New features in FLUKA for activation studies

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for the FLUKA Collaboration

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Outline

1. Nuclear interactions in FLUKA

- Overview
- *Physics improvements* →
  - Peanut energy range
  - Spin-parity in Fermi breakup
  - Direct (p,α) and (p,d) reactions
  - BME improvements

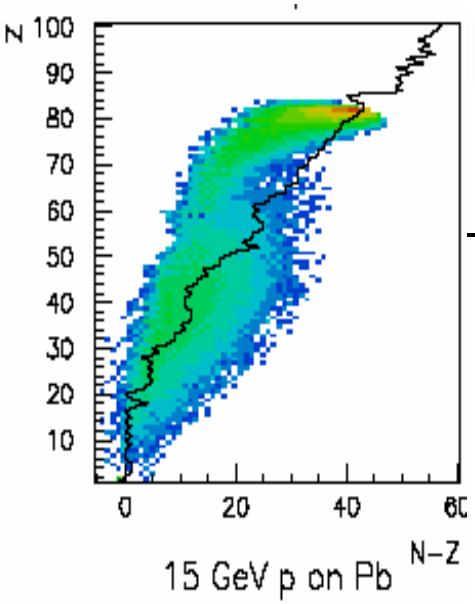
2. Radioactive decays

- Overview
- *Physics improvements* →
  - Alpha decay radiation
  - New database
  - Isomers
  - ^{9}C decay
- Geometry features

3. Application

- LHC Present and future

Nuclear interactions – *Overview (1)*



General properties

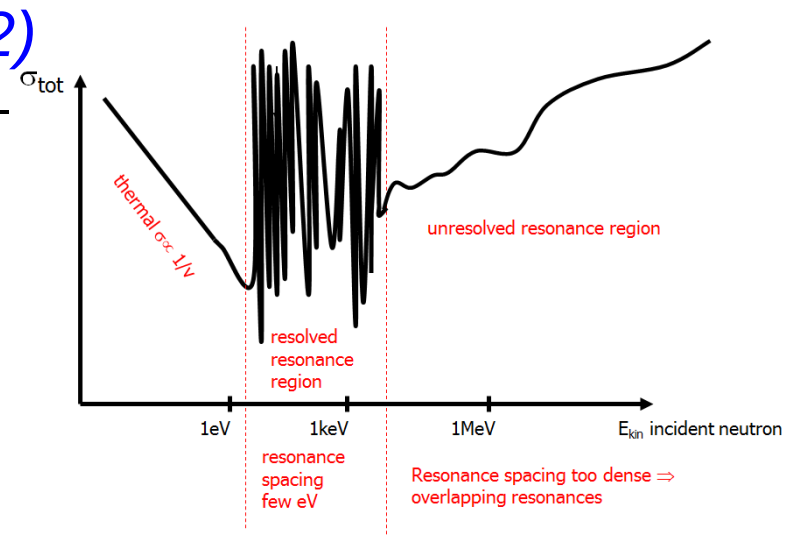
- **"Microscopic" interactions models for nuclear reactions** (except low energy neutrons)
- Consideration of 60 different particles and (any) heavy ions
- Nuclear interactions (hadron-nucleus and nucleus-nucleus) in wide energy range (**from threshold up to 10000 TeV/n**)
- Detailed treatment of photonuclear interactions (GDR, quasi-deuteron, delta resonance, VMD)

- Predictions for nuclide production follow directly from these models for (almost) arbitrary projectile-target combinations and energy (predictive power!)
- **Detailed and comprehensive benchmarks** of radionuclide production available

Isotope	Copper	Iron	Titanium	Stainless Steel	Aluminum	Concrete
^{7}Be 53.29d	1.47 ± 0.19 M	1.55 ± 0.22	1.50 ± 0.19	0.98 ± 0.24 M C,N	0.71 ± 0.09 Al	1.17 ± 0.14 O, C
	0.84 ± 0.25	0.90 ± 0.15				
^{22}Na 2.60y	0.72 ± 0.11	0.70 ± 0.13 M	0.85 ± 0.11	—	0.76 ± 0.07 Al	0.86 ± 0.09 Ca,(Si,Mg)
^{24}Na 14.96h	0.42 ± 0.03	0.48 ± 0.02	0.63 ± 0.02	0.37 ± 0.02 Fe,(Cr,Si)	0.81 ± 0.03 Al,Mg	0.62 ± 0.02 Ca,(Si,Al)
^{27}Mg 9.46m			0.79 ± 0.14 M		1.52 ± 0.25 Al,Mg	
^{28}Mg 20.91h	0.25 ± 0.04 -	0.23 ± 0.03 -	0.31 ± 0.02 -	0.29 ± 0.10 M- Fe,Ni,Si)		0.29 ± 0.02 - Ca,(Si)
^{28}Al 2.24m	0.25 ± 0.03 -	0.21 ± 0.02 -	0.31 ± 0.02 -	0.29 ± 0.10 M- Fe,Ni,Si)		0.29 ± 0.03 - Ca,(Si)
^{29}Al 6.56m			0.93 ± 0.25 M			
^{35}S 2.84h	—	—	0.60 ± 0.12 -	—		
^{36,37}Cl 32.00m		0.91 ± 0.19 M	1.19 ± 0.18	0.77 ± 0.15 Fe,Cr,(Mn)		1.25 ± 0.07 Ca
^{36}Cl 37.24m		0.81 ± 0.06	0.60 ± 0.01	0.58 ± 0.07 Fe,Cr,(Mn)		
^{38}Cl 55.60m		0.84 ± 0.11 M	0.73 ± 0.08	0.66 ± 0.12 Fe,Cr,(Mn)		
^{41}Ar 1.82h	0.39 ± 0.06	0.48 ± 0.05	0.47 ± 0.04 -	0.38 ± 0.05 Fe,Cr,(Mn)		0.88 ± 0.14 Ca
^{38}K 7.64m	—	—		—		1.76 ± 0.20 - Ca
^{39}K 12.36h	0.86 ± 0.10	0.83 ± 0.06	0.95 ± 0.05	0.76 ± 0.09 Fe,Cr,(Mn)		1.21 ± 0.08 Ca
^{41}K 22.30h	0.81 ± 0.10 -	0.77 ± 0.05	0.85 ± 0.03	0.74 ± 0.04 Fe,Cr,(Mn)		1.16 ± 0.05 Ca
^{42}K 22.13m			—			
^{43}K 17.30m			—			
^{47}Ca 4.54d	0.59 ± 0.16	0.56 ± 0.17 M	0.73 ± 0.12	0.51 ± 0.15 M Fe,Cr,(Mn)		0.79 ± 0.12 Ca
^{43}Sc 3.89h	0.40 ± 0.07 -	1.01 ± 0.14	1.28 ± 0.29 -	0.93 ± 0.15 Fe,Cr,(Mn)		
^{44}Sc 3.93h	0.89 ± 0.07	1.08 ± 0.06	0.98 ± 0.05	0.96 ± 0.09 Fe,Cr,(Mn)	—	0.83 ± 0.06 Fe,(Ti)
^{m44}Sc 58.60h	0.95 ± 0.12	1.20 ± 0.09	2.13 ± 0.12	1.24 ± 0.09 Fe,Cr,(Mn)	1.08 ± 0.17 Fe,Mn	1.67 ± 0.22 Fe,(Ti)
^{46}Sc 83.79d	0.81 ± 0.07	0.86 ± 0.07	0.93 ± 0.08	0.89 ± 0.08 Fe,Cr,(Mn)	0.79 ± 0.18 Mn,(Ti,Fe)	0.88 ± 0.10 Fe,(Ti)
^{47}Sc 80.28h	1.08 ± 0.14	1.17 ± 0.10 -	0.87 ± 0.07	1.06 ± 0.09 Fe,Cr,(Mn)	1.04 ± 0.15 Mn,(Ti,Fe)	1.00 ± 0.09 Fe,Ti,(Ca)
^{48}Sc 43.67h	1.39 ± 0.16	1.47 ± 0.10	1.10 ± 0.04	1.42 ± 0.08 Fe,Cr,(Mn)		1.38 ± 0.25 Fe,Ti,(Ca)
^{48}V 15.97d	1.16 ± 0.08	1.45 ± 0.06	1.11 ± 0.07	1.44 ± 0.11 Fe,Cr,(Mn)	1.07 ± 0.13 Fe,Mn	1.63 ± 0.16 Fe
^{48}Cr 21.56h	0.92 ± 0.14	0.97 ± 0.07		1.02 ± 0.08 Fe,(Cr)		1.06 ± 0.23 M Fe
^{49}Cr 42.30m	1.00 ± 0.22 M	1.24 ± 0.12 -		1.06 ± 0.12 Fe,(Cr)		
^{51}Cr 27.70d	1.06 ± 0.13	1.15 ± 0.12	0.64 ± 0.24 M	1.24 ± 0.16 Fe,Cr	0.86 ± 0.16 Fe,Mn	1.33 ± 0.22 Fe
^{52}Mn 5.59d	0.88 ± 0.06	1.15 ± 0.04		1.09 ± 0.03 Fe,(Mn)	0.88 ± 0.07 Fe,Mn	1.39 ± 0.07 Fe
^{m52}Mn 21.10m	1.88 ± 0.35	1.24 ± 0.09		1.12 ± 0.10 Fe,(Mn)		1.75 ± 0.79 M Fe
^{54}Mn 312.12d	1.13 ± 0.12	1.01 ± 0.10		1.08 ± 0.11 Fe,(Mn)	0.96 ± 0.12 Mn,Fe	1.06 ± 0.13 Fe
^{56}Mn 2.58h	0.81 ± 0.08	0.99 ± 0.05		1.33 ± 0.10 Fe	1.53 ± 0.25 Mn	1.03 ± 0.25 Mn,Fe
^{52}Fe 8.28h	—	1.09 ± 0.13		0.99 ± 0.19 M Fe,(Mn)		
^{53}Fe 8.51m		—				
^{59}Fe 44.50d	0.82 ± 0.09					
^{55}Co 17.53h	0.66 ± 0.09	0.76 ± 0.04		1.03 ± 0.05 Fe,Ni		—
		1.13 ± 0.10				
^{56}Co 77.27d	1.04 ± 0.09	1.15 ± 0.10		1.37 ± 0.11 Fe,Ni	—	0.80 ± 0.20 M Fe
		1.79 ± 0.15				
^{57}Co 271.79d	0.85 ± 0.08	0.38 ± 0.08 M		1.16 ± 0.13 Ni	0.66 ± 0.24 M Cu,Zn,Ni	
^{58}Co 70.82d	0.91 ± 0.09	0.31 ± 0.06 M		0.98 ± 0.10 Ni	0.82 ± 0.19 Cu,Zn,Ni	—
^{60}Co 5.27y	0.90 ± 0.08					
^{61}Co 99.00m	0.68 ± 0.08					
^{57}Co 90.00s						
^{57}Ni 35.60h	0.76 ± 0.11			1.44 ± 0.07 Ni		
^{65}Ni 2.52h	1.46 ± 0.29					
^{66}Cu 23.70m	0.78 ± 0.08					
^{61}Cu 3.33h	0.87 ± 0.25					
^{64}Cu 12.70h	0.63 ± 0.10					
^{62}Zn 9.19h	1.05 ± 0.23					
^{63}Zn 38.47m	—					
^{65}Zn 244.26d	0.62 ± 0.08					
	0.97 ± 0.20					

