffs (**EMFCUT**) for prompt radiation.
Coulomb corr		Flag for generating β^+/β^-spectra with Coulomb and screening corrections (on by default).

Recalls on FLUKA cards from the Beginner’s lectures 2/3

- **IRRPROFI** defines an irradiation profile (duration and intensity) for radioactive decay calculations

IRRPROFI	Δt: =6*day	p/s: 5.88E10
	Δt: =12*hour	p/s: 0.0
	Δt: =1*day	p/s: 6.67E10

Δt Irradiation time in seconds

p/s Beam intensity in primaries/s (e.g. particles/s, collisions/s for colliders, …).
Several cards can be issued up to a maximum of 2500 irradiation intervals.
Sequence order is assumed from first card (top) to last (bottom)

- **DCYTIMES** defines the cooling times with respect to the end of the irradiation for scoring purposes

Cooling times at 0s, 1h and 30 days

DCYTIMES	t1: 0.0	t2: 3600	t3: 2592000
	t4:	t5:	t6:

t1-t6 Cooling time in seconds.
Several cards can be combined, and each cooling time is assigned an index, following the order in which it has been input. This index can be used in the card **DCYSCORE** to assign that cooling time to one or more scoring detectors.
A negative decay time is also admitted: scoring will be performed at the chosen time "during irradiation“.

Recalls on FLUKA cards from the Beginner's lectures 3/3

- **DCYSCORE** associates selected scoring detectors of given estimator type with user-defined decay times or with combined prompt-decay particle scoring. When the **DCYSCORE** option is applied to a given detector, all quantities are expressed per unit time.

USRBIN			Unit: 21 BIN ▾	Name: Act
	Type: R-Φ-Z point ▾	Rmin: 0	Rmax: 5	NR: 50
	Part: ACTOMASS ▾	X: 0	Y: 0	NΦ: 1
		Zmin: 0	Zmax: 10	NZ: 100
DCYSCORE		Cooling t: 3600 ▾	Kind: USRBIN ▾	
		Det: Act ▾	to Det: Act ▾	Step:

Cooling t	Cooling time index to be associated with the detector(s): FLAIR offers a convenient drop-down menu (See Lecture on Radioactive Sources for other options).
Kind	Identifies the kind of estimator under consideration, e.g. **RESNUCLE**, **USRBIN**, **USRTRACK**, ...
Det … to Det	Detectors (of the same type as specified in Kind) which should be associated to the cooling time indicated in Cooling t
Step	Step length in assigning indices

Estimation of nuclide yields/activities with event-based methods

RESNUCLE 1/4

- **RESNUCLE** allows to **score nuclei stopped in a given region** once they have been de-excited down to their ground or isomeric state.
  - Also protons, ^{2}H, ^{3}H, ^{3}He and ^{4}He are scored at the end of their path
- Stable nuclides created in a region that already contains these nuclides in the material description of the region and remain in the region are not scored.
  - One should pay attention when interested in the production of H or He.
- Radioactive decay of the residual nuclei over time can be simulated if the **RADDECAY**, **IRRPROFI**, **DCYTIMES** and **DCYSCORE** cards are issued.
- The output units are:
  - #nuclides/primary if no normalization is provided, and no association to a cooling time is made
  - #nuclides/g/primary (or #nuclides/cm^3/primary) if the mass (or volume) is provided and no association to a cooling time is made
  - Bq if no normalization is provided, and the scoring is associated to a cooling time
  - Bq/g (or Bq/cm^3) if the mass (or volume) is provided, and the scoring is associated to a cooling time

RESNUCLE 2/4

⚠ RESNUCLEI		Type: All ▾	Unit: 30 BIN ▾	Name: TAR_RES
	Max Z:	Max M:	Reg: TARGET ▾	Vol:

Type	Type of products to be scored: • Spallation: Spallation products (all inelastic interactions except those induced by neutrons below the threshold for multigroup treatment). • Low Energy: Low energy products, i.e. those produced by neutrons below the threshold for multigroup treatment. • **All: All residual nuclei are scored**.
Unit	Logical output unit.
Max Z	Maximum atomic number Z of the residual nuclei distribution. The default value is selected according to the Z of the element(s) of the material assigned to the scoring region
Max M	Maximum M = N - Z - (NMZ)min of the residual nuclei distribution. The default value is selected according to the A and Z of the element(s) of the material assigned to the scoring region
Reg	Scoring region number or name (Default = 1.0). If set to -1.0 or `@ALLREGS` scoring will include all regions
Vol	Volume of the region in cm^3 or, more in general, a **normalization factor by which the scoring shall be divided**. The default value is 1.0
Name	Character string identifying the detector (max. 10 characters)

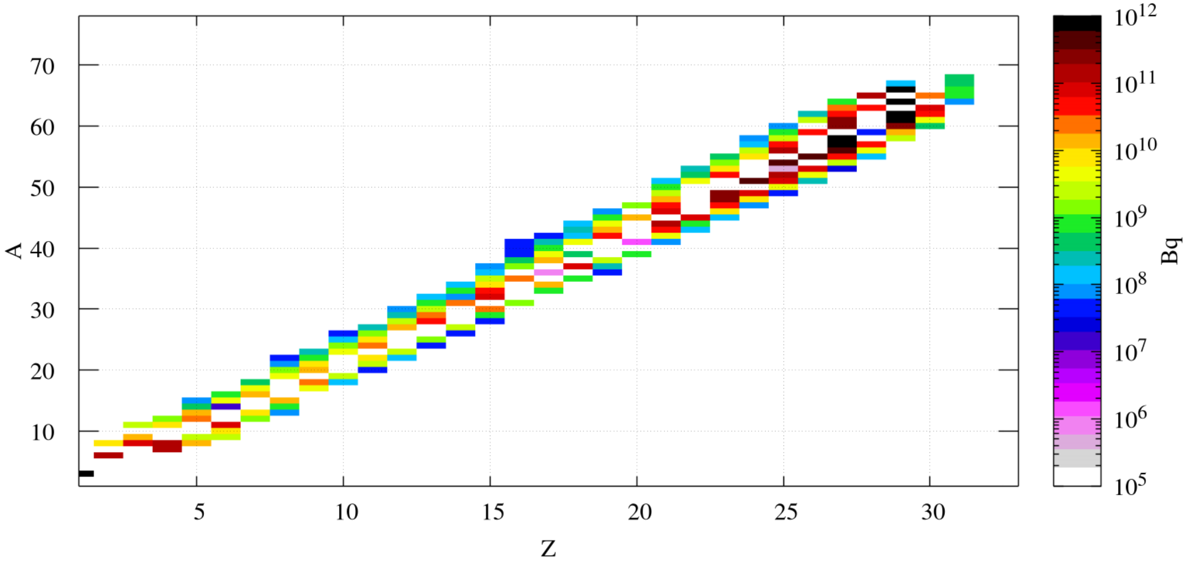
RESNUCLE 3/4

- **RESNUCLE** output

```
# Detector n:      1
TAR_RES
# A/Z Isotopes:
   68   31   3.8580E+08    36.27
   68   32    0.000        0.000
   68   33    0.000        0.000
   67   23    0.000        0.000
   67   24    0.000        0.000
   67   25    0.000        0.000
   67   26    0.000        0.000
   67   27    0.000        0.000
   67   28    0.000        0.000
   67   29   1.2860E+08    55.71
   67   30    0.000        0.000
   67   31   8.1447E+08    22.05
   67   32    0.000        0.000
   67   33    0.000        0.000
   66   23    0.000        0.000
   66   24    0.000        0.000
   66   25    0.000        0.000
   66   26    0.000        0.000
   66   27    0.000        0.000
   66   28   4.2867E+07    99.00
   66   29   7.4155E+11   0.7681
   66   30    0.000        0.000
   66   31   1.0717E+09    20.00
...
```

```
# A/Z/m Isomers:
  24   11    1   9.0020E+09    4.582
  24   13    1   2.1433E+07    99.00
  26   13    1   1.0824E+10    4.254
  34   17    1   7.8660E+09    5.716
  38   17    1   7.0944E+09    6.076
  38   19    1   3.3007E+09    6.718
  42   21    1   5.4655E+09    7.040
  44   21    1   7.7031E+10    1.612
  45   21    1   9.2678E+10    1.590
  46   21    1   5.1119E+10    1.839
  46   23    1   4.2009E+09    8.196
  50   21    1   1.7147E+08    30.79
  50   25    1   3.6651E+09    9.220
  52   25    1   1.3235E+11    1.507
  52   26    1   6.0228E+09    6.781
  53   26    1   4.3167E+10    1.826
  54   27    1   1.9719E+09    11.27
  58   25    1   3.2579E+09    7.914
  58   27    1   7.9449E+11   0.3885
  60   25    1   2.1433E+07    99.00
  60   27    1   3.8475E+11   0.4975
  62   27    1   4.0252E+10    2.101
```

- The **`*tab.lis`** output is easier to read and post-process.
- The **`*sum.lis`** output provides additional information, e.g. the total weight of the primary histories run, and the integral over the region.
- Visualization with FLAIR is also possible.



