Materials

Advanced FLUKA Course

Materials under irradiation

- The prediction of the structural damage to materials under irradiation is essential to evaluate consequences due to long term employment of construction materials in nuclear reactors and charged particle accelerators.
- There are several effects and quantities that are important for studying the material behavior under irradiation and FLUKA is capable in predicting several of them:
  - Heating total energy deposition
    → could be used for temperature rise, stresses, deformations …
  - Energy deposition due to EMF → radiolysis calculations …
  - Dose calculation → medical applications …
  - Gas production
  - Non Ionizing Energy Losses (NIEL)
  - Displacement per Atoms (dpa)

  → material damage …
  - Silicon 1MeV Neutron Equivalent (Si1MeVEq)
  - Single Event Upsets to electronics (SEU)

  → electronics

For all the above you need to input the proper MATERIAL properties

Material definition

Single-element material definition

	atomic number Z	atomic weight	density (g/cm³)	material number	Alternate material to use for dE/dx	mass number (A)	name
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+...							
MATERIAL	24.0	51.9961	7.18	26.0	0.0	0.0	CHROMIUM

MATERIAL	Name: PHOSPHO	#	ρ: 2.2
Z: 15	Am: 30.973761	A:	dE/dx:

Notes:

- if $\rho<0.01$: gas (default: at atmospheric pressure)
- Atomic Weight is **calculated by the code** using the internal database
  → it is better to leave empty
- Material number use it **ONLY** if you want to **override** a predefined one
- Mass Number to define specific **ISOTOPES**
  Do not confuse with the Atomic weight
- Choose a name corresponding to the **LOW-ENERGY neutron database**
  Section 10.4 in the manual

Predefined ICRU materials

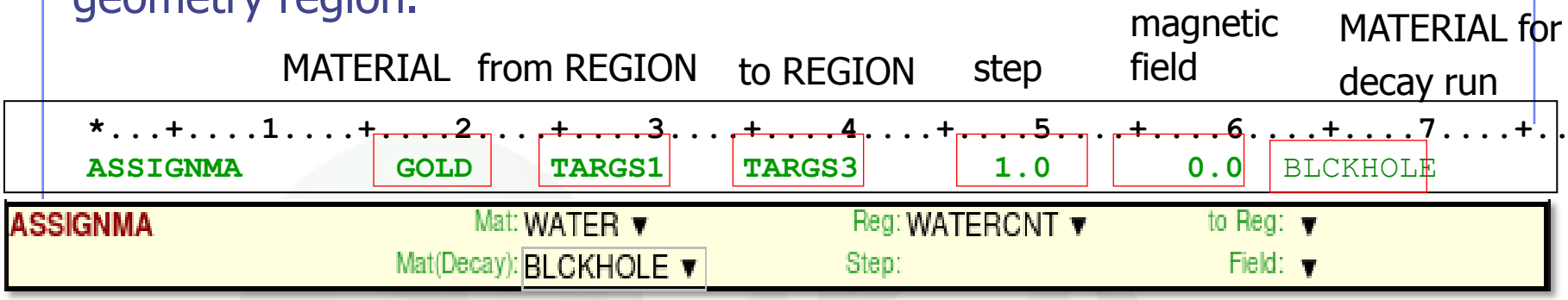
In the new version of FLUKA, the code contains several predefined materials with the composition suggested by ICRU

FLUKA	Material	FLUKA	Material
AIR	Dry air 20°C	BONECOMP	Compact bone
WATER	Water	BONECORT	Cortical bone
POLYSTYR	Polystyrene	MUSCLESK	Skeletal muscle
PMMA	Polymethyl methacrylate	MUSCLEST	Striated muscle
POLYETHY	Polyethylene	ADTISSUE	Adipose tissue
PLASCINT	Plastic scintilator	KAPTON	Kapton

- The materials can be used WITHOUT the need of an explicit MATERIAL / COMPOUND cards
- If the user defines a MATERIAL card in the input with the same name as the predefined ones IT WILL OVERRIDE THE PREDEFINED.

Material Assignment

A (single-element or compound) material is assigned to each geometry region.