M. Brugger, S. Roesler *et al.*,
Nuclear Instruments and Methods A 562 (2006) 814

Nuclear interactions – *Overview (2)*



Low energy neutrons (E<20MeV)

- Special treatment because of: complex cross sections, interactions down to meV, calculation by models difficult/impossible
- Use of **evaluated nuclear data files** (ENDF, JENDL, JEFF, etc.)
- **Transport in energy "groups"** (260), point-wise transport available only for few specific reactions (e.g.,^{1}H, ^{7}Li), extension planned

- Nuclide production also based on data files
- Residual nuclei produced "at rest", except recoil protons from hydrogen and ^{14}N(n,p) as well as αand 3H fragments from neutron capture in ^{6}Li and ^{10}B

Material		Temp.	Origin	RN	Name	Identifiers			Gam
9Be	Beryllium 9	296K	ENDF/B-VIIR0	Y	BERYLLIU	4	9	296	Y
9Be	Beryllium 9	87K	ENDF/B-VIIR0	Y	BERYLLIU	4	9	87	Y
B	Natural Boron	296K	ENDF/B-VIIR0	Y	BORON	5	-2	296	Y
B	Natural Boron	87K	ENDF/B-VIIR0	Y	BORON	5	-2	87	Y
10B	Boron 10	296K	ENDF/B-VIIR0	Y	BORON-10	5	10	296	Y
10B	Boron 10	87K	ENDF/B-VIIR0	Y	BORON-10	5	10	87	Y
11B	Boron 11	296K	ENDF/B-VIIR0	Y	BORON-11	5	11	296	Y
11B	Boron 11	87K	ENDF/B-VIIR0	Y	BORON-11	5	11	87	Y
C	Free gas natural Carbon	296K	ENDF/B-VIIR0	Y	CARBON	6	-2	296	Y
C	Graphite bound nat. Carbor	296K	ENDF/B-VIIR0	Y	CARBON	6	-3	296	Y
C	Free gas natural Carbon	87K	ENDF/B-VIIR0	Y	CARBON	6	-2	87	Y
N	Natural Nitrogen	296K	ENDF/B-VIIR0	Y	NITROGEN	7	-2	296	Y
N	Natural Nitrogen	87K	ENDF/B-VIIR0	Y	NITROGEN	7	-2	87	Y
14N	Nitrogen 14	296K	ENDF/B-VIIR0	Y	NITRO-14	7	14	296	Y
14N	Nitrogen 14	87K	ENDF/B-VIIR0	Y	NITRO-14	7	14	87	Y
16O	Oxygen 16	296K	ENDF/B-VIR8	Y	OXYGEN	8	16	296	Y
16O	Oxygen 16	87K	ENDF/B-VIR8	Y	OXYGEN	8	16	87	Y
19F	Fluorine 19	296K	ENDF/B-VIR8	Y	FLUORINE	9	19	296	Y
19F	Fluorine 19	87K	ENDF/B-VIR8	Y	FLUORINE	9	19	87	Y
23Na	Sodium 23	296K	JENDL-3.3	Y	SODIUM	11	23	296	Y
23Na	Sodium 23	87K	JENDL-3.3	Y	SODIUM	11	23	87	Y
Mg	Natural Magnesium	296K	JENDL-3.3	Y	MAGNESIU	12	-2	296	Y
Mg	Natural Magnesium	87K	JENDL-3.3	Y	MAGNESIU	12	-2	87	Y
27Al	Aluminium 27	296K	ENDF/B-VIIR0	Y	ALUMINUM	13	27	296	Y
27Al	Aluminium 27 SelfShielded	296K	ENDF/B-VIIR0	Y	ALUMINUM	13	1027	296	Y

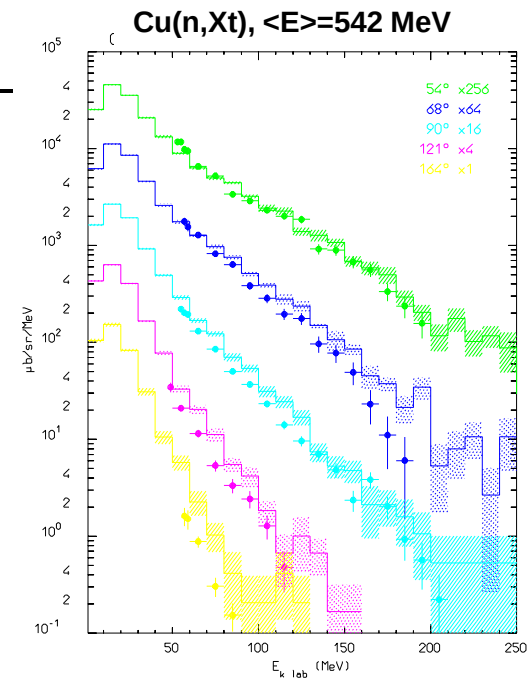
etc.

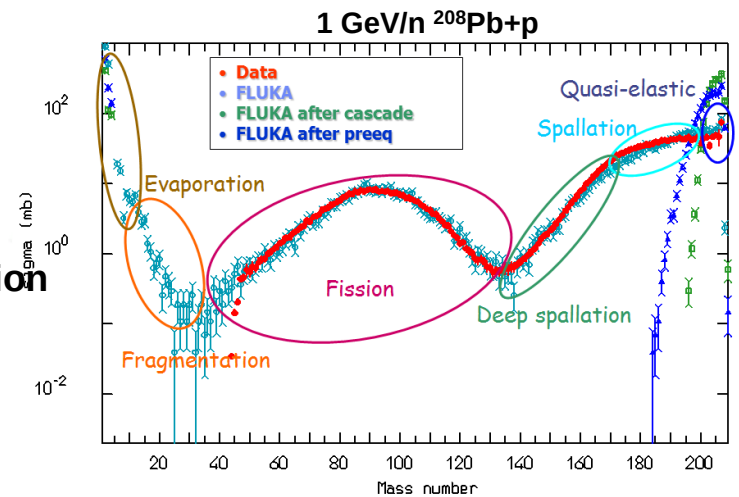
Nuclear interactions – *Overview (3)*

Peanut

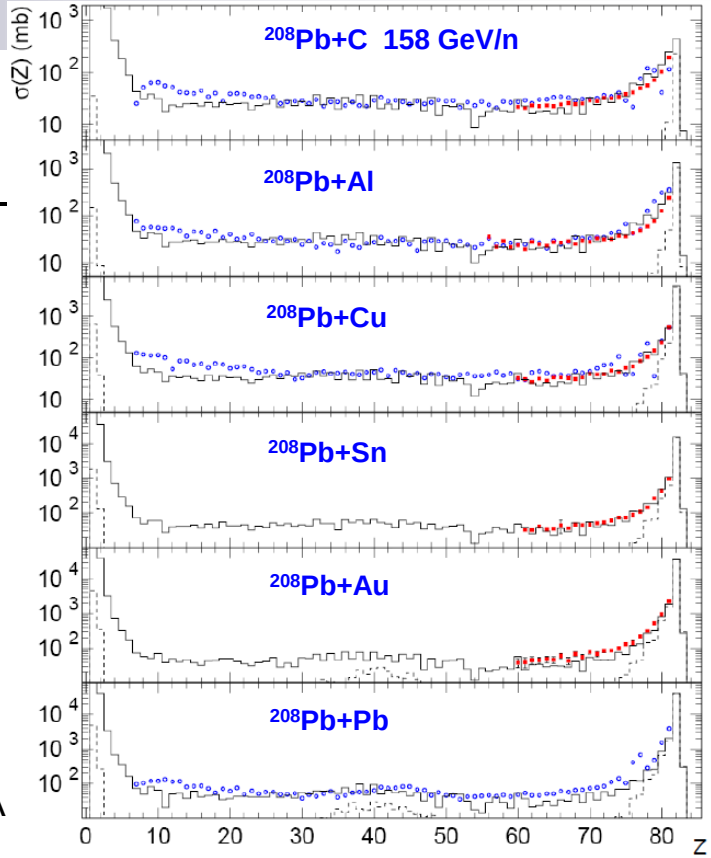
- Originally, model for nuclear interactions below few GeV, including a **sophisticated generalized intranuclear cascade and nuclear models** (interactions at high energy using a more simplified intranuclear cascade and nuclear models).
- Recently, its **extension to high (all) energies**, by including Glauber-Gribov multiple interactions and the Dual Parton Model (DPM), has become the default in FLUKA.
- Sequence of interaction steps (in time) considered in Peanut:
  1. Glauber-Gribov cascade with formation zone and DPM
  2. Generalized intranuclear cascade
  3. Preequilibrium stage with current exciton configuration and excitation energy
  4. Evaporation / fragmentation / fission
  5. Gamma-deexcitation

- All steps embedded in detailed description of target nucleus (density distribution, Fermi motion, *etc.*)
- **Production of nuclides is result of last step of the interaction sequence**, influenced by all previous stages. Very universal, however, production of individual nuclides might be influenced by specific models features (or short-comings..).





Nuclear interactions – *Overview (4)*

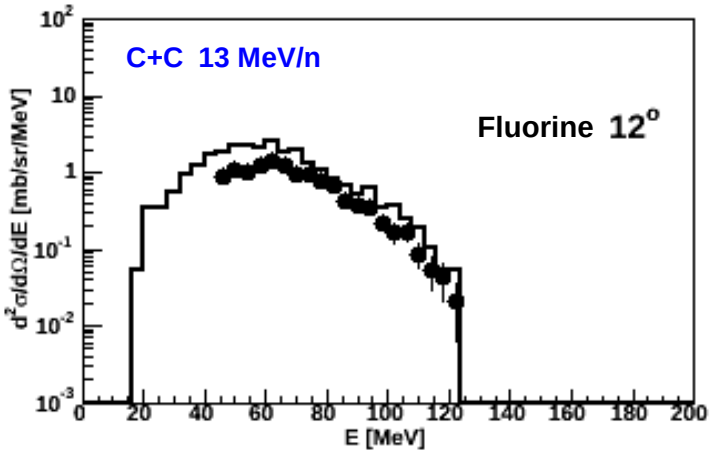


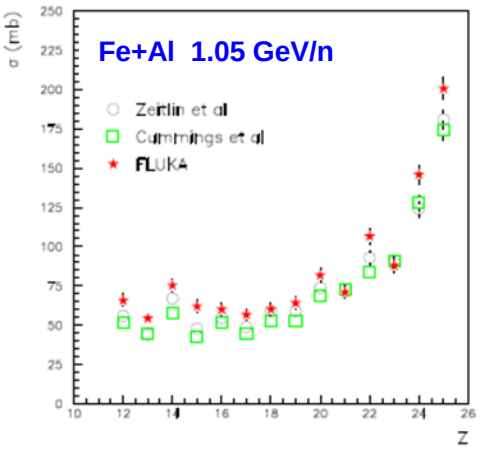
Heavy ions

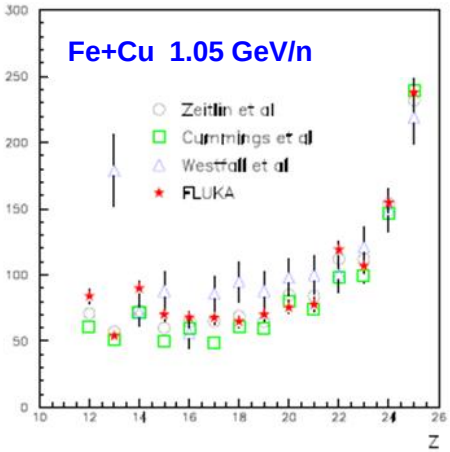
- **Different models** depending on energy