RESNUCLE 4/4

- Sometimes it can be more convenient to reformat the **RESNUCLE** output in a more readable and user-friendly format which can be then used for additional post-processing.
- The **flurenucle_formatter.py** (distributed from FLUKA4-5.0 onwards) is a simple, yet effective, formatter code that can be used for this task:
  - Use of the convention **<element symbol>-<mass number>**
  - **M** is added for the first metastable state
  - The absolute uncertainty is reported
  - Several formats: **txt**, **csv**, **Excel**, **JSON**
  - Additional normalization can be applied

```
usage: fluresnucle_formatter.py [-h] -i INPUT_FILE [-o OUTPUT_FILE] [-fmt {json,excel,csv,txt}] [-nf NORMALIZATION_FACTOR]

options:
  -h, --help            show this help message and exit
  -i INPUT_FILE, --input-file INPUT_FILE
                        Name of the input file; tab.lis format expected
  -o OUTPUT_FILE, --output-file OUTPUT_FILE
                        Name of the output file
  -fmt {json,excel,csv,txt}, --output-format {json,excel,csv,txt}
                        Format of the output
  -nf NORMALIZATION_FACTOR, --normalization-factor NORMALIZATION_FACTOR
                        Multiplicative factor for normalization of yields/activities
```

TAR_RES

	Act	Act_uncert
H-3	5.870100e+11	2.474834e+09
He-6	1.071700e+11	1.805814e+09
He-8	7.673100e+09	6.907325e+08
Li-8	8.472000e+10	2.093431e+09
Li-9	1.646100e+10	8.072474e+08
Li-11	3.557900e+09	3.244093e+08
Be-7	1.201000e+11	2.092142e+09
Be-8	1.055600e+11	2.162924e+09
Be-10	9.502300e+04	1.872903e+03
Be-11	6.495500e+09	4.163616e+08
Be-12	1.671800e+09	2.400705e+08
B-8	1.136000e+10	8.500688e+08
B-9	1.328900e+09	2.426571e+08
B-12	2.566000e+10	9.312014e+08
B-13	1.076000e+10	7.097296e+08
B-14	6.430000e+08	1.716810e+08
B-15	8.573300e+07	5.956729e+07
C-9	1.328900e+09	2.426571e+08
C-10	8.273300e+09	4.997073e+08
C-11	7.428800e+10	1.619478e+09
C-14	1.029000e+07	4.292988e+05
C-15	4.886800e+09	5.209329e+08
C-16	5.572700e+08	1.593792e+08
N-12	7.716000e+08	1.910482e+08
N-13	7.630300e+09	4.356901e+08
N-16	1.663200e+10	7.698953e+08
N-17	4.972500e+09	4.434973e+08
N-18	2.572000e+08	9.552408e+07
N-19	4.286700e+07	4.243833e+07
O-13	1.714700e+08	1.019389e+08
O-14	1.114500e+09	2.668113e+08
O-15	1.178800e+10	7.032721e+08
O-19	4.186800e+09	4.588733e+08
O-20	7.716000e+08	1.807859e+08
O-21	3.429300e+08	1.055881e+08
O-22	4.286700e+07	4.243833e+07
F-17	3.643700e+09	4.139243e+08
F-18	2.036200e+10	7.994121e+08
F-20	1.564600e+10	7.921570e+08
F-21	5.444100e+09	5.256823e+08
F-22	9.859300e+08	1.918620e+08
F-23	3.429300e+08	1.222888e+08
F-24	4.286700e+07	4.243833e+07
Ne-18	4.286700e+08	1.424042e+08
Ne-19	2.186200e+09	3.270555e+08
Ne-23	5.444100e+09	5.434301e+08
Ne-24	1.628900e+09	3.078621e+08
Ne-25	1.286000e+08	7.164306e+07
Na-20	8.573300e+07	5.956729e+07
Na-21	1.586100e+09	2.804225e+08
Na-22	7.972600e+09	2.786424e+08
Na-24	1.962800e+10	8.867930e+08
Na-24M	9.002000e+09	4.124716e+08
Na-25	8.530500e+09	5.102945e+08
	...	

USRBIN: ACTIVITY and ACTOMASS

- Activity and mass specific activity can be scored on a mesh basis with the **USRBIN** card and the generalized particles **ACTIVITY** and **ACTOMASS**.
- The scoring must be a **point-mesh scoring** since activity and specific activity cannot be scored along a step like track length (i.e. fluence).

USRBIN			Unit: 21 BIN ▾	Name: Act
	Type: R-Φ-Z point ▾	Rmin: 0	Rmax: 5	NR: 50
	Part: ACTOMASS ▾	X: 0	Y: 0	NΦ: 1
		Zmin: 0	Zmax: 10	NZ: 100

- The output will be in Bq/cm^3 (for **ACTIVITY**) or Bq/g (**ACTOMASS**) with Cartesian or cylindrical binning. For point-region scoring the output will be Bq or Bq cm^3/g and the result will have to be divided by the region volume to have meaningful units.
- Additional filtering by nuclide or generating particle can be performed with **AUXSCORE** or by means of user routines.

AUXSCORE

- **AUXSCORE** also allows to filter scoring detectors according to auxiliary (generalised) particle distributions or ion isotopic ranges.
- For instance, it is possible to **filter nuclide contributions** when scoring **ACTIVITY** or **ACTOMASS**. By default, the field Isomer is set to 0 and this will include all ground and isomeric states: to select only the ground state the value 9 should be entered.

USRBIN			Unit: 21 BIN ▾	Name: Act_Mn54
	Type: R-Φ-Z point ▾	Rmin: 0	Rmax: 7.5	NR: 15
	Part: ACTIVITY ▾	X: 0	Y: 0	NΦ: 1
		Zmin: 0	Zmax: 80	NZ: 80
AUXSCORE		Type: USRBIN ▾	Part: ▾	Set: ▾
	Delta Ray: ▾	Z: 25	A: 54	Isomer: 0
		Det: Act_Mn54 ▾	to Det: ▾	Step:

- Since FLUKA4-4.0, the card has also been provided with the additional option **RESNUCLE** to **filter by the projectile particle species** producing the nuclides.

RESNUCLEI		Type: All ▾	Unit: 31 BIN ▾	Name: PR_Res
	Max Z:	Max M:	Reg: TARGET ▾	Vol:
AUXSCORE		Type: RESNUCLE ▾	Part: PROTON ▾	Set: ▾
	Delta Ray: ▾	Det: PR_Res ▾	to Det: ▾	Step:

User routines for scoring

- **FLUKA already offers a wide variety of built-in scoring capabilities** that do not require the User to write a single line of code. These should be fully explored and exploited first.
- One may still need additional flexibility (e.g. to extract information not directly obtainable) and can rely on user routines at the cost of (FORTRAN) programming, and possibly post-processing the results.
- Among the different user routines, `comscw.f`, `usrrnc.f`, and `fluscw.f` can be particularly handy for advanced scoring. These routines are activated with the `USERWEIG` card.

USERWEIGHT ϕ Weight: FLUSCW+ ▾ Resnuclei: USRRNC ▾ Density Weight: COMSCW+ ▾

`WHAT(3) > 0`

`fluscw.f`

Weighting fluence, current and yield

`WHAT(5) > 0`

`usrrnc.f`

Called each time a residual nucleus is stopped

`WHAT(6) > 0`

`comscw.f`

Weighting deposited energy, stars or residual nuclei

comscw.f

```
      DOUBLE PRECISION FUNCTION COMSCW ( IJ    , XA    , YA    , ZA    ,
     &                                  MREG  , RULL  , LLO   , ICALL )
...
*                                                                      *
*     Input variables:                                                 *
*                                                                      *
*           Ij = (generalized) particle code                           *
*     Xa,Ya,Za = position                                              *
*         Mreg = region number                                         *
*         Rull = amount to be deposited                                *
*          Llo = particle generation                                   *
*        Icall = call id                                               *
*                                                                      *
*     Output variables:                                                *
*                                                                      *
*       Comscw = factor the scored amount will be multiplied by        *
*       Lsczer = logical flag, if true no amount will be scored        *
*                regardless of Comscw                                  *
*                                                                      *
...
*     Useful variables (common SCOHLP):                                *
*                                                                      *
*     Energy/Star binnings/scorings (Comscw):                          *
*          ISCRNG = 3 --> Residual nuclei scoring                      *
*          ISCRNG = 4 --> Momentum transfer density binning            *
*          ISCRNG = 5 --> Activity density binning                     *
*          ISCRNG = 7 --> Residual nuclei density binning              *
*          JSCRNG = # of the binning/detector                          *
...
```

- This function is called **before scoring** if the card **USRWEIG** is issued with **WHAT(6) > 0**:
  - It provides access to information about the generalized particle being scored and the type of scoring.
  - The User can **apply a weighting factor to the scored amount**.
- Additional useful commons to include:
  - **rsnccm.inc** to access information on the residual nuclei being scored.
  - **usrbin.inc** to access information on the **USRBIN** scorings.
- A simplified example for a possible usage in Radiation Protection studies is provided in the following slide and more will be discussed during the exercise session.

comscw.f: example

```
      DOUBLE PRECISION FUNCTION COMSCW ( IJ    , XA    , YA    , ZA    ,
     &                                   MREG  , RULL  , LLO   , ICALL )
...
      ! Default return value
      COMSCW = ONEONE
...
1     IF ( ISCRNG .EQ. 5 ) THEN
         ! The current scoring is an activity density binning
         ! Get the detector name (the USRBIN's SDUM)
2        SCORING_NAME = TITUSB(JSCRNG)

         ! Check the scoring name
3        IF ( SCORING_NAME(1:6) .EQ. "CLMn54" ) THEN

            ! Obtain the present isotope from the common block /RSNCCM/
            AA  = IARSDL(1)
4           ZZ  = IZRSDL(1)
            SS  = ISRSDL(1)

            ! Apply the weight
            IF (ZZ .EQ. 25 .AND. AA .EQ. 54) THEN
               COMSCW = ONEONE / 1.0D-1   **
5           ELSE
               COMSCW = ZERZER
            ENDIF

         ENDIF

      ENDIF

      RETURN
*=== End of function Comscw ===========================================*
      END
```

- In this simplified example, the `comscw.f` routine is used to obtain the activity distribution of ^{54}Mn weighted by the corresponding nuclide clearance limit.

1. The routine first checks that the scoring is an activity density binning.
2. Then the detector name is retrieved.
3. The weighting is applied only if the scoring name matches a given string.
4. The information on the present isotope is retrieved.
5. If the isotope is ^{54}Mn, a weighting is applied while other nuclides are discarded.
6. No weighting is applied for all other cases.

** **NB**: The specific clearance limits depend on national or international regulations

usrrnc.f

```
      SUBROUTINE USRRNC ( IZ, IA, IS, X, Y, Z, MREG, WEE, ICALL )
...
*                                                                      *
*     Input variables:                                                 *
*                                                                      *
*           IZ = atomic number of the residual nucleus                 *
*           IA = mass number of the residual nucleus                   *
*           IS = isomeric state of the residual nucleus                *
*      X, Y, Z = position of the stopped residual nucleus              *
*         MREG = number of the current region                          *
*          WEE = residual nucleus statistical weight                   *
*        ICALL = internal code calling flag (not for general use)      *
*                                                                      *
...
```

- This subroutine is called **every time a residual nucleus is stopped** if the card **USRWEIG** is issued with **WHAT(5) > 0**:
  - It provides access to all the information of the residual.
- It can be used to **create dump files** or to discard radionuclides:
  - Dump files can be read by source routines in two-step calculations
- Only a simple example is provided here: the **usrrnc.f** subroutine is used to filter out all residual nuclei except ^{60}Co and to dump the final position of the generated ^{60}Co.

```
      SUBROUTINE USRRNC ( IZ, IA, IS, X, Y, Z, MREG, WEE, ICALL )
...

      IF (IZ .NEQ. 27 .OR. IA .NEQ. 60) THEN
         WEE = ZERZER
      ELSE
         WRITE(90,*) IZ, IA, IS, X, Y, Z, MREG, WEE, ICALL
      ENDIF

      RETURN
*=== End of subroutine Usrrnc =========================================*
      END
```

Estimation of nuclide yields/activities with fluence-based methods

Fluence-based methods 1/4

- The most straightforward approach in estimating induced radioactivity is by directly scoring the residual nuclei produced during particle transport as a result of nuclear interactions.