In the new version of FLUKA:

- WHAT(5) is controlling the magnetic & electric field for the prompt and radioactive decay product transport
- WHAT(6) is permitting to assign a different material for the radioactive decay product transport.
  Only **VACUUM** and **BLCKHOLE** are allowed

MAT-PROP

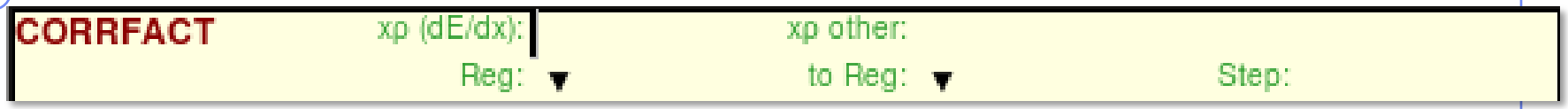
- Supply extra information on gaseous materials (pressure)
- Create materials with fictitious or effective density
- Override the default ionization potential

- Set the DPA energy damage threshold (WARNING in eV)

- Enable the call to USRMED routine when a particle enters in the desired materials

There is a last option (sdum=LOWNTEMP) to change the material temperature for the neutron treatment at thermal energies.
HOWEVER ***it cannot be applied with the new library with 260 groups***

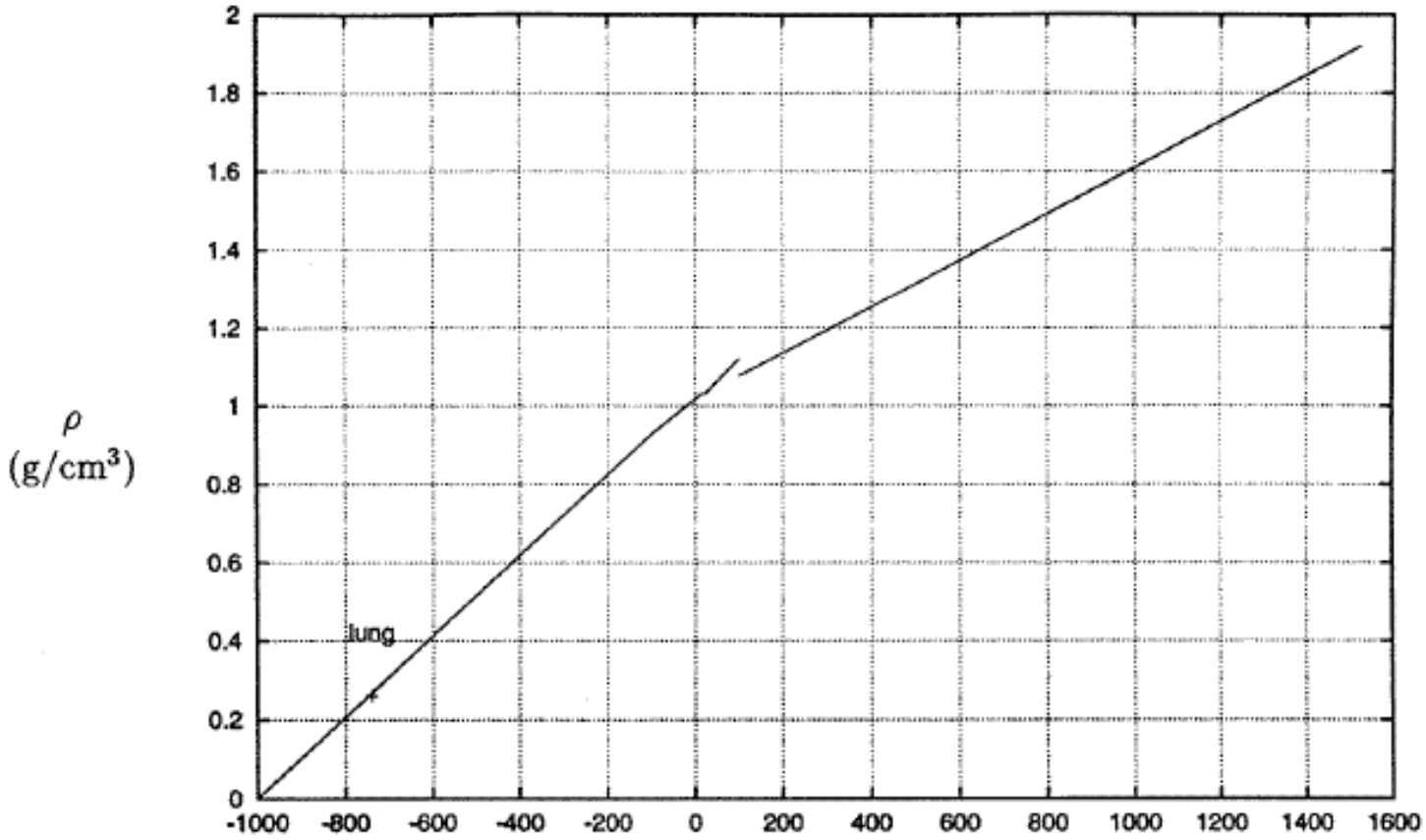
CORRFACT: Region dependent – 1



- CORRFACT card allows to alter material density for dE/dx and nuclear processes