  > 5 GeV/n : Dual Parton Model (DPMJET-III)
  0.1 - 5 GeV/n : Relativistic Quantum Molecular Dynamics model (based on RQMD-2.4)
  < 0.1 GeV/n : Boltzmann Master Equation theory

- Model implementations of stand-alone codes adopted and interfaced to FLUKA (except BME), *i.e.*, partially not making use of the Peanut nuclear model.
- Extensive benchmarking of individual codes and within FLUKA







Nuclear interactions – *Physics improvements (1)*

Spin-parity in Fermi Break-up

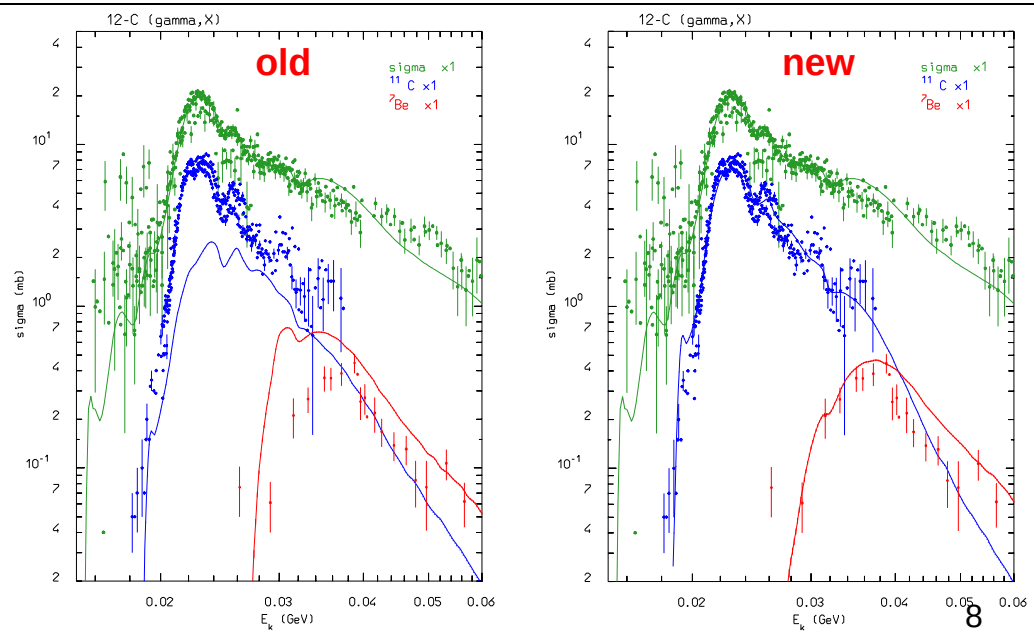
- Fragmentation by A≤17 fragments by Fermi break-up model
- Considered fragment configurations include all stable states and particle unstable levels with sizable gamma-decay branching
- Final configuration selected from probability distribution of the configurations and kinematics following n-body phase space distributions and Coulomb effects
- ***New:*** if spin and parity of excited nucleus are known conservation laws, constraints on available configurations and centrifugal barrier are enforced in fragment production (presently limited to specific channels, e.g., GDR, as FLUKA event generators are not tracing consistently spin-parity evolution)
- ***New:*** broad ^{8}Be* 1st excited state accounted for in Fermi break-up

Example:

^{12}C(g,n)^{11}C at GDR energies

- initial state is $J^{\pi} = 1^{-}$
- disintegration into 3α or α+^{8}Be energetically favored but impossible in l=0
- branching of α-channels suppressed and those of n,^{11}C increased

→ Factor 3 on ^{11}C production



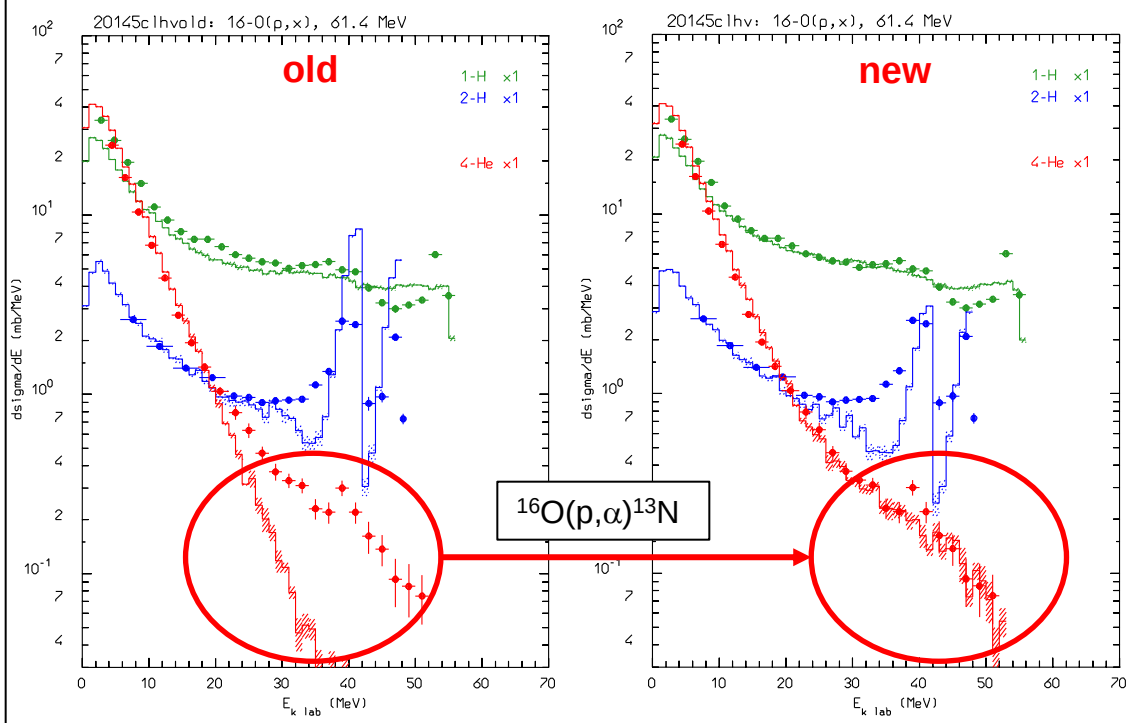
Nuclear interactions – *Physics improvements (2)*

Direct (p,α) and (p,d) reactions

- ***New:*** model for "first interaction" deuteron production for light nuclei
- Effect on production of β^+ emitter, important for medical applications (online PET simulations)

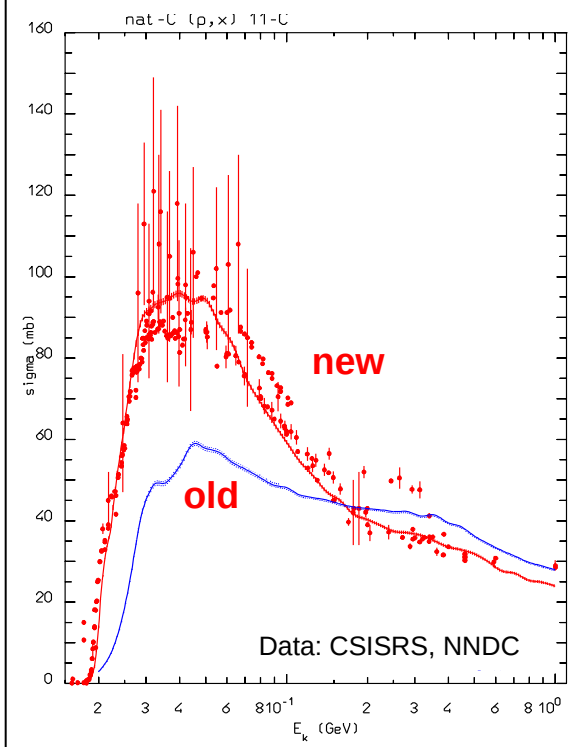
Example 1:

Angle-integrated p, d, and α spectra by 62 MeV protons on Oxygen



Example 2:

Excitation function C(p,X)^{11}C



Nuclear interactions – *Physics improvements (3)*

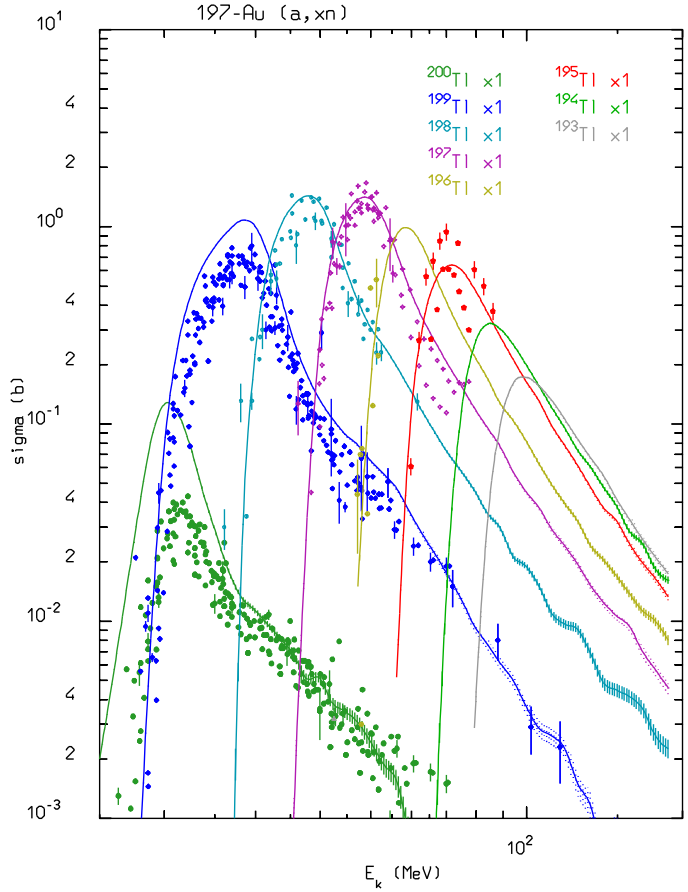
BME (< 0.1 GeV/n) :

- Pre-equilibrium particle spectra pre-computed following BME theory for certain configurations and energies only (presently mostly for ^{16}O and ^{12}C projectiles and various targets)
- For all other configurations: coupling to Peanut for pre-equilibrium emissions
- In particular, very light projectile reactions are not included in BME database. However, pre-equilibrium emissions dominate high energy tail in excitation functions (see example)

- α (re)interactions important for many applications: hadron-therapy, damage to electronics, radiation protection)
- ***New:*** A=3 projectile interactions now also simulated with BME through Peanut for pre-equilibrium emissions

Example:

Excitation function for the production of radioisotopes from a interactions on Au



Radioactive decays – *Overview (1)*

General properties

- The generation and transport of radioactive decay radiation (γ, β^-, β^+, X-rays, Conversion Electrons emissions and ***new*** α) is possible during the same simulation which produces the radio-nuclides (one-step method).
- It uses a database of decay emissions created for FLUKA, based mostly on information obtained from NNDC, sometimes supplemented with other data and checked for consistency.