- However, for regions in which the interaction probability is small, **fluence-based methods can offer a more efficient approach**.

- A possible workflow for the implementation of a fluence-based method is:
  1. Score particle's fluence energy spectra (**`USRTRACK`**): typically, one should consider particles that contribute significantly to activation i.e. protons, charged pions, neutrons, photons.
  2. Weight the particle's fluence energy spectra with radionuclide production cross sections to obtain radionuclide production yields.
     - The weighting can be done either offline (post-processing) or during transport/scoring time with dedicated User routines (**see examples and exercise**)
     - The cross section can be evaluated with experimental data or calculated with Monte Carlo transport codes.
  3. Perform build-up and decay of radionuclides (Bateman equations) for an arbitrary irradiation history and cooling times to obtain nuclide activities.
     - This can also be performed either offline or online, depending on the code used.

Fluence-based methods 2/4

- The fluence-based methods typically have improved convergence with respect to event-based methods but are more difficult to implement from scratch.
- Fluence-based methods have been implemented in several codes, for example:
  - ActiWiz (CERN)
  - JEREMY (CERN)
  - DCHAIN-PHITS (OECD/NEA, JAEA)
  - CINDER (RSSIC)
  - ORIGEN (ORNL)

  } Typical workflow: scoring of particle energy fluence spectra and offline post-processing

  - Fluence Conversion Coefficients method (CERN)

  } Typical workflow: pre-computation of energy- and particle- dependent coefficients applied online during transport
- For the exercise part, a simple, yet instructive, implementation of a fluence-based method will be illustrated. The usage of the above codes will be showcased in examples from advanced applications.

Fluence-based methods 3/4

- To understand a simple implementation of a fluence-based method via the `fluscw.f` routine in FLUKA and the exercise related to this session, we can introduce some basic formalism.
- The production rate/yield P_r of radionuclide r in a given material of density ρ containing N_e elements can be expressed as

$$P_r = \sum_{e}^{N_e} \rho \frac{N_{AV}}{M_e} m_e \sum_{i=p,\pi^{\pm},n,\gamma,\dots} \int \sigma_{i,e,r}(E)\, \phi_i(E)\, dE$$

- $\phi_i(E)$ is the fluence energy spectrum of particle i.
- $\sigma_{i,e,r}(E)$ is the production cross section of radionuclide r from element e due to particle i.
- N_{AV}, M_e, m_e are the Avogadro's number, the element atomic weight and the mass fraction of element e in the compound.
- The unit of P_r will be #nuclides/cm^3/s or #nuclides/cm^3 depending on whether $\phi_i(E)$ is differential in time or not.
- Note that only the energy dependence was written explicitly. The particle fluence energy spectrum may easily depend on the position and on time if the primary source also changes with time.
- Activities can be computed from the production yields applying exponentials and Bateman coefficients.

Fluence-based methods 4/4

$$P_r = \sum_{e}^{N_e} \rho \frac{N_{AV}}{M_e} m_e \sum_{i=p,\pi^{\pm},n,\gamma,\dots} \int \sigma_{i,e,r}(E)\, \phi_i(E)\, dE$$

Discretization in energy bins: k identifies the energy bin and E_k is the energy bin centre

$$P_r = \sum_{e}^{N_e} \rho \frac{N_{AV}}{M_e} m_e \sum_{i=p,\pi^{\pm},n,\gamma,\dots} \sum_{k} \sigma_{i,e,r}(E_k)\, \phi_i(E_k)\, \Delta E_k$$

OFFLINE approach

$$P_r = \sum_{e}^{N_e} \rho \frac{N_{AV}}{M_e} m_e \sum_{i=p,\pi^{\pm},n,\gamma,\dots} \sum_{k} \sigma_{i,e,r}(E_k)\, \phi_i(E_k)\, \Delta E_k$$

Estimate $\phi_i(E_k)$ (e.g. USRTRACK) and then compute the production yield. Examples: ActiWiz, JEREMY

ONLINE approach

$$P_r = \sum_{i=p,\pi^{\pm},n,\gamma,\dots} \sum_{k} \left(\sum_{e}^{N_e} \rho \frac{N_{AV}}{M_e} m_e \sigma_{i,e,r}(E_k) \right) \phi_i(E_k)\, \Delta E_k$$

Pre-compute the term in parenthesis (energy and particle dependent coefficient) and weight the fluence scoring during the calculation by means of user routines. Example: Fluence Conversion Coefficients method.

User routines for scoring (reminder)

- **FLUKA already offers a wide variety of built-in scoring capabilities** that do not require the User to write a single line of code. These should be fully explored and exploited first.
- One may still need additional flexibility (e.g. to extract information not directly obtainable) and can rely on user routines at the cost of (FORTRAN) programming, and possibly post-processing the results.
- Among the different user routines, `comscw.f`, `usrrnc.f`, and `fluscw.f` can be particularly handy for advanced scoring. These routines are activated with the `USERWEIG` card.

USERWEIGHT   ϕ Weight: FLUSCW+ ▾   Resnuclei: USRRNC ▾ Density Weight: COMSCW+ ▾

WHAT(3) > 0	WHAT(5) > 0	WHAT(6) > 0
`fluscw.f`	`usrrnc.f`	`comscw.f`
Weighting fluence, current and yield	Called each time a residual nucleus is stopped	Weighting deposited energy, stars or residual nuclei

fluscw.f

```
      DOUBLE PRECISION FUNCTION FLUSCW ( IJ    , PLA    , TXX    , TYY    ,
     &                                   TZZ    , WEE    , XX     , YY     ,
     &                                   ZZ     , NREG   , IOLREG, LLO    ,
     &                                   NSURF )
...
*                                                                      *
*     Input variables:                                                 *
*                                                                      *
*           Ij = (generalized) particle code (Paprop numbering)        *
*          Pla = particle laboratory momentum (GeV/c) (if > 0),        *
*                or kinetic energy (GeV) (if <0 )                      *
*     Txx,yy,zz = particle direction cosines                           *
*          Wee = particle weight                                       *
*      Xx,Yy,Zz = position                                             *
*         Nreg = (new) region number                                   *
*       Iolreg = (old) region number                                   *
*          Llo = particle generation                                   *
*        Nsurf = transport flag (ignore!)                              *
*                                                                      *
*     Output variables:                                                *
*                                                                      *
*       Fluscw = factor the scored amount will be multiplied by        *
*       Lsczer = logical flag, if true no amount will be scored        *
*                regardless of Fluscw                                  *
*                                                                      *
*     Useful variables (common SCOHLP):                                *
*                                                                      *
*     Flux like binnings/estimators (Fluscw):                          *
...
*          ISCRNG = 2 --> Track length      binning     i.e. USRBIN    *
*          ISCRNG = 3 --> Track length      estimator   i.e. USRTRACK  *
*          JSCRNG = # of the binning/detector                          *
...
```

- This function is called **before scoring** if the card **USRWEIG** is issued with **WHAT(3) > 0**:
  - It provides access to information about the generalized particle being scored and the type of scoring.
  - The user can **apply a weighting factor to the scored amount**.
- **fluscw.f** is used for fluence-like quantities and is specular to **comscw.f** which is used for “event-like” quantities
- Additional useful commons to include:
  - **usrbin.inc**, **usrtrc.inc** to access information on the **USRBIN** scorings and **USRTRACK** scorings.
- A simplified example for a possible usage in Radiation Protection studies is provided in the following slide and more will be discussed during the exercise session.

fluscw.f: example

```
      DOUBLE PRECISION FUNCTION FLUSCW ( IJ     , PLA    , TXX    , TYY    ,
     &                                   TZZ    , WEE    , XX     , YY     ,
     &                                   ZZ     , NREG   , IOLREG, LLO    ,
     &                                   NSURF )
...   ! Default return value
      FLUSCW = ONEONE
...
1     IF ( ISCRNG .EQ. 2 ) THEN
         ! The current scoring is a fluence binning
         ! Get the detector name (the USRBIN's SDUM)
2        SCORING_NAME = TITUSB(JSCRNG)

         ! Check the scoring name
3        IF ( SCORING_NAME(1:4) .EQ. "Ar41" ) THEN

            ! New default value if the scoring name matches
4           FLUSCW = ZERZER

            ! Check the particle type
5           IF ( IJ .EQ. 8 ) THEN
               ! EKIN is the particle kinetic energy (computed elsewhere
               ! in the routine)
               ! Call to a user written function for table look-up
6              ! Apply any additional normalization
               FLUSCW = NORM * GETTABULATEDXS( EKIN )
            ENDIF

         ENDIF

      ENDIF

      RETURN
*=== End of function Fluscw ===========================================*
      END
```

- In this simplified example, the **fluscw.f** routine is used to fold the neutron fluence spectrum with a pre-tabulated cross section.
  1. The routine first checks that the scoring is a fluence binning.
  2. Then the detector name is retrieved.
  3. The weighting is applied only if the scoring name matches a given string.
  4. A new default return value is set.
  5. The weighting is applied only if the particle is a neutron.
  6. A user written function is called to return the pre-tabulated cross section at the corresponding neutron energy **EKIN**.

Example of application: activation of cooling fluids 1/3

- A very common case in which fluence-based methods can be used is to assess the environmental impact of the activation of (cooling) fluids such as air and water.