- First two inputs specify a density scaling factor (restricted to the interval [2/3,3/2]) for charged particle ionization processes (WHAT(1)) and for all other processes (WHAT(2)) to the region(s) specified by the inputs WHAT(4-6)
- This is especially important in ion beam therapy to force the MC to follow the same semi-empirical Hounsfield Units-range calibration curve as the Treatment Planning System (TPS) for dosimetric comparisons.
- Typically, a user has to deal with a CT stoichiometric calibration, i.e. a segmentation of the CT scan (expressed in Hounsfield units (HU)) into materials of defined elemental composition (for example Schneider *et al* 45 2000).

CORRFACT: Region dependent – 2

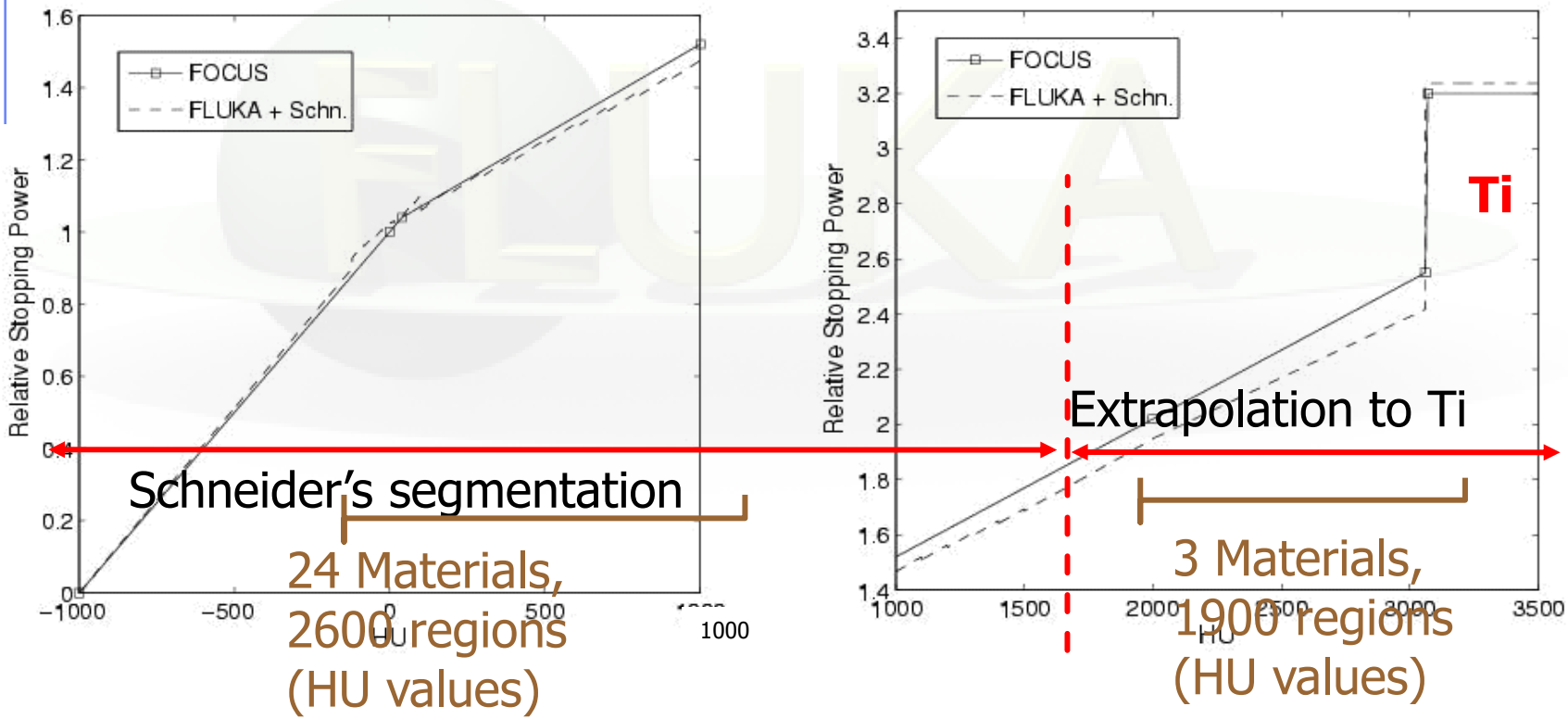
- A "nominal density", e.g., using the density at the center of each HU interval (Jiang et al MP 2004) is assigned to each material. But "real density" (and related physical quantities) varies continuously with HU values.