- The FLUKA simulation can proceed in ***two modes***

1. Semi-analytical mode ("Activation study case")

   - Prediction of residual nuclei by FLUKA models
   - Radioactive built-up and decay calculated for certain (arbitrary) irradiation pattern and fixed cooling time(s) analytically (run-time) with an exact solution of the Bateman equation

$$\frac{dN_i}{dt} = -\sum_{j \neq i}\left[\lambda^d_{ji} + \bar{\sigma}_{ji}\bar{\varphi}\right]N_i + \sum_{j \neq i}\left[\lambda^d_{ij} + \bar{\sigma}_{ij}\bar{\varphi}\right]N_j$$

λ^d_{ji} Decay constant nuclide i->j

σ_{ji} Cross section for transmutation of nuclide i->j

$$\bar{\varphi} = \int \varphi(E)dE \qquad \bar{\sigma}_{ji} = \frac{1}{\bar{\varphi}}\int \varphi(E)\sigma_{ji}(E)dE$$

2. Semi-analogue mode (pure Monte Carlo method)

   - Each radioactive nucleus is treated like all other unstable particles
   - times are sampled randomly from the correspondent exponential distribution, radiation and daughters also randomly, all secondary particles/nuclei carry time stamp ("age")

Radioactive decays – *Overview (2)*

Decay radiation

- Up to 4 different decay branching for each isotope/isomer
- All gamma lines down to 0.1-0.01% branching, including X-ray lines following conversion electron emissions
- All beta emission spectra down to 0.1-0.01% branching, sampling of the β^-/β^+ spectra includes screening Coulomb corrections
- Auger and conversion electrons included

Isomers

- The production of **metastable states** is not yet simulated by the FLUKA nuclear models (it would require spin/parity dependent calculations in evaporation).
- Thus, isomer production is based on a rough estimate: equal sharing among states
- Exception ***(New):*** isomer production by neutrons below 20 MeV (see next slide)
- Metastable states in the subsequent decay chain are always populated and decayed according to the correct branching ratios.

Radioactive decays – *Physics improvements*

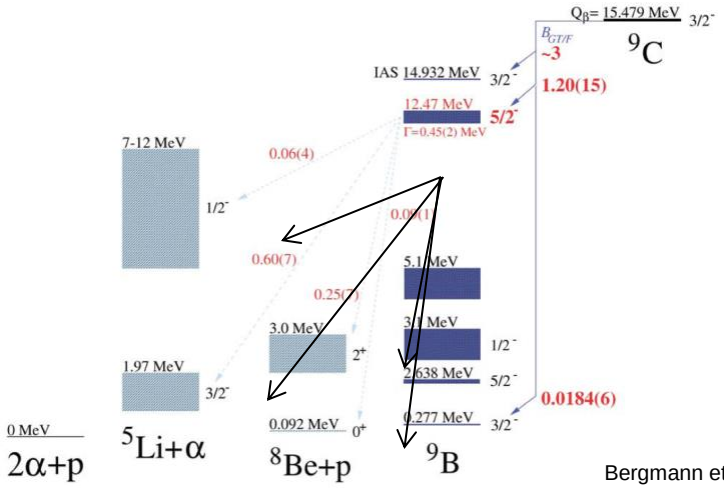
New

- Emission of α particles in radioactive decays, however no re-interactions considered in analytical mode ("Activation study case")

- New masses/half-lives/decays/radiations database
  - Old database: last update many years ago (>15 years for masses, >3 years for levels, etc.). Since then, significant amount of new data has become available
  - New database based on RIPL (Reference Input Parameter Library), using ENSDF to complete missing information (e.g., EC/β^+ branchings) and solving numerous inconsistencies
  - Now available: increased precision on excess masses, additional isotopes (15%) and isomers (50%)

- Branchings for isomer production by neutrons below 20 MeV now based on JEFF activation file and no longer on the assumption of equal sharing among the different states

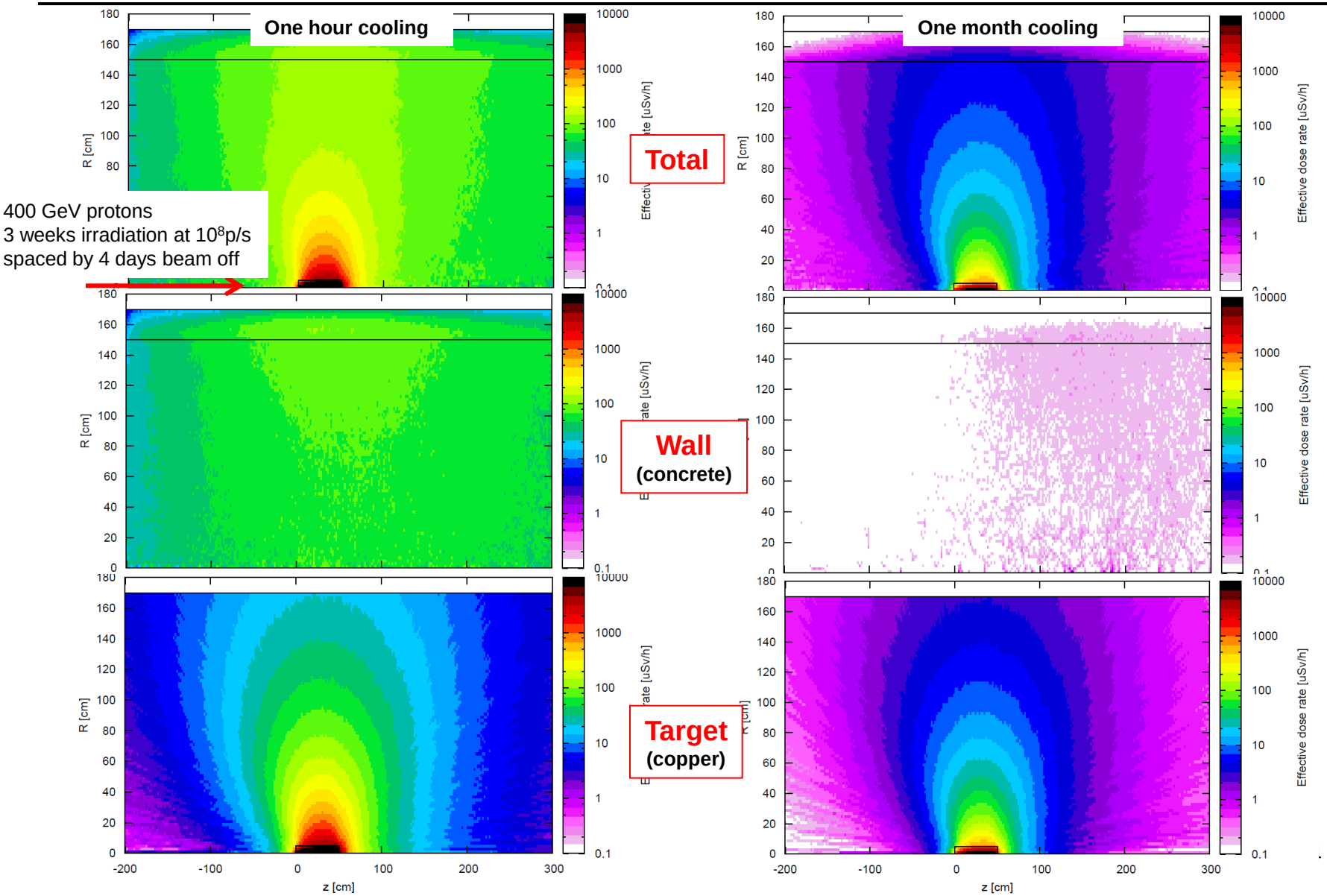
- Special decay model for ^{9}C



Bergmann et al., NPA 692 (2001) 427

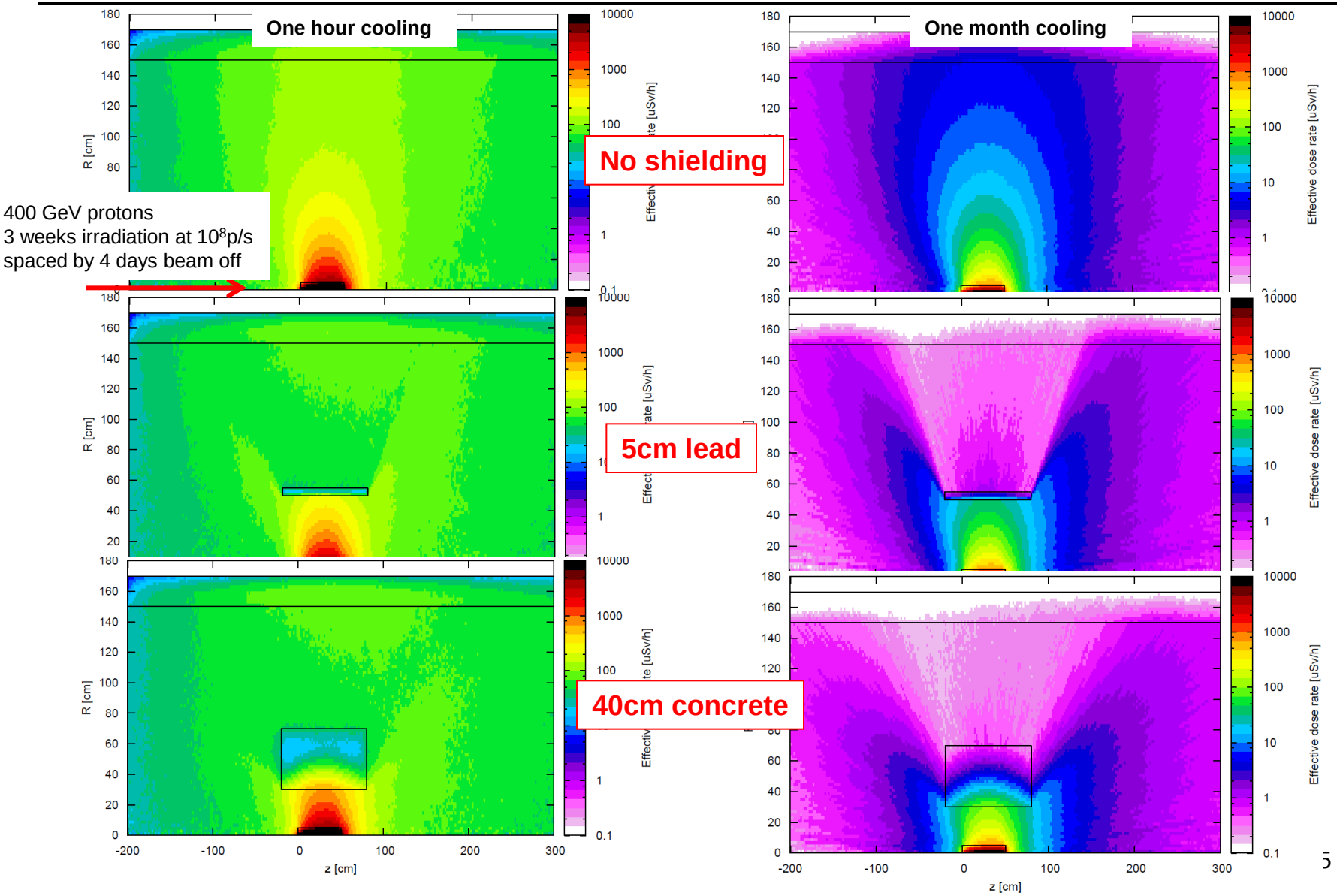
Radioactive decays – *Geometry features (1)*