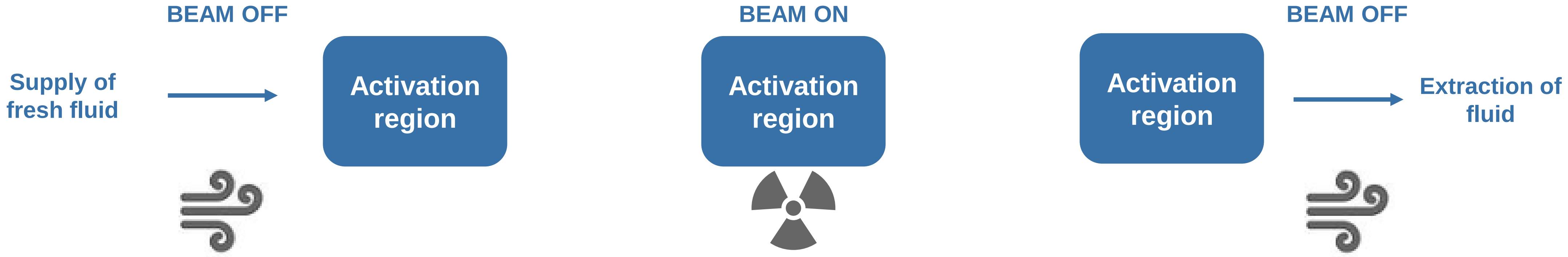
- Gases and fluids are often non-stationary materials (forced flow, natural convection) and an additional complication lies in the choice of an appropriate model for fluid movement during activation and transit to the release point.

- Two of the most common approaches are:
  - **Simple static model**: The fluid is stationary during activation and moves directly to the release point.
  - **Complete mixing model**: The fluid in the irradiation region is completely mixed and only a small fraction is removed regularly. This approach takes into account the effect of ventilation.

- The additional problem concerning the dispersion of the radionuclides after they have been released will not be discussed here. In any case this can be reasonably decoupled from the flow model.

Example of application: activation of cooling fluids 2/3

- **Simple static model**: the fluid is stationary during activation and moves directly to the release point.
  - This “brute force” approach can be used for rough preliminary estimates or when no other information on the flow is provided.



  - For a simple decay chain, time-independent production rate during an interval t and zero initial concentration, one obtains the well-known formulas*

$$\frac{dN_r}{dt} = P_r(t) - \lambda_r N_r$$

Net change = Production - Decay

$$N_r(t) = \frac{P_r}{\lambda_r}\left(1 - e^{-\lambda_r t}\right)$$

Saturation concentration

$$A_r(t) = P_r\left(1 - e^{-\lambda_r t}\right)$$

Saturation activity

* NB: In this simple illustration we do not explicitly take into account the production of radionuclide r from the decay of other radionuclides. If transmutation is negligible, the system of equations that results is linear, and the superposition principle applies (see backup slides).

Example of application: activation of cooling fluids 3/3

- **Complete mixing model**: the fluid in the irradiation region is completely mixed and only a small fraction is removed regularly.
  - Define the fluid exchange rate $\Gamma = Q/V_{irr}$ where Q is the volume of fluid cycled through the region per unit time, and V_{irr} is the volume of the region.

  - For a simple decay chain, constant production rate during an interval t and zero initial concentration, one obtains the well-known formulas*

$$\frac{dN_r}{dt} = P_r(t) - \lambda_r N_r - \Gamma N_r$$

Net change = Production - Decay - Removal

$$N_r(t) = e^{-(\lambda_r+\Gamma)t}\left(\int_0^t P_r(\tau)e^{(\lambda_r+\Gamma)\tau}d\tau\right) = \frac{P_r}{\lambda_r+\Gamma}\left(1-e^{-(\lambda_r+\Gamma)t_{irr}}\right)$$

$$A_r^{inside}(t) = \lambda_r N_r(t) = \boxed{\frac{\lambda_r P_r}{\lambda_r+\Gamma}}\left(1-e^{-(\lambda_r+\Gamma)t_{irr}}\right)$$

Saturation activity in presence of ventilation

$$A_r^{extracted}(t) = \Gamma\lambda_r N_r(t) = \frac{\Gamma\lambda_r P_r}{\lambda_r+\Gamma}\left(1-e^{-(\lambda_r+\Gamma)t_{irr}}\right)$$

* NB: In this simple illustration we do not explicitly take into account the production of radionuclide r from the decay of other radionuclides. If transmutation is negligible, the system of equations that results is linear, and the superposition principle applies (see backup slides).

Example of application: soil and/or groundwater activation

- Although event-based methods can be often employed to assess the activation in the soil and groundwater surrounding an accelerator facility, fluence-based methods can also be a choice due to their faster convergence.

- Estimating the amount that ultimately reaches public consumption is a much more complex problem involving several processes for which data is not always precise or not known:
  - Geological and hydrogeological data around the site (e.g. percolating water, seeping)
  - Chemical data, for instance leaching of nuclides from the rock/soil: ^{3}H and ^{22}Na are of typical concern since they are leachable and have long half-lives.

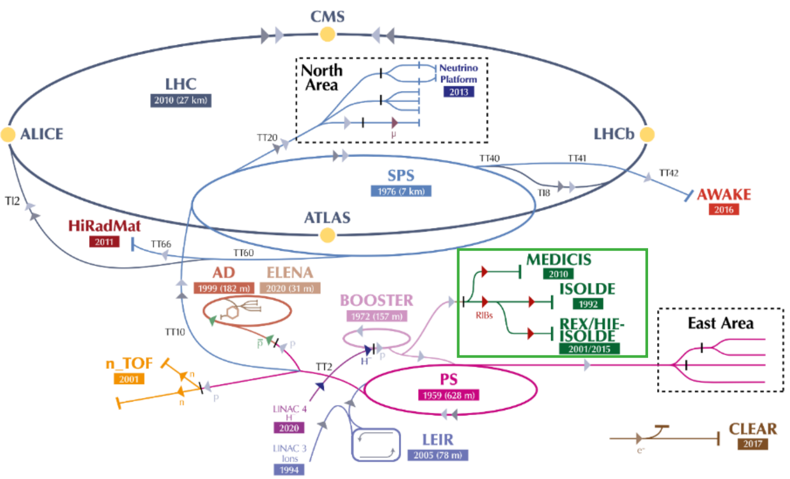
- Just as dispersion models for fluid releases into the environment can be decoupled from activity computations, so can transport models in soil and groundwater.

- The assessment assumptions (e.g. leachability, water content in soil/rock) depend on the site specificities and limits depend on national or international regulations (e.g. EU Directives).

Examples of applications to recent assessments for CERN facilities

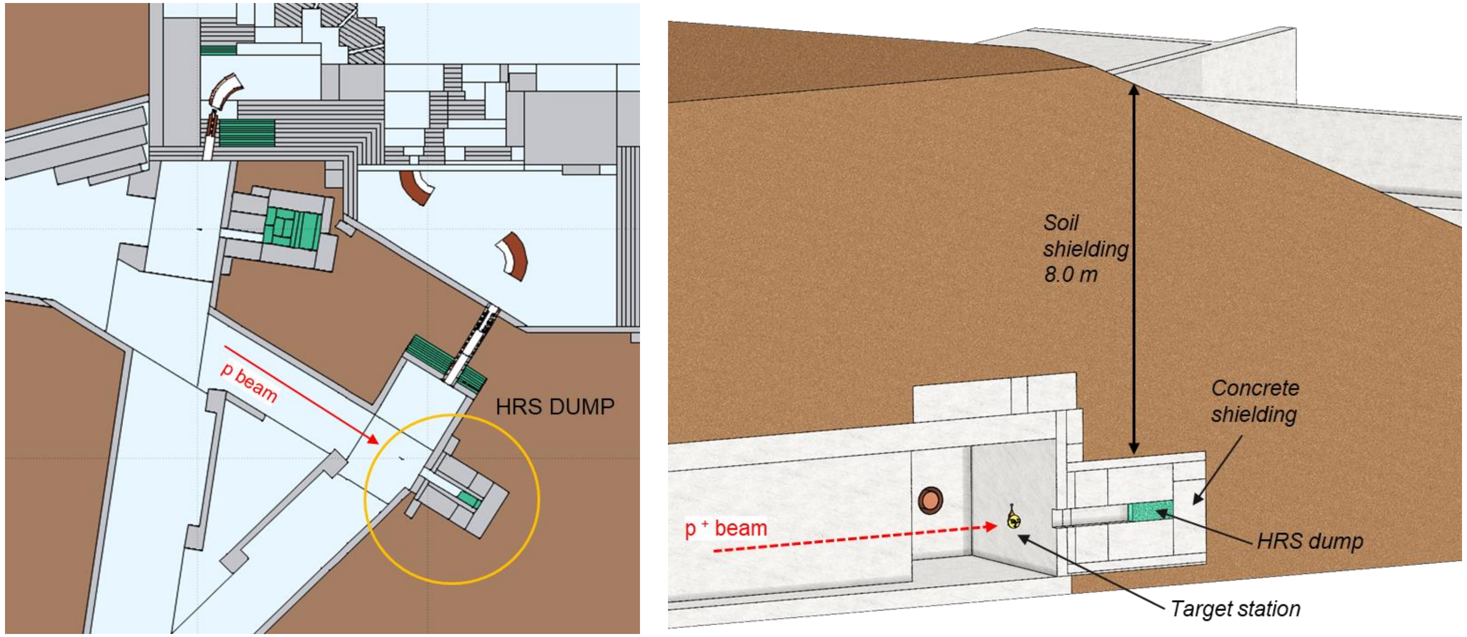
ISOLDE beam dump and surrounding shielding

A. Formento, F. Pozzi et al., *Radiological characterization of the beam dumps and their surrounding shielding of the ISOLDE facility at CERN,* AccApp'24, JLAB



- **I**sotope mass **S**eparator **O**n-**L**ine **DE**vice:
  - Pulses of 1.4 GeV protons, max 2.8 kW
  - Production of more than 1000 radio-isotopes from 2 target stations.
- Two beam dumps to be upgraded to allow for a beam energy (2 GeV) and intensity (12 kW) increase:
  - Characterization of shielding and soil needed.
  - FLUKA simulations were performed to benchmark soil activation samples.