Contributions by different parts of the geometry



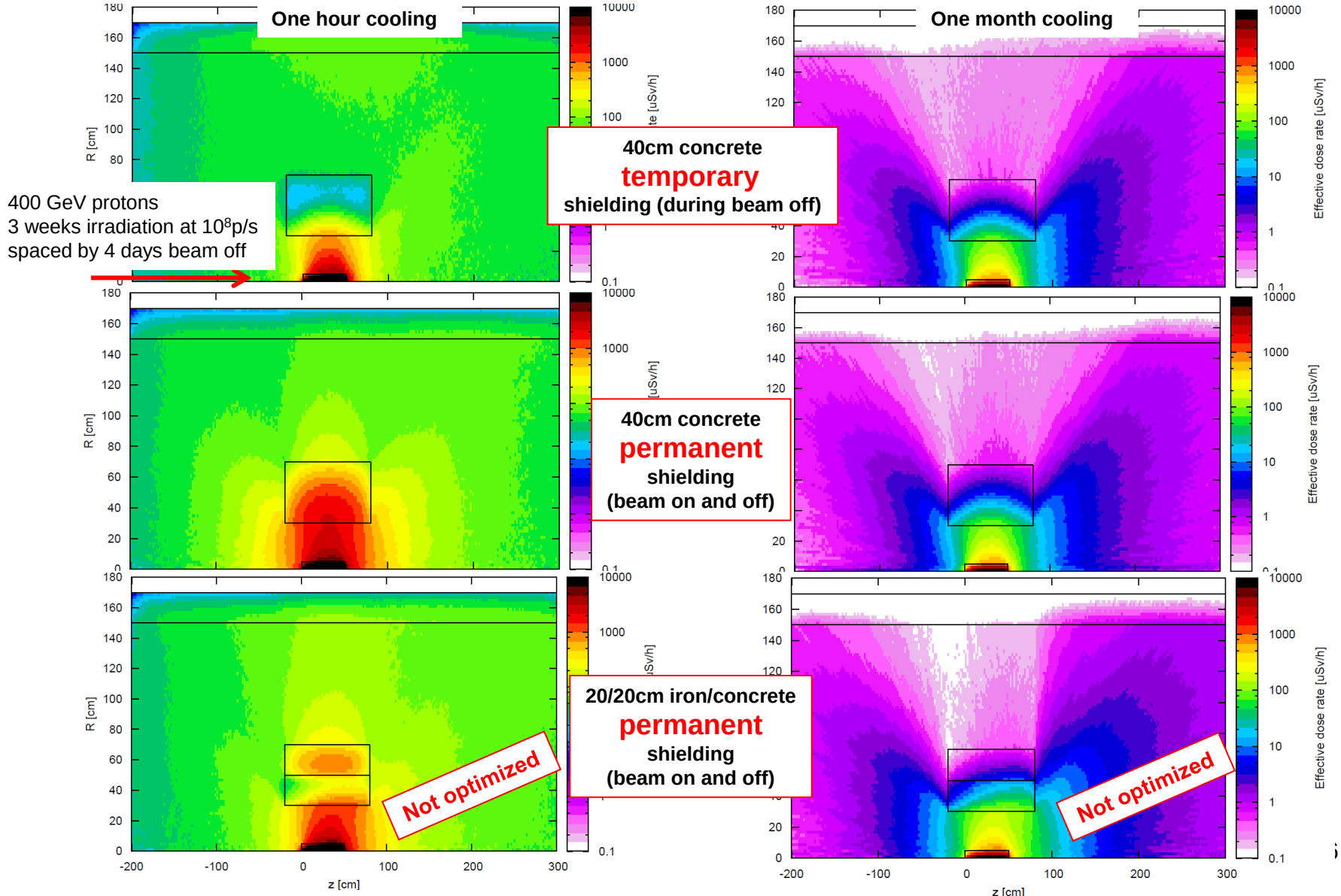
Radioactive decays – *Geometry features (2)*

Effect of different shielding material

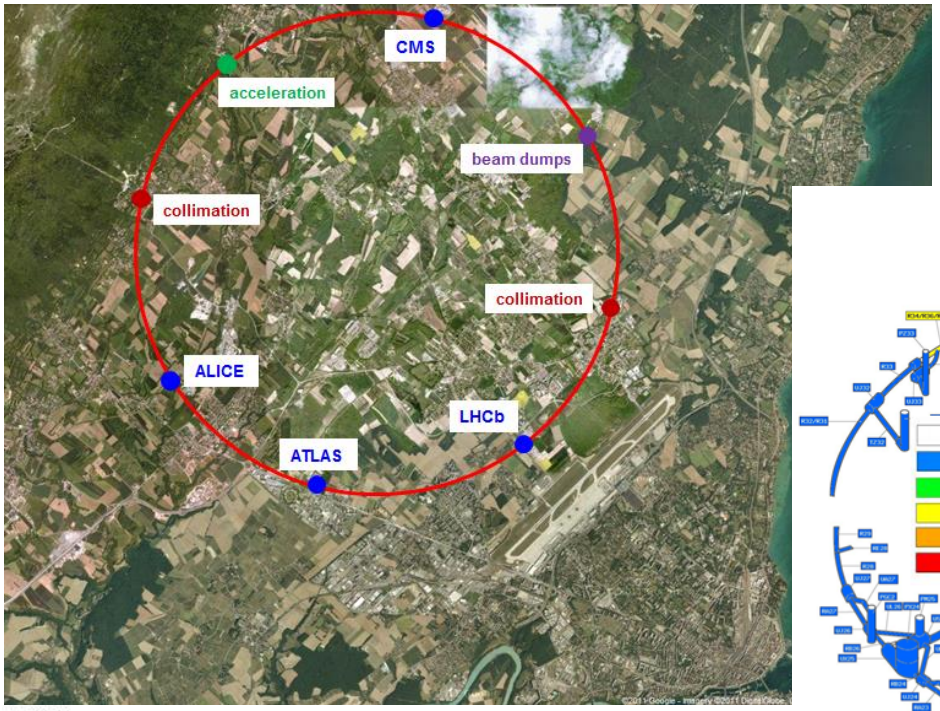


Radioactive decays – *Geometry features (3)*

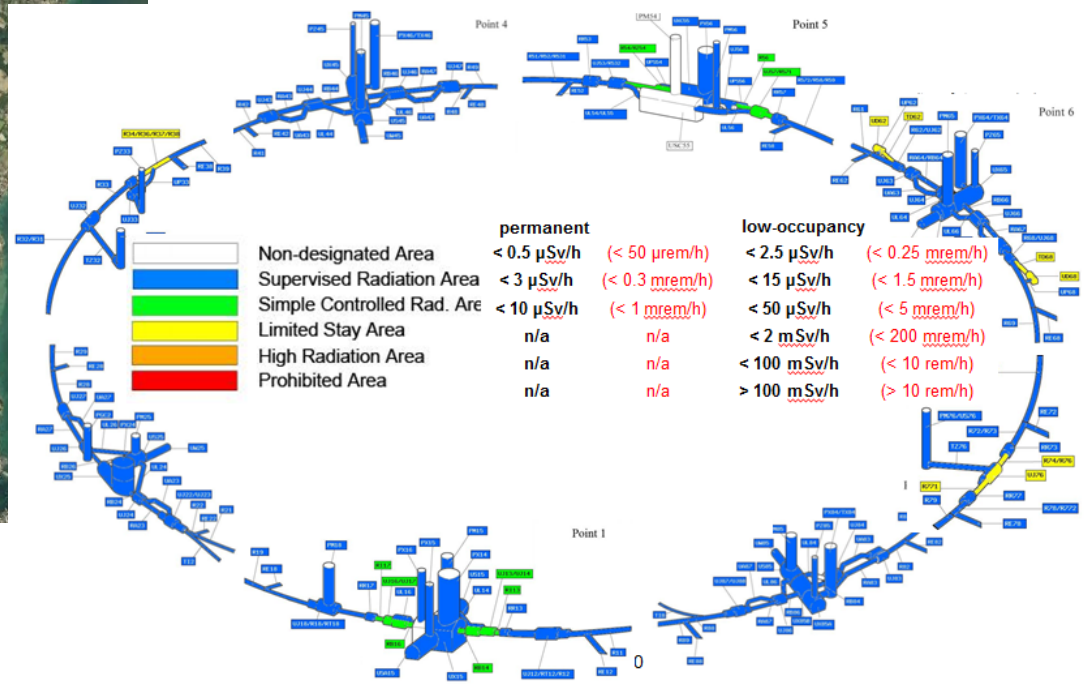
Permanent vs. temporary shielding

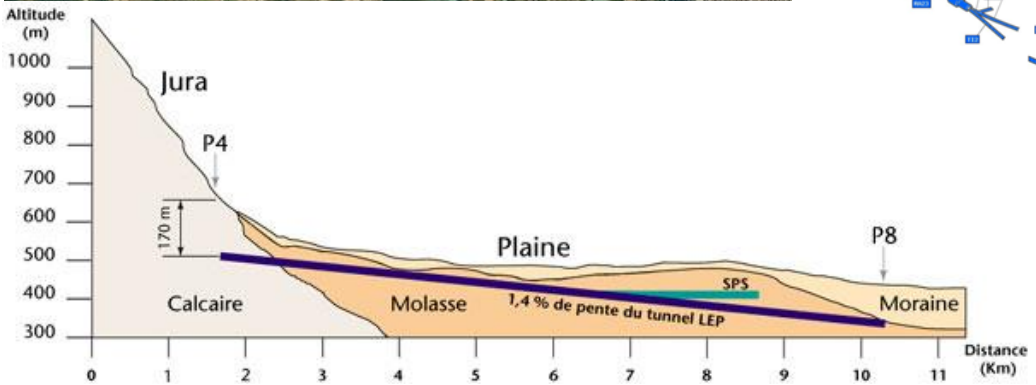


Application – *Large Hadron Collider*



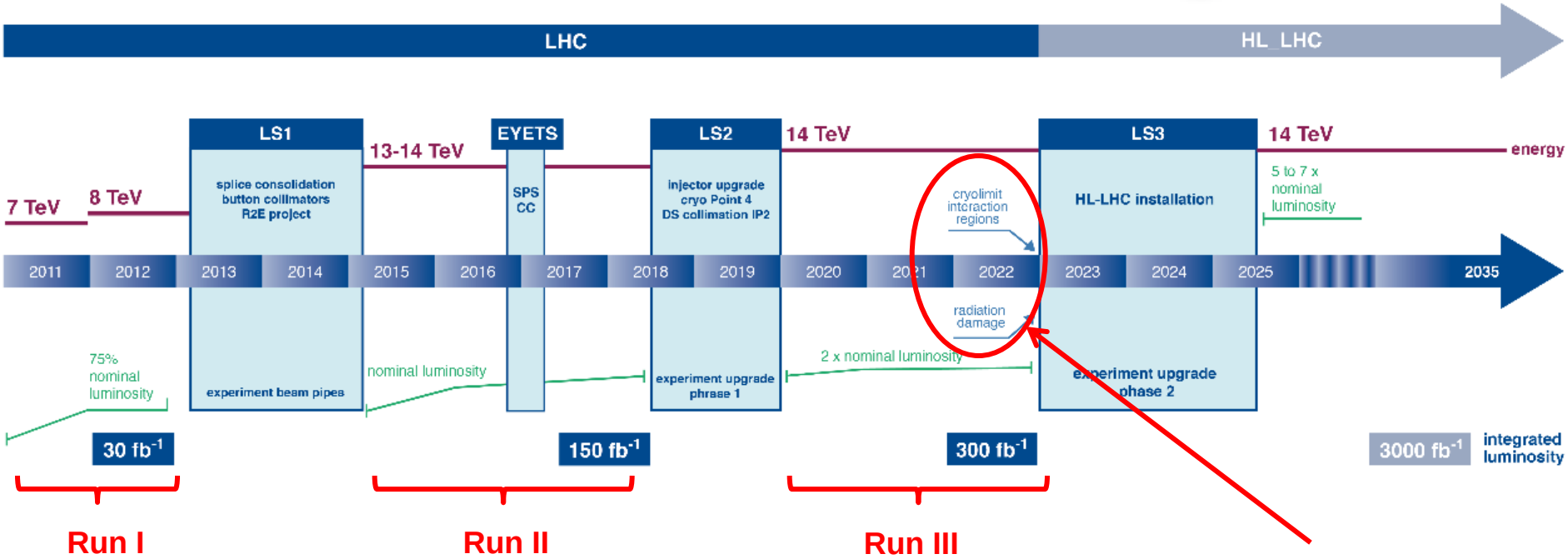
Radiological classification during Run I (2012)





Application – *LHC long-term schedule*

http://hilumilhc.web.cern.ch/about/hl-lhc-project



Run I

0.75×10^{34} cm^{-2}s^{-1}
50 ns bunch spacing

Run II

1.5×10^{34} cm^{-2}s^{-1}
25 ns bunch spacing
(**nominal LHC**)

Run III

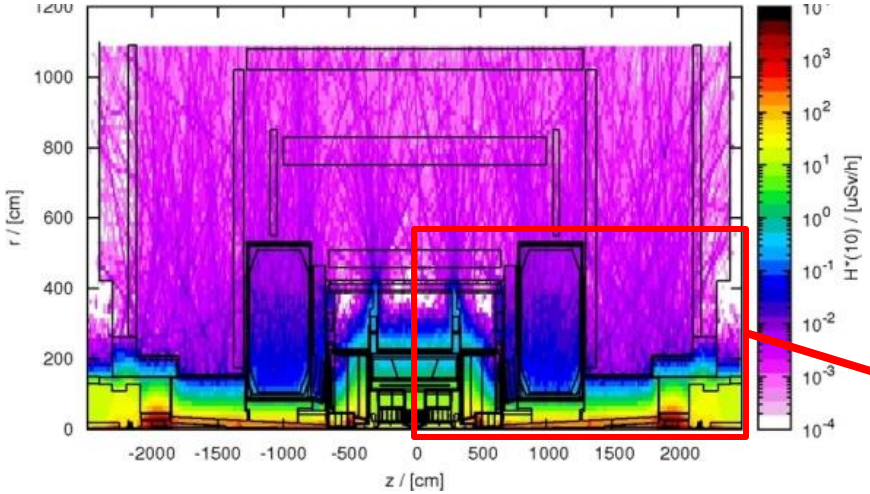
$1.7 – 2.2 \times 10^{34}$ cm^{-2}s^{-1}
25 ns bunch spacing
(**ultimate LHC**)

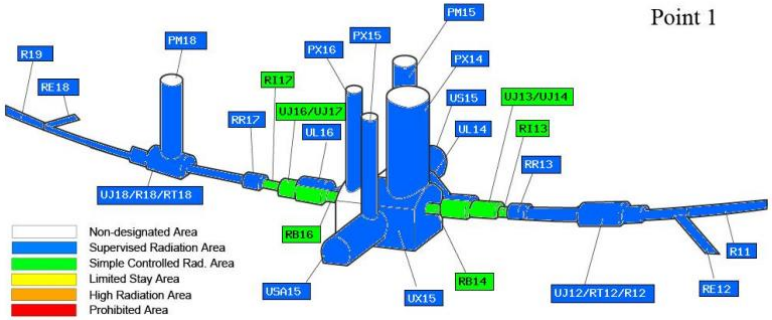
Technical limits to further luminosity increase (accelerator and experiments)

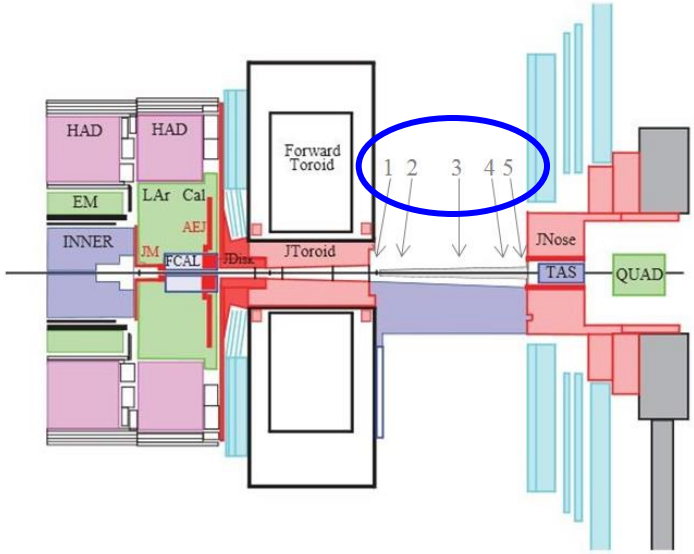
Application – *LHC present situation (1)*

Comparison calculation vs. measurement for ATLAS

Courtesy: C.Urscheler et al.



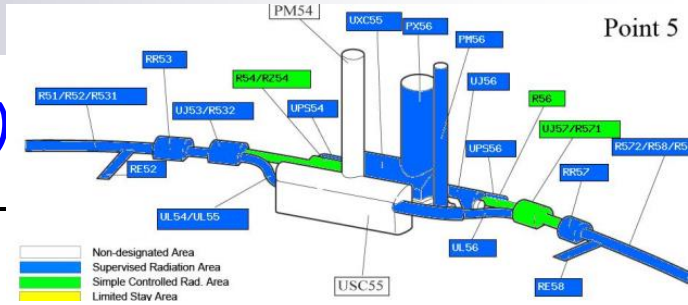




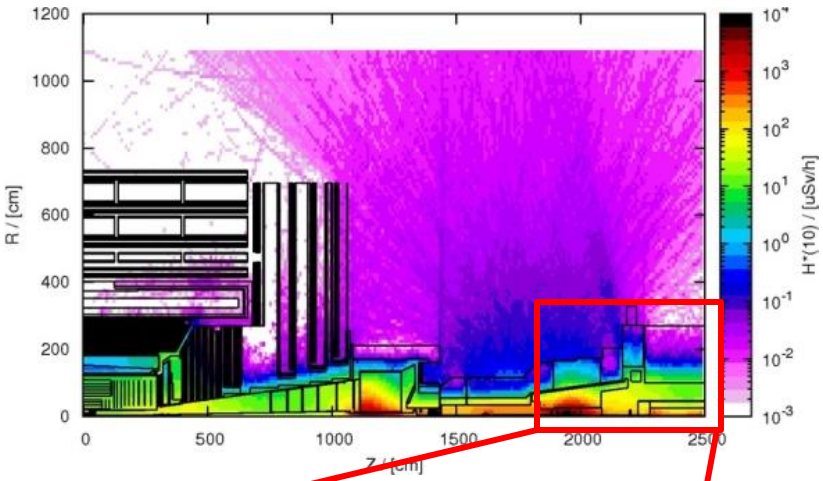
Location	Measurement [μSv/h]	FLUKA [μSv/h]
1	19	13 (±0.3)
2	10	13 (±0.3)
3	7.2	10 (±0.2)
4	47	46 (± 0.5)
5	42	72 (± 0.5)

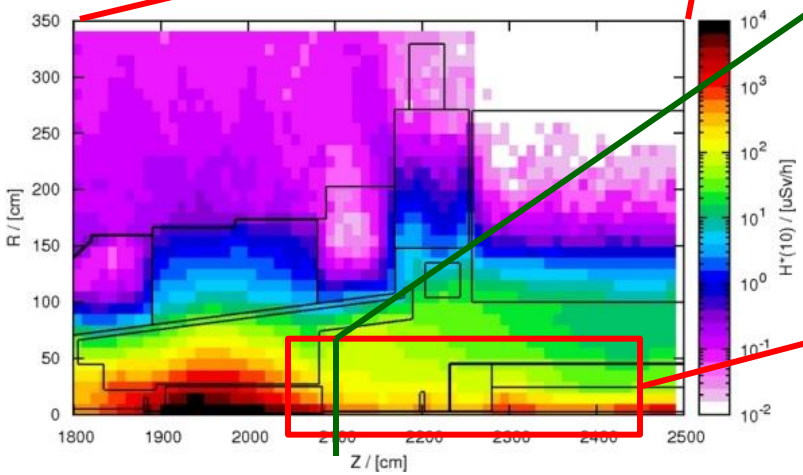
Application – *LHC present situation (2)*