View of ISOLDE at beam height and detail of one target station



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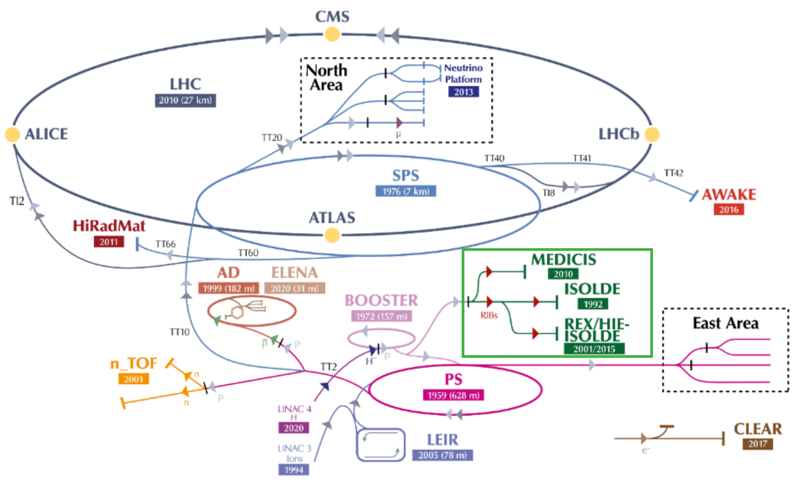

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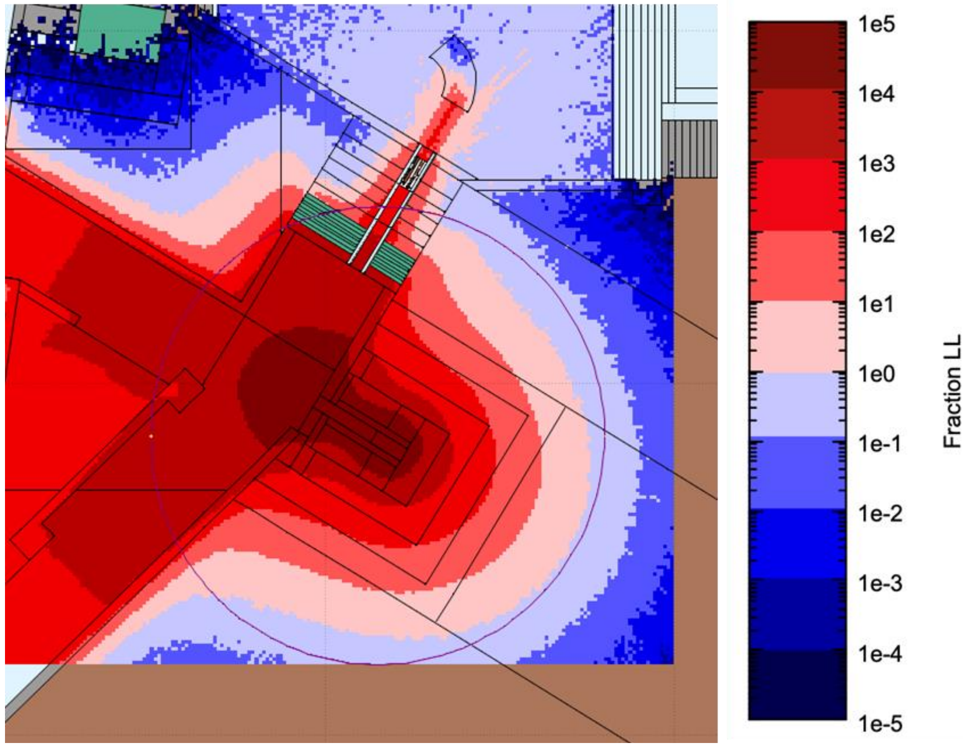
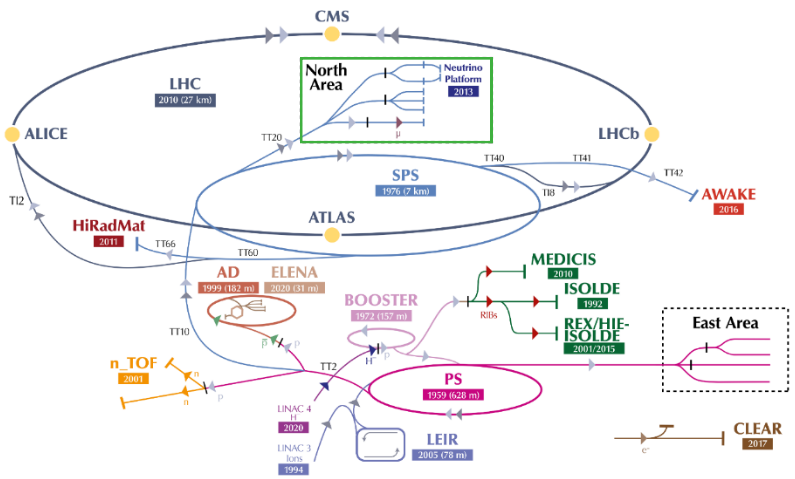


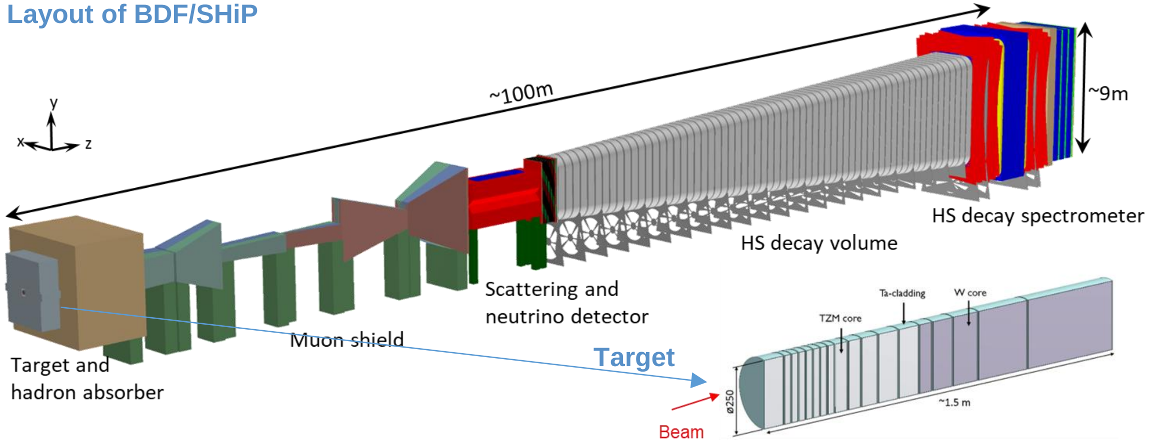
Estimation of soil activation in terms of multiples of Swiss clearance limits using a fluence-based method (Fluence Conversion Coefficients)

RP studies for CERN HI-ECN3 Facility

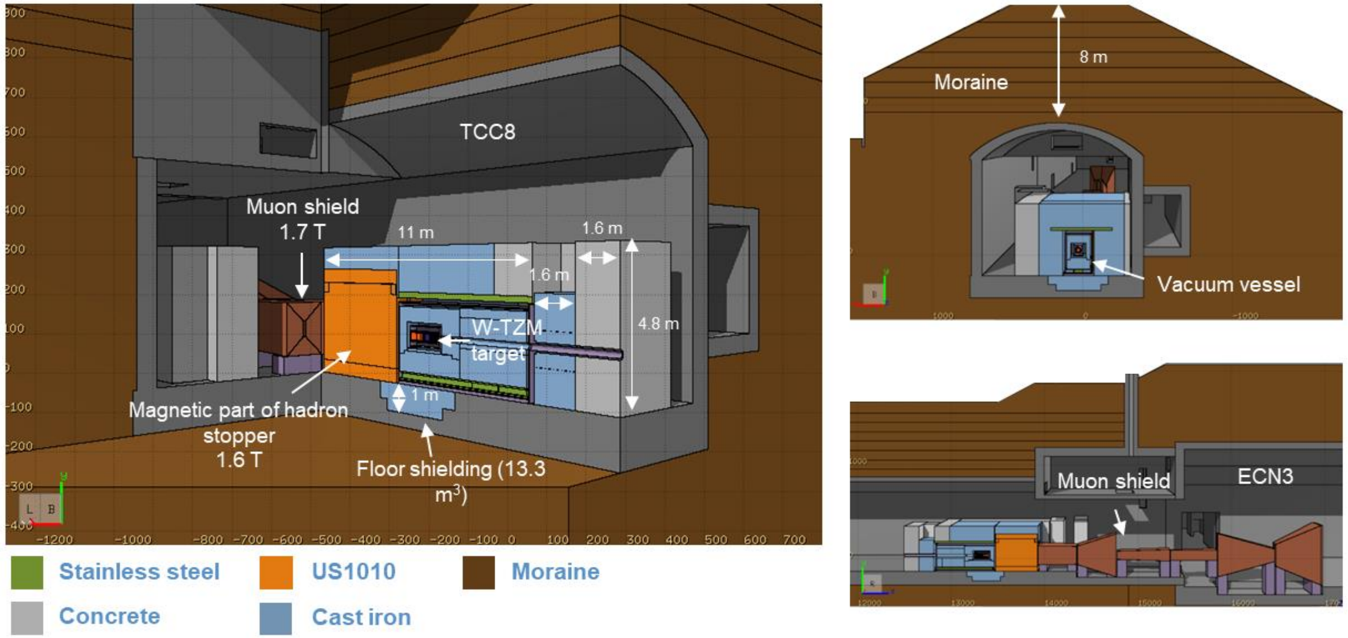
C. Ahdida et al., *Radiation Protection Studies for CERN's HI-ECN3 Facility,* SATIF-16, 28-31 May 2024, Frascati



Layout of BDF/SHiP



Simulation geometry of the complex built with Flair



- Underground experimental cavern at the CERN's SPS North Area
  - Future experiment (SHiP) for the search of hidden particles.
  - 400 GeV/c protons in spills of $4{\times}10^{13}$ p/spill.
  - Avg. beam power of 356 kW, $60{\times}10^{19}$ POT over 15 years.
- RP studies based on FLUKA simulations were performed for a design optimization of the future experiment