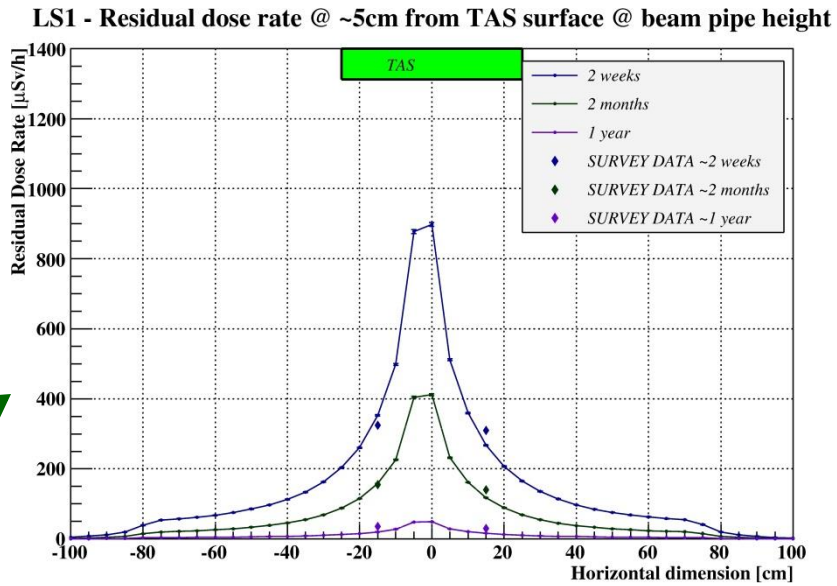
Comparison calculation vs. measurement for CMS

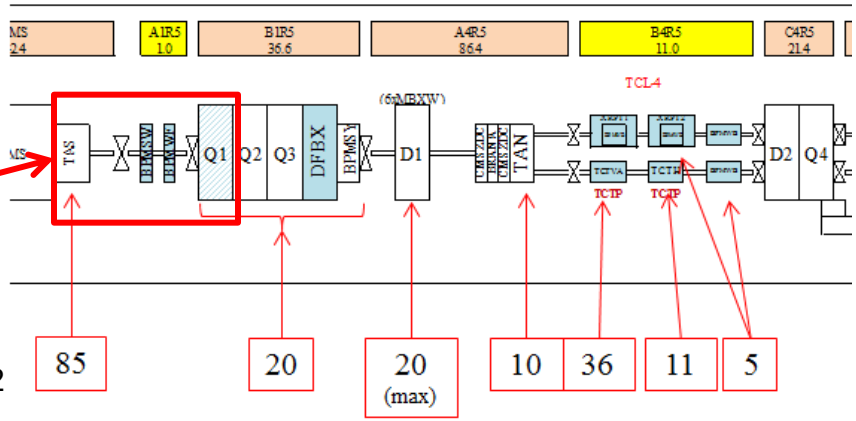


Courtesy: C.Urscheler et al.

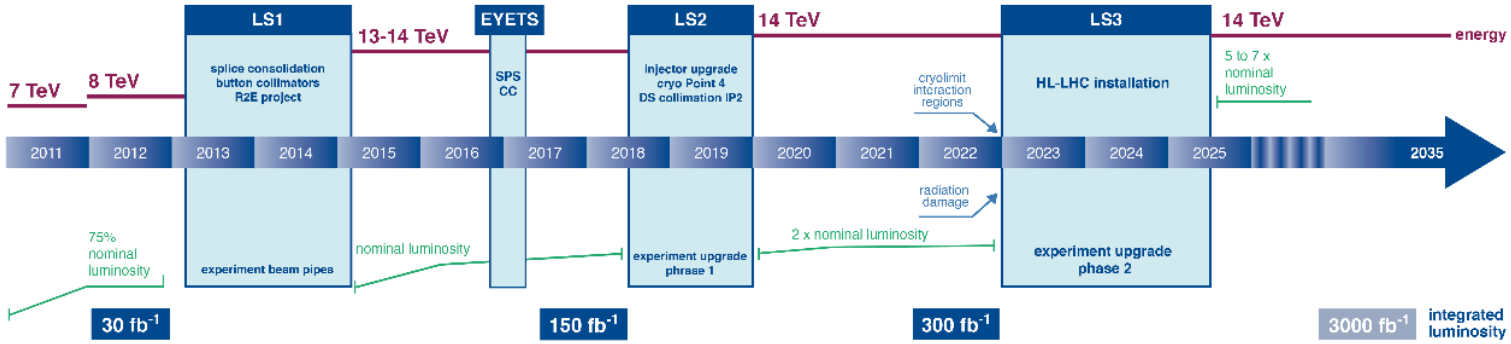


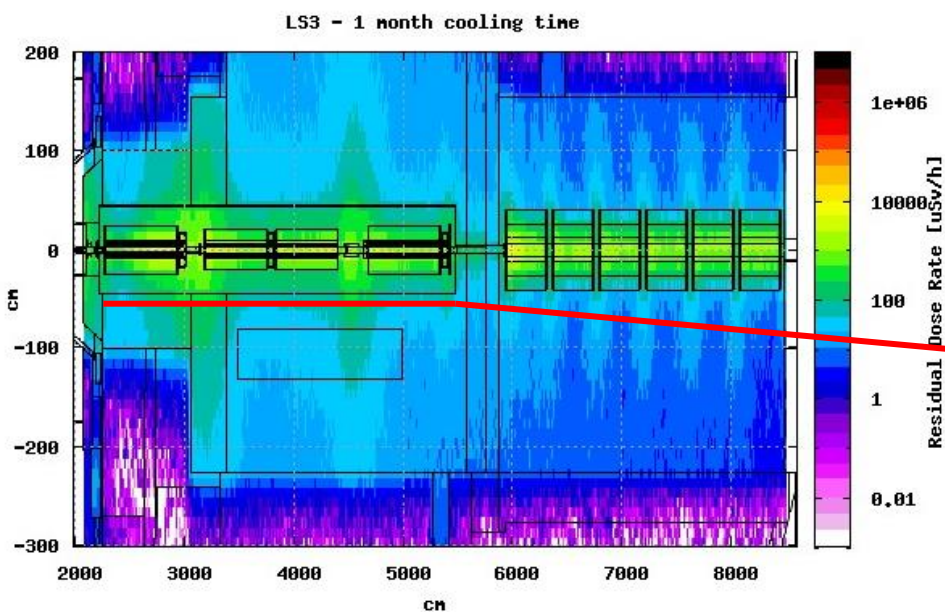


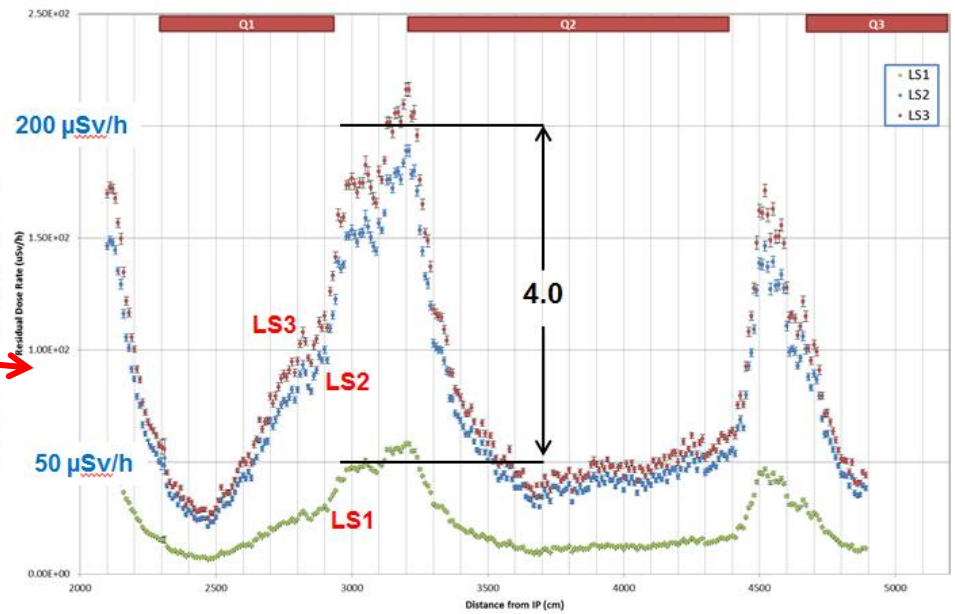




Application – *LHC dose rate evolution (1)*

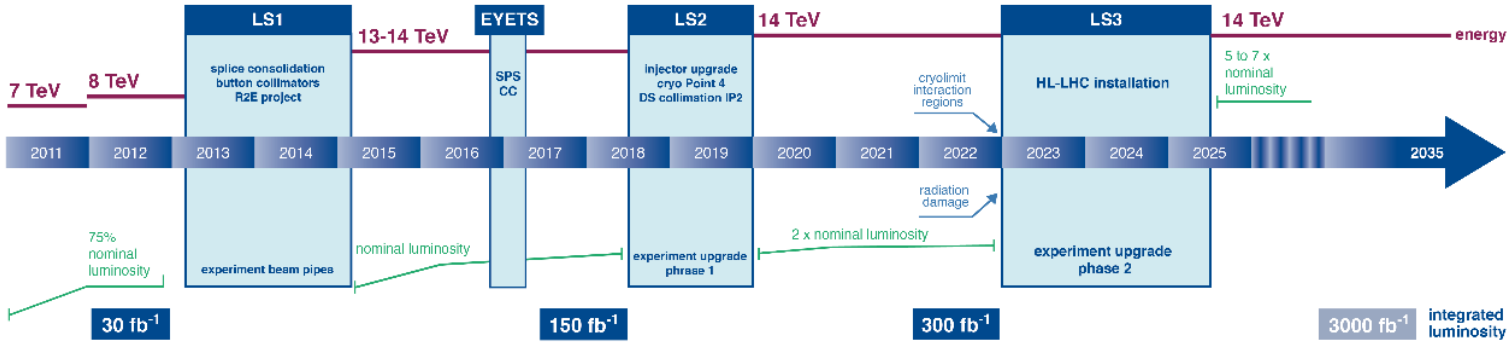


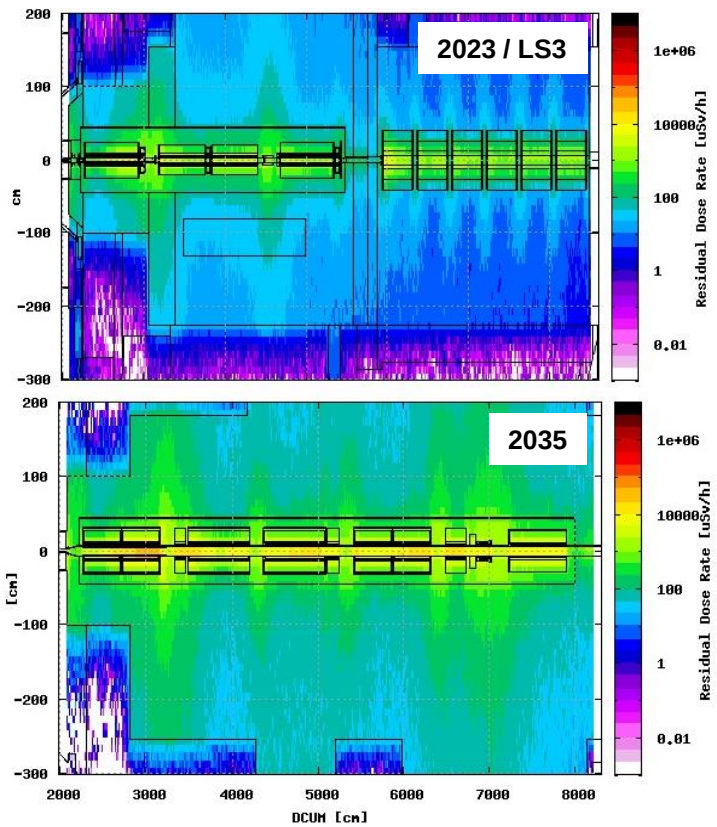


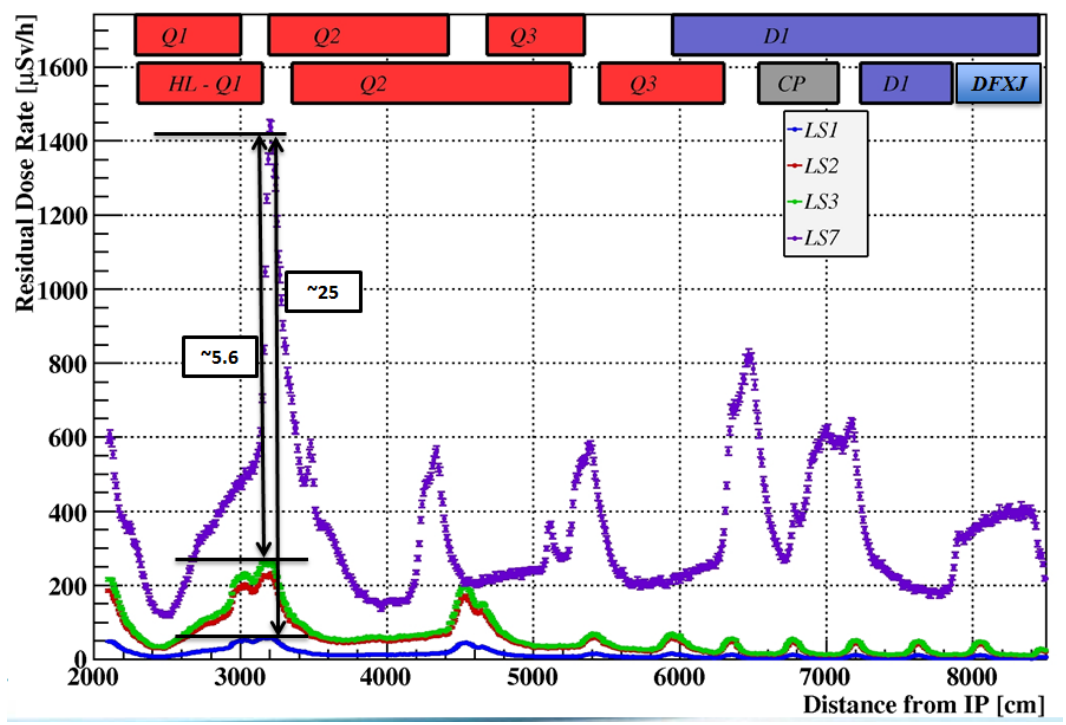


Courtesy: C.Adorisio

Application – *LHC dose rate evolution (2)*



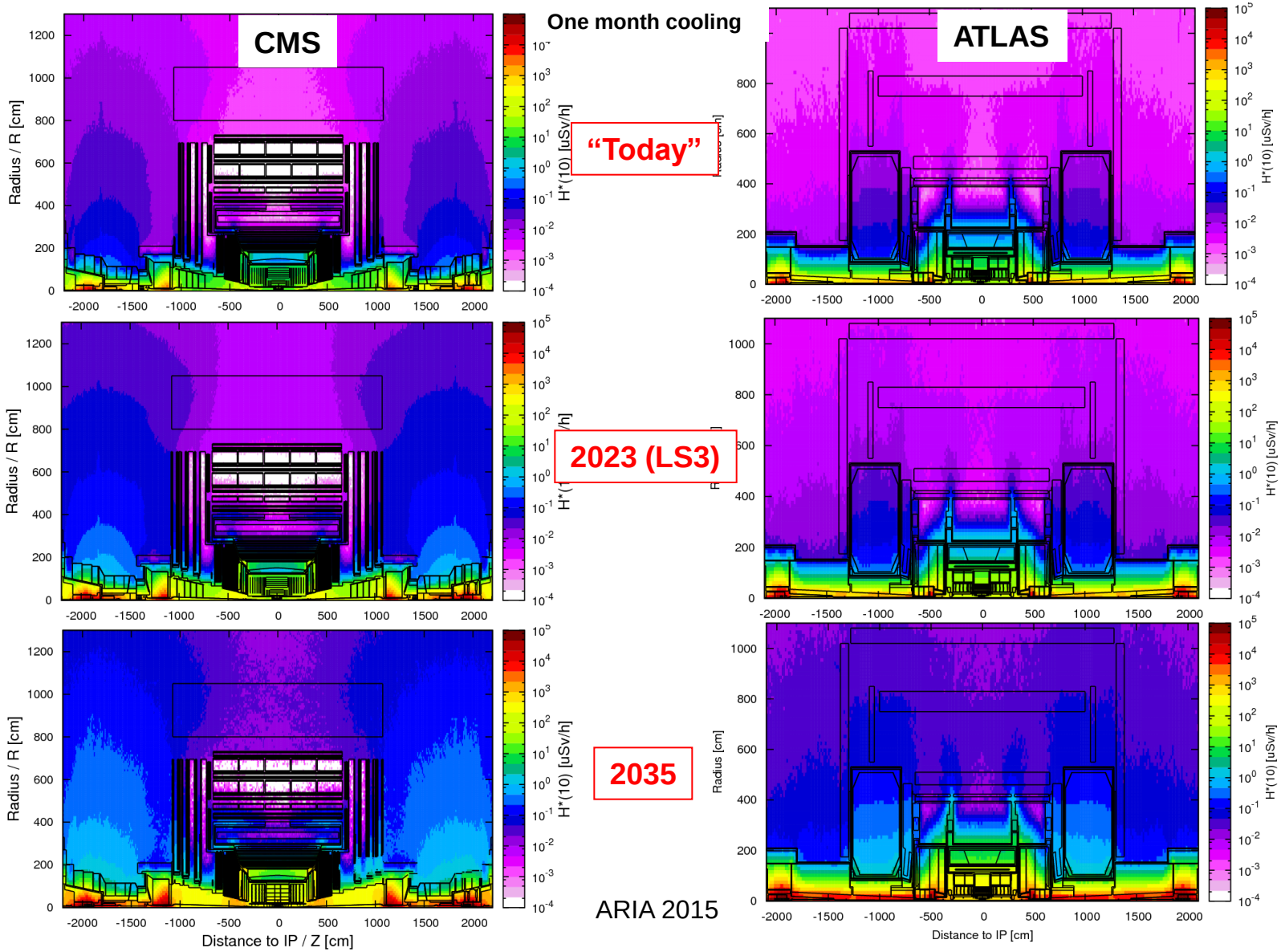




Courtesy: C.Adorisio

Application – *LHC dose rate evolution (3)*

Courtesy: I.Bergstrom and K. Zabrzycki



(Future) application… – *Future Circular Collider at 100TeV*

Alignment | **Shaft Tools**

Choose alignment option

100km quasi-circular

Tunnel depth at centre: 263mASL

Gradient Parameters

Azimuth (°): -20

Slope Angle x-x(%): .65

Slope Angle y-y(%): 0

CALCULATE

Alignment centre

X: 2500119 Y: 1108575

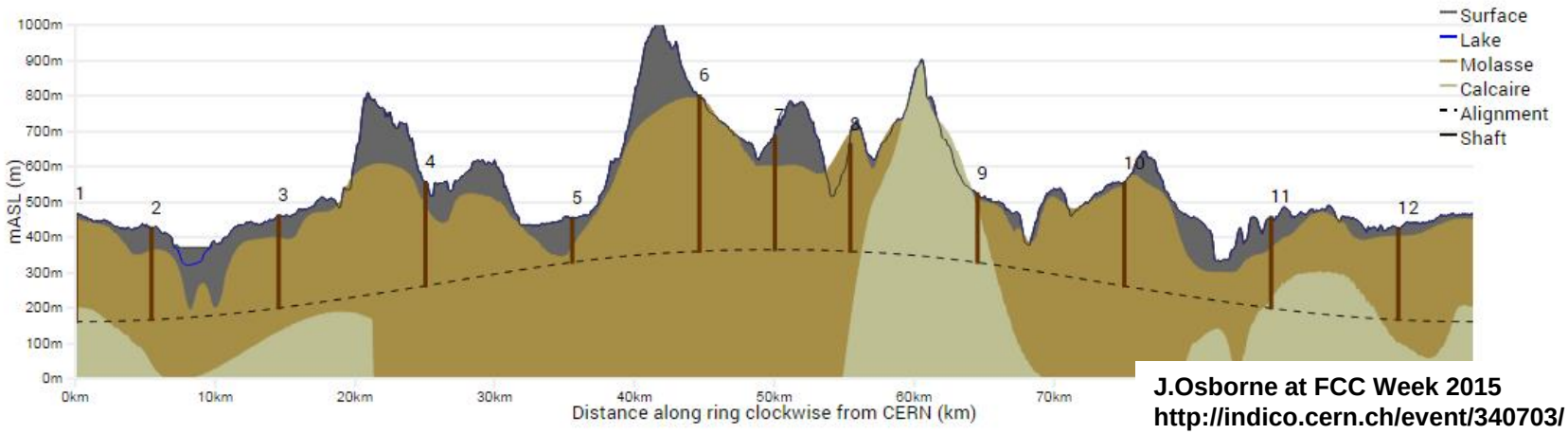
LHC Intersection	IP 1	IP 2
Angle	-65°	65°
Depth	221m	180m

Alignment Location

Geology Intersected by Shafts | **Shaft Depths**

Shaft	Shaft Depth (m) Actual	Min	Mean	Max	Geology (m) Moraine	Molasse	Calcaire
1	304	303	305	306	16	248	40
2	260	260	263	271	65	195	0
3	261	249	258	262	62	199	0
4	293	269	296	322	64	229	0
5	125	124	127	129	85	40	0
6	440	432	441	451	10	431	0
7	321	302	332	368	85	235	0
8	302	235	304	358	0	333	0
9	195	184	195	204	15	18	161
10	291	289	296	307	7	285	0
11	257	247	252	257	89	149	19
12	259	258	262	266	23	236	0
Total	3309	3152	3331	3501	521	2597	220

Alignment Profile



J.Osborne at FCC Week 2015
http://indico.cern.ch/event/340703/

Summary

- FLUKA continues to provide unique features for activation studies
- Recent improvements include
  - Extension of energy range at which detailed nuclear model (Peanut) is used
  - Use of evaluated isomer production cross sections for low-energy neutron reactions
  - (Re)interactions of light nuclei
  - Geometry modifications between simulation of activity production and decay
- The code is being used extensively for all radiological studies at the LHC
  - Best adapted: direct link to DPMJET-III, used since first days of design, very convenient for residual dose rate assessments (one-step calculations!), extensively benchmarked, well-known to authorities..
  - Comparison of FLUKA predictions with measurements for highly non-trivial setups (like an LHC experiment) show remarkable agreement
  - Now applied to design the LHC Upgrade and predict evolution of radiological quantities for the next two decades of LHC operation