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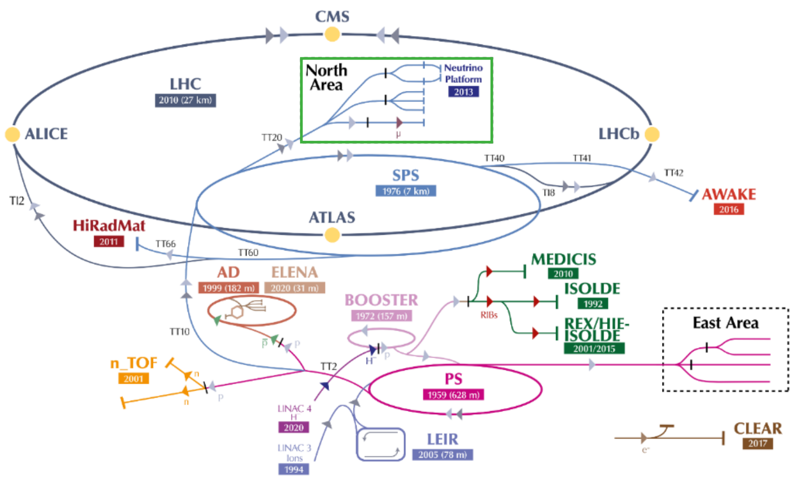

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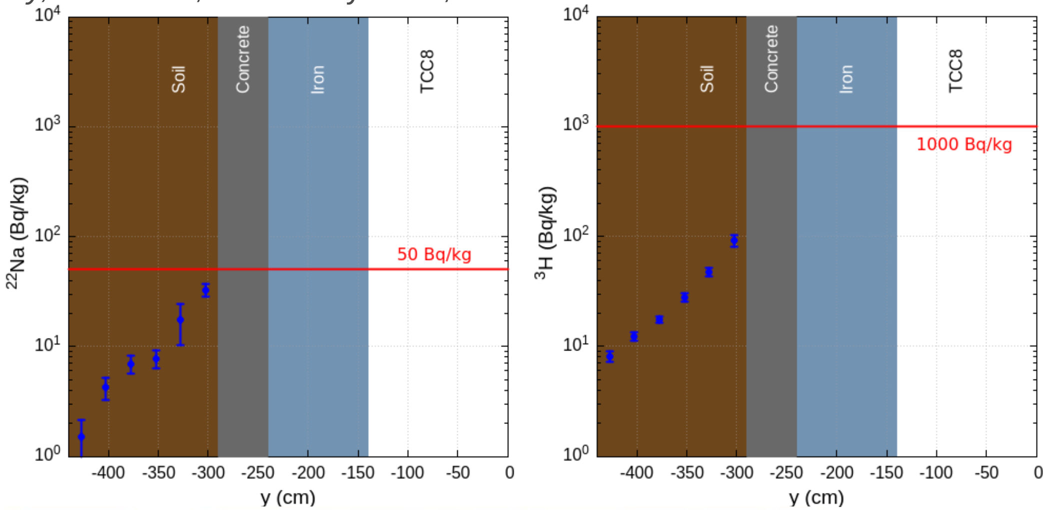
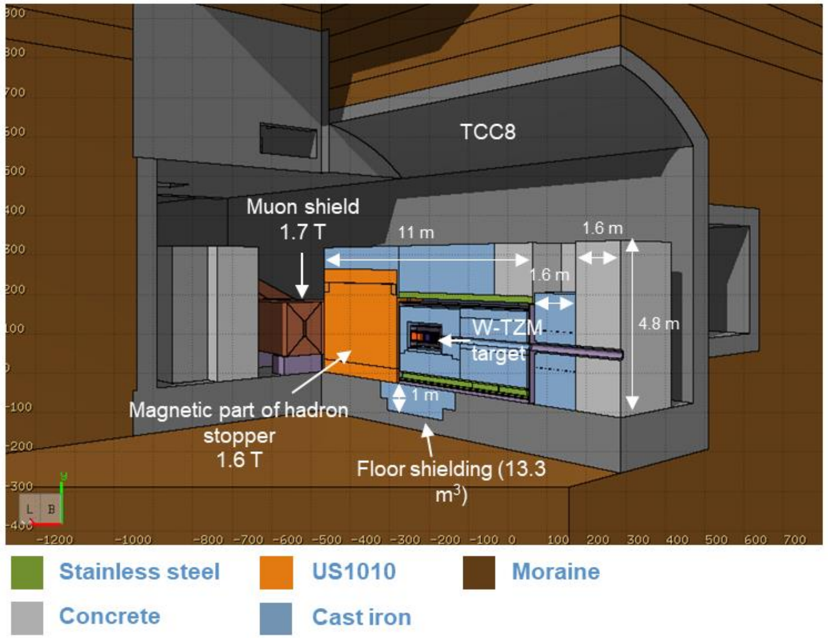


Estimation of ^{22}Na specific activity in the soil below TCC8 with an event-based method (`USRBIN ACTOMASS`)



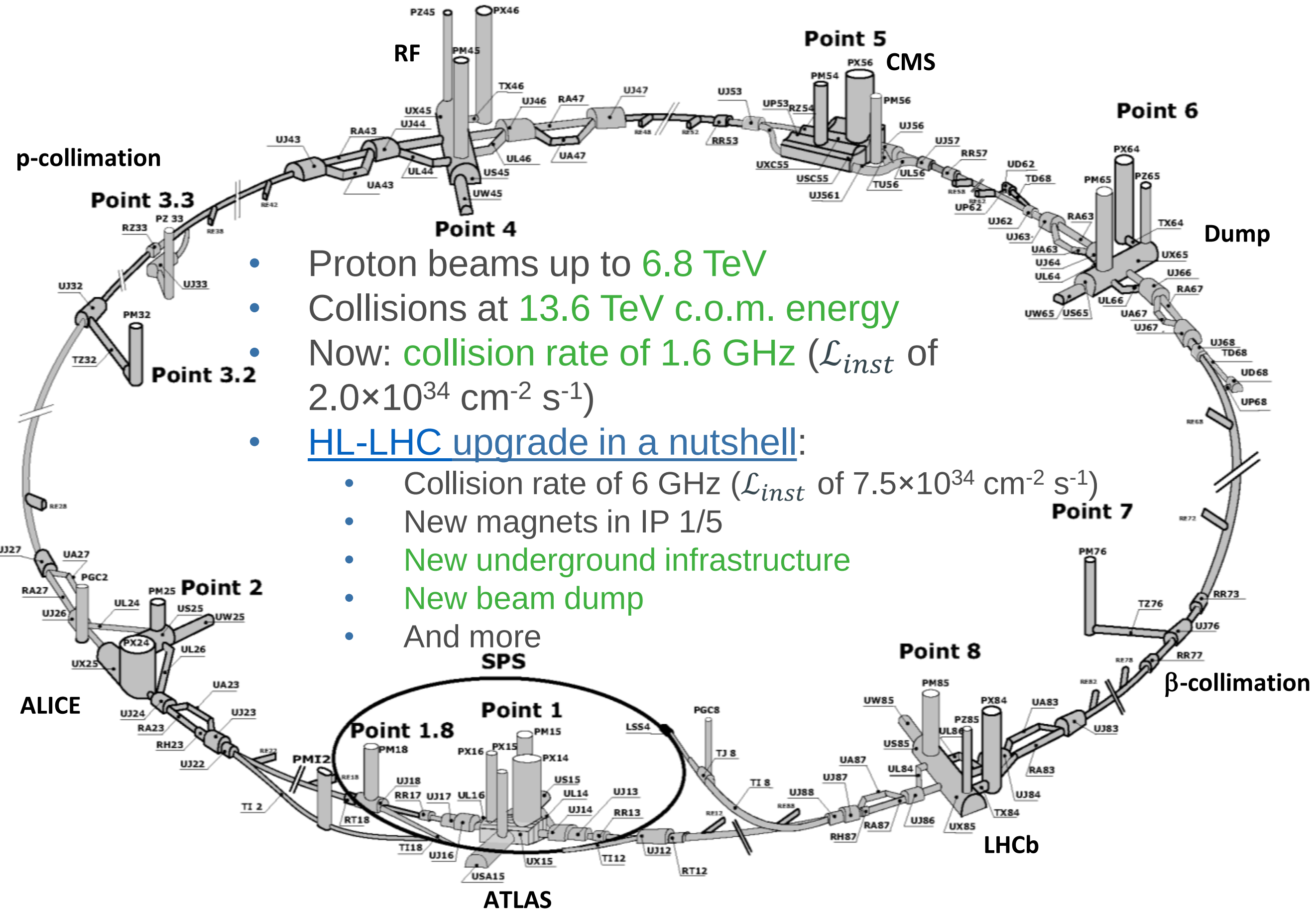
Air activation in the target complex was studied with FLUKA and Actiwiz (fluence based method)

CASE 1 - *Air*			
Radionuclide	Half life	A [Bq]	%
Ar-41	110 min	2.44×10^6	66.31
Be-7	53.3 d	4.55×10^5	12.35
C-11	20.4 min	2.54×10^5	6.878
N-13	10 min	2.31×10^5	6.259
Ar-37	35 d s	9.19×10^4	2.493
C-14	5700 y	7.71×10^4	2.091
H-3	12.32 y	7.49×10^4	2.032
Cl-39	55.6 min	2.44×10^4	0.661
S-35	87.37 d s	1.15×10^4	0.312
Cl-38	37.24 min	7.56×10^3	0.205
Sum		3.68×10^6	99.59

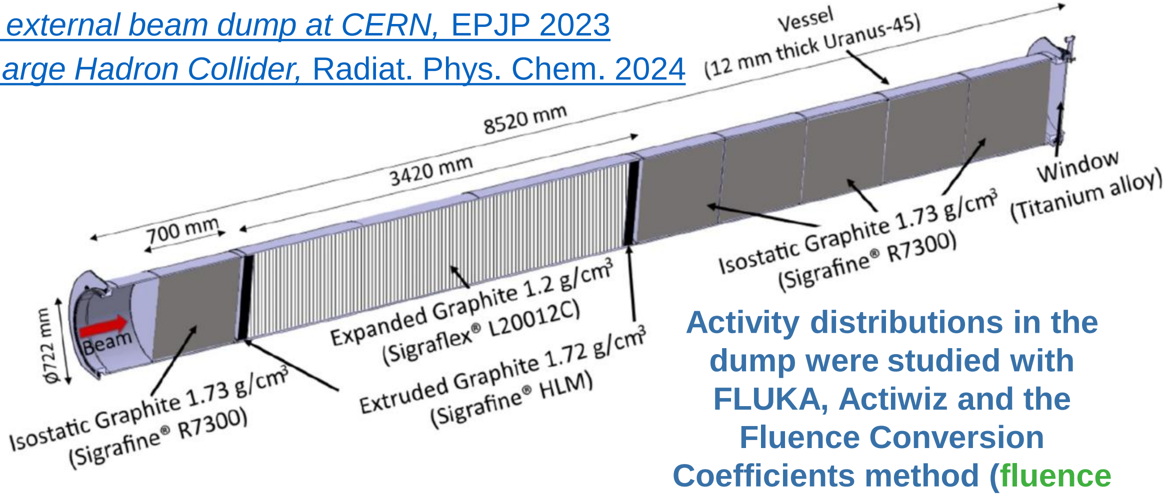
RP studies for the LHC operation and future projects

A. Infantino et al., [Radiological characterization for the disposal of a decommissioned LHC external beam dump at CERN,](#) EPJP 2023

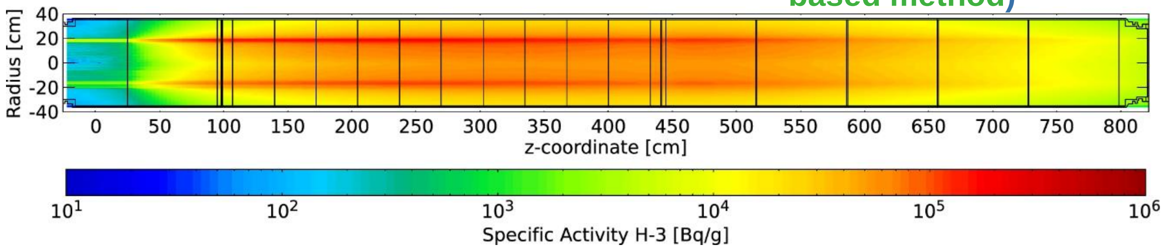
D. Bozzato et al., [Advanced simulation techniques for Radiation Protection studies at the Large Hadron Collider,](#) Radiat. Phys. Chem. 2024

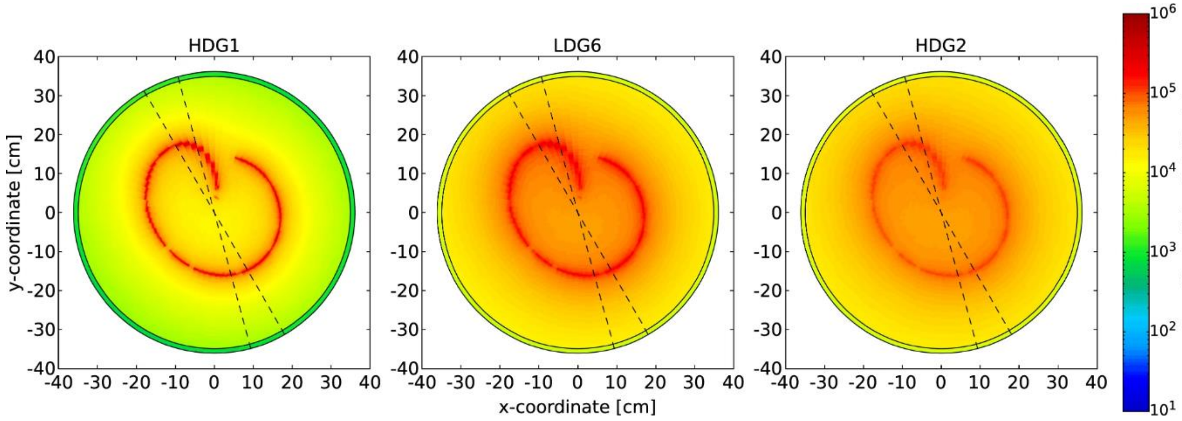


- Proton beams up to 6.8 TeV
- Collisions at 13.6 TeV c.o.m. energy
- Now: collision rate of 1.6 GHz ($\mathcal{L}_{inst}$ of 2.0×10^{34} cm^{-2} s^{-1})
- [HL-LHC upgrade in a nutshell](#):
  - Collision rate of 6 GHz ($\mathcal{L}_{inst}$ of 7.5×10^{34} cm^{-2} s^{-1})
  - New magnets in IP 1/5
  - New underground infrastructure
  - New beam dump
  - And more



Activity distributions in the dump were studied with FLUKA, Actiwiz and the Fluence Conversion Coefficients method (fluence based method)



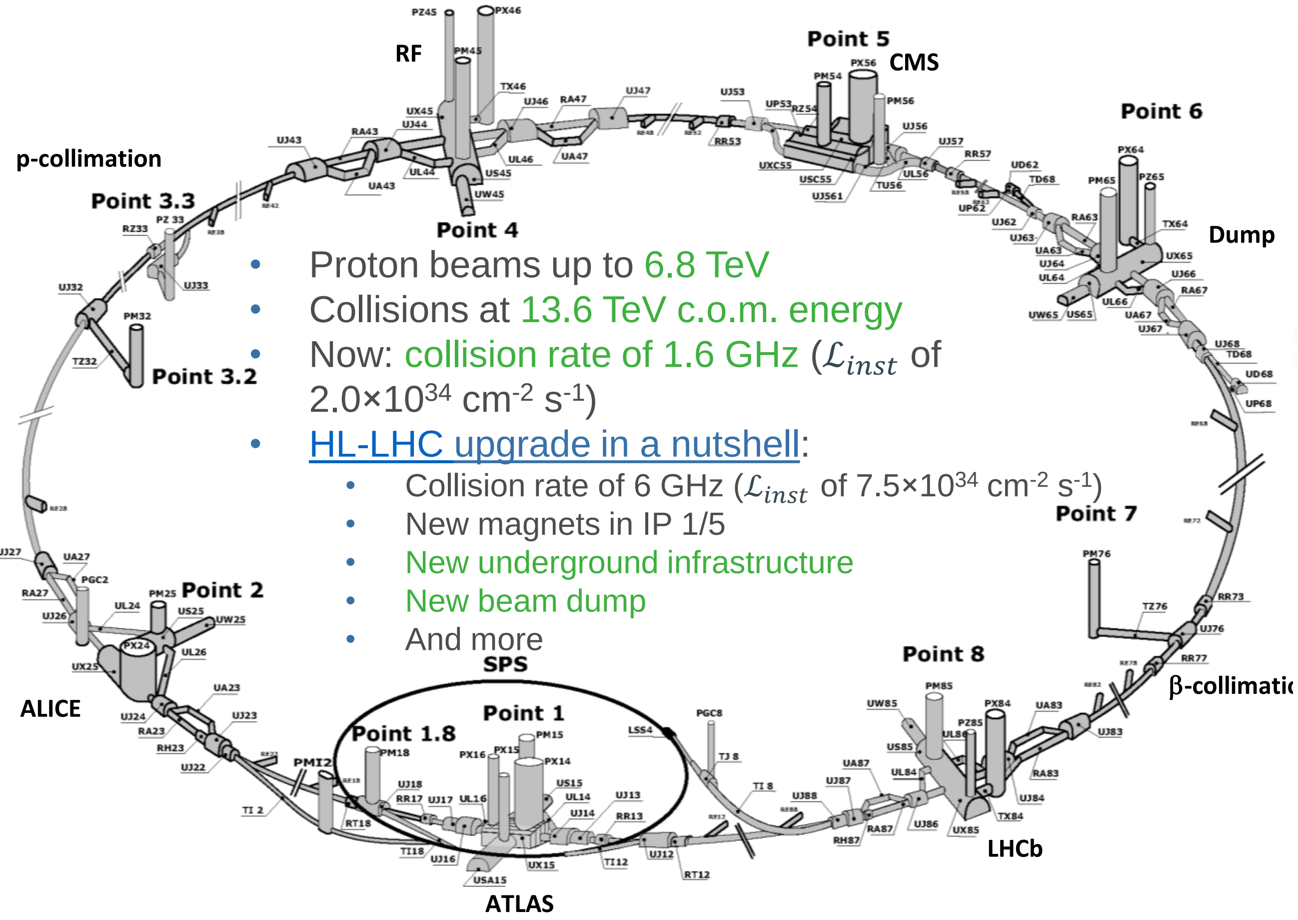


RP studies based on FLUKA simulations were performed for the dismantling of 800 m of beam lines, preconditioning of the beam dumps, design of HL-LHC infrastructure

RP studies for the LHC operation and future projects

A. Infantino et al., *Radiological characterization for the disposal of a decommissioned LHC external beam dump at CERN,* EPJP 2023

D. Bozzato et al., *Advanced simulation techniques for Radiation Protection studies at the Large Hadron Collider,* Radiat. Phys. Chem. 2024



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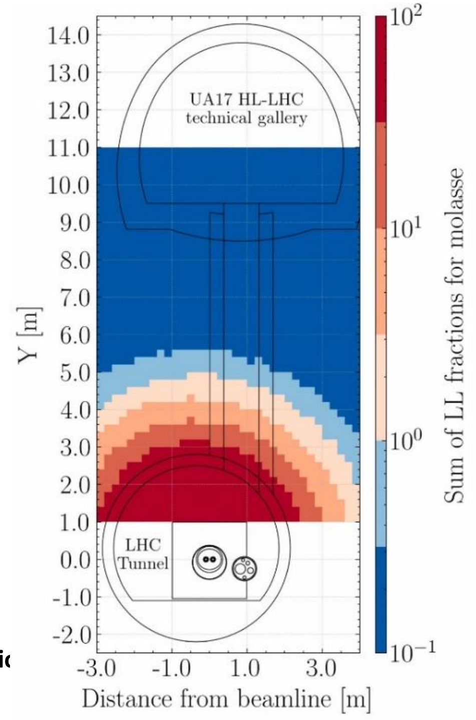
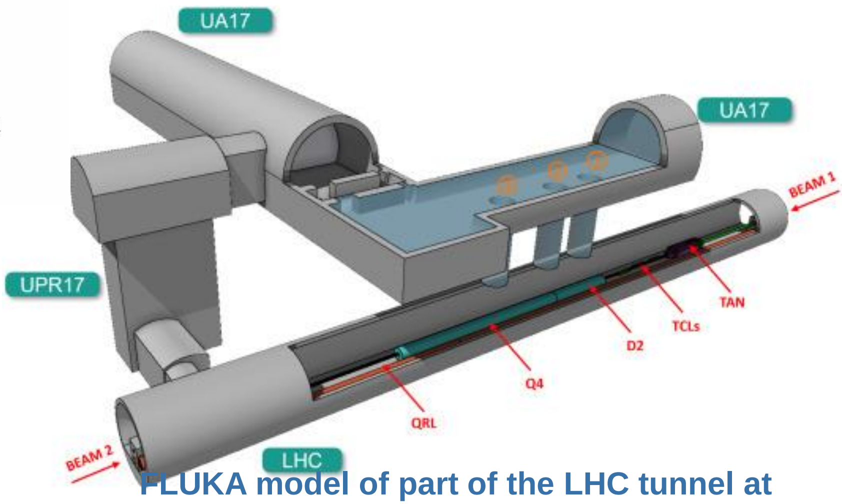


For the excavation of new technical underground areas, the estimation of the rock activation in terms of multiples of Swiss clearance limits was performed using a fluence-based method (Fluence Conversion Coefficients)



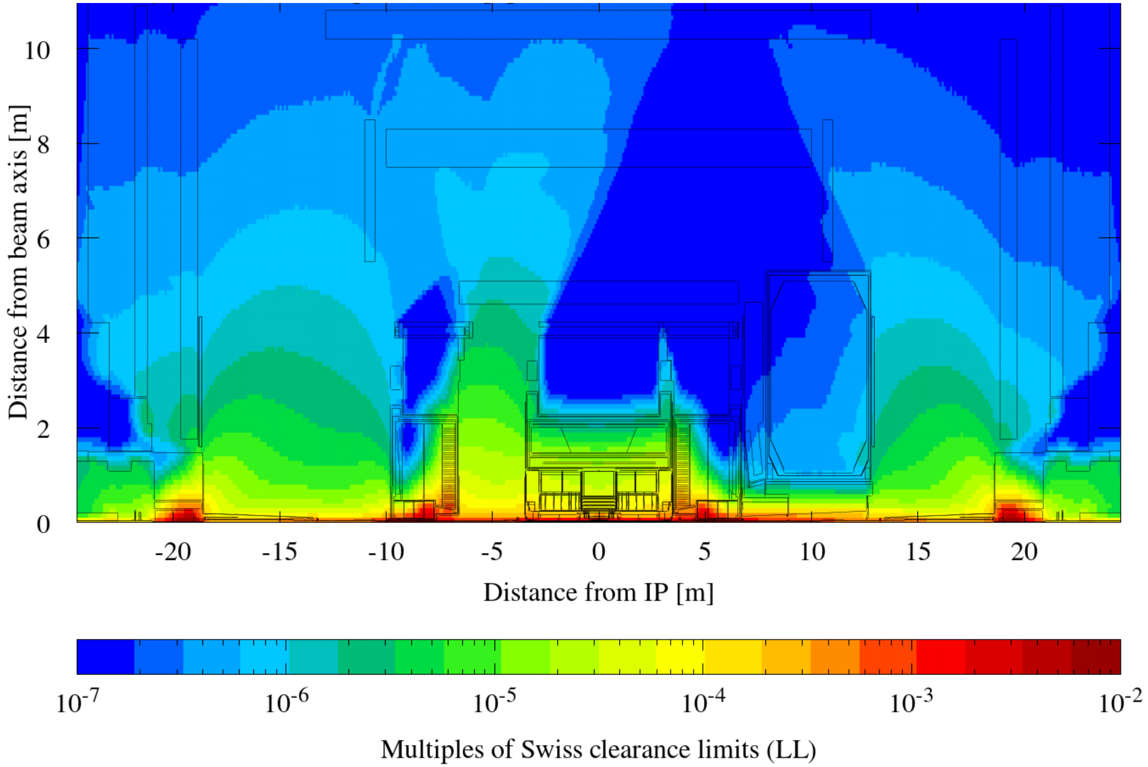
FLUKA model of part of the LHC tunnel at Point 1 and of the new HL-LHC galleries

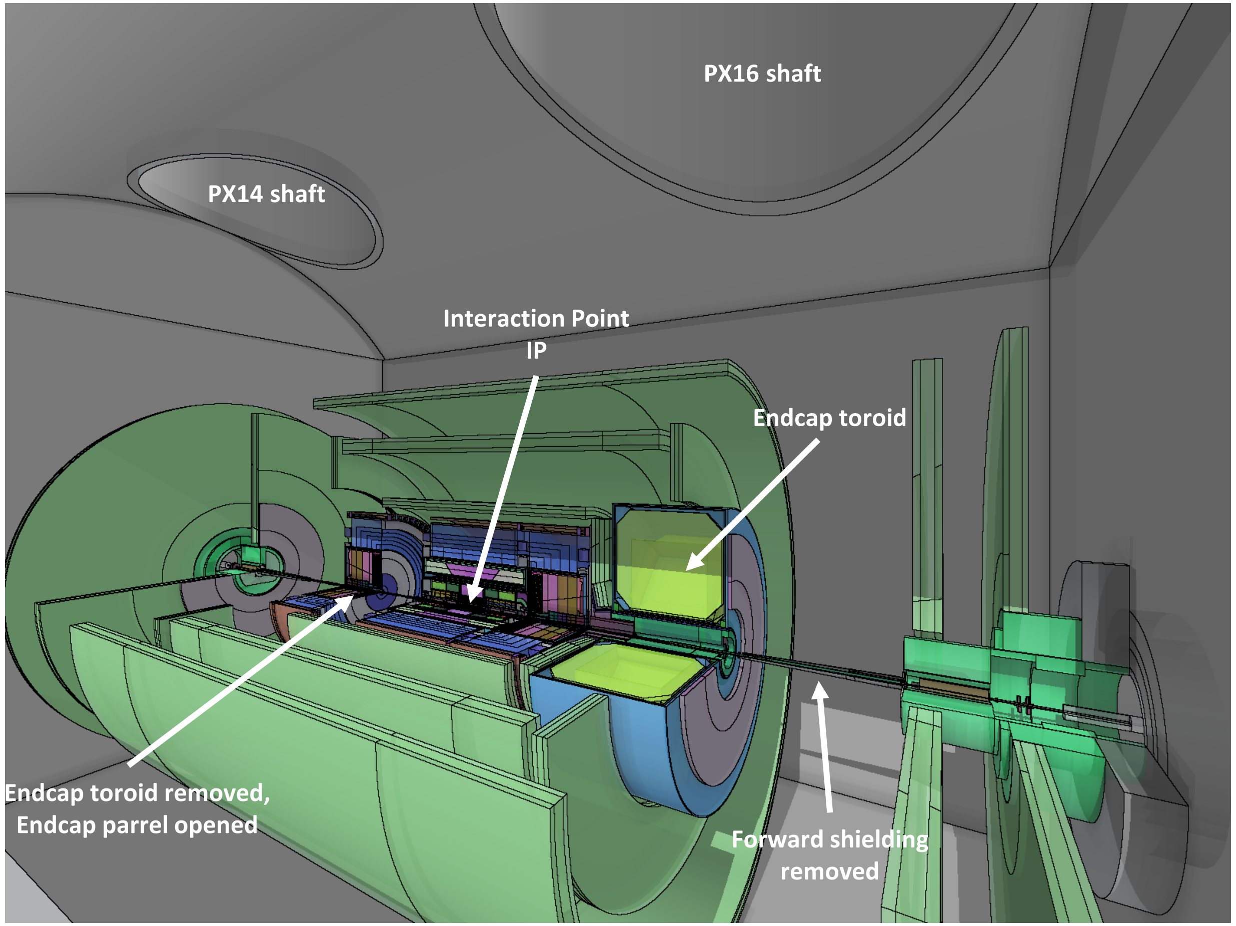
RP studies based on FLUKA simulations were performed for the dismantling of 800 m of beam lines, preconditioning of the beam dumps, design of HL-LHC infrastructure

RP studies for the LHC Experiments

D. Bozzato et al., [Radiological Characterization with a Fluence Conversion Coefficients–Based Method: A Practical Example of the Preparatory Studies to the Pilot Beam at the CERN Large Hadron Collider, NSE 2024]

- ATLAS is the large detector installed at LHC Point 1
- Nominal operation: collisions at 13.6 TeV c.o.m. energy, 1.6 GHz collision rate, magnetic field on.
- [2021 LHC Pilot Beam] conducted with exceptional configuration: open detector, collisions at injection energy, magnetic field switched off.





The estimation of the additional induced activation in terms of multiples of Swiss clearance limits was performed using a fluence-based method (Fluence Conversion Coefficients)

Summary

Summary of the lecture 1/2

- We have recalled that the production and simulation of the decay of nuclides can be activated with the **RADDECAY** card. Activities can be estimated if **IRRPROFI**, **DCYTIME**, and **DCYSCORE** cards are also issued.
- We have also revised the most important **PHYSICS** settings for activation simulations.
- We have seen that there are many built-in options to estimate induced radioactivity with FLUKA which implement event-based methods.

Quantity	Scoring card(s)	Output
Nuclide's production yields	RADDECAY	**Inventory** averaged over the scoring region
Nuclide's activities/specific activities	RADDECAY + DCYSCORE	**Inventory** averaged over the scoring region
Activity	USRBIN (ACTIVITY) + DCYSCORE	Spatial **distribution** of total activity, average specific activity in a region or over a mesh
Specific activity	USRBIN (ACTOMASS) + DCYSCORE	Spatial **distribution** of specific activity, average specific activity in a region or over a mesh

- With **AUXSCORE** it is possible to filter **ACTIVITY** and **ACTOMASS** by radionuclide, and **RADDECAY** by particle.

Summary of the lecture 2/2

- There are several user routines activated with the **`USERWEIG`** card which can be particular handy:
  - **`comscw.f`** to weigh / filter activity density binnings;
  - **`usrrnc.f`** called every time a residual nucleus is stopped;
  - **`fluscw.f`** to weight particle fluences: this allows simple implementation of fluence-based methods;

- We have seen that fluence-based methods can be useful and complementary approaches to estimated induced radioactivity.
  - Typical applications include:
    - Activation of air, water, or cooling fluids in general;
    - Activation of soil and groundwater;
  - They are a bit more difficult to implement from scratch, but several codes already exist.
  - Simple implementations are still possible on the User side with user routines (**`fluscw.f`**).

FLUKA