Schneider et al PMB 45 2000

Forcing FLUKA to follow the same range calibration curve as TPS for protons @ MGH

The CORRFACT ionization scaling factors (WHAT(2) in the CORRFACT card) were obtained from the ratio between TPS and FLUKA (+Schneider et al “mass” density)



Parodi et al MP 34, 2007, Parodi et PMB 52, 2007

STERNHEIme card

- Below the δ-ray threshold, energy losses are treated as "continuous", with some special features:
  - Fluctuations of energy loss are simulated with a FLUKA-specific algorithm
  - The energy dependence of cross sections and dE/dx is taken into account exactly
  - Latest recommended values of ionization potential and density effect parameters implemented for elements (Sternheimer, Berger & Seltzer), but can be overridden by the user with (set yourself for compounds!) the

STERNHEI C X0 X1 a m δ0 MAT

- In addition, the card MAT-PROP can be used a to override the value of the average ionization potential used by the program

MAT-PROP Gasp Rhosc Iion Mat1 Mat2 Step

dpa: Displacements Per Atom

- Is a measure of the amount of radiation damage in irradiated materials
  For example, 3 dpa means each atom in the material has been displaced from its site within the structural lattice of the material an average of 3 times
- Displacement damage can be induced by all particles produced in the hadronic cascade, including high energy photons.
  The latter, however, have to initiate a reaction producing charged particles, neutrons or ions.
- The dpa quantity is directly related with the total number of defects (or Frenkel pairs)

$$dpa = \frac{1}{\rho} \sum_i N_i N_F^i$$

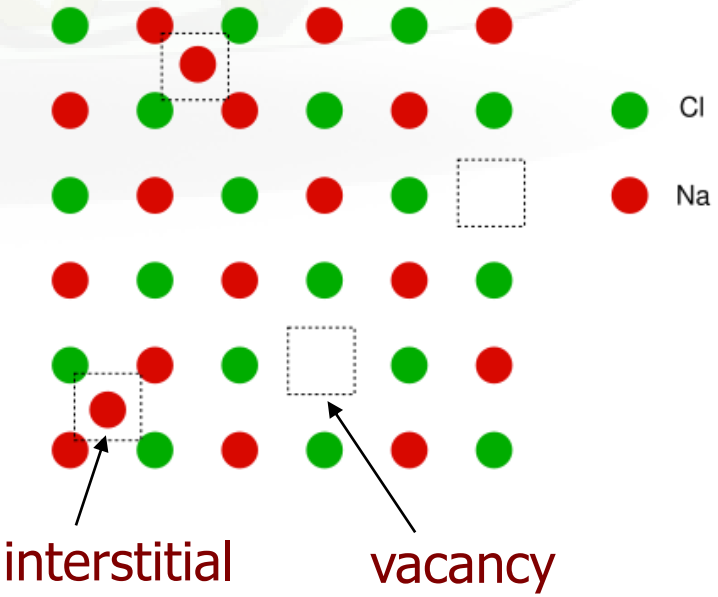
ρ atoms/cm^3
N_i particles per interaction channel i
N_f^i Frenkel pairs per channel

Frenkel pairs

- Frenkel pairs N_F (defect or disorder), is a compound crystallographic defect in which an interstitial lies near the vacancy. A Frenkel defect forms when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial)

$$N_{NRT} \equiv N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

N_{NRT}	Defects by Norgert, Robinson and Torrens
κ=0.8	is the displacement efficiency
T	kinetic energy of the primary knock-on atom (PKA)
$\xi(T)$	partition function (LSS theory)
$\xi(T)$ T	directly related to the NIEL (non ionizing energy loss)
E_{th}	damage threshold energy



E_{th} Damage Threshold Energy

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

- E_{th} is the value of the threshold displacement energy averaged over all crystallographic directions or a minimum energy to produce a defect

Element	Eth (eV)	Element	Eth (eV)
Lithium	10	Co	40
C in SiC	20	Ni	40
Graphite	30..35	Cu	40
Al	27	Nb	40
Si	25	Mo	60
Mn	40	W	90
Fe	40	Pb	25

Typical values used in NJOY99 code

- FLUKA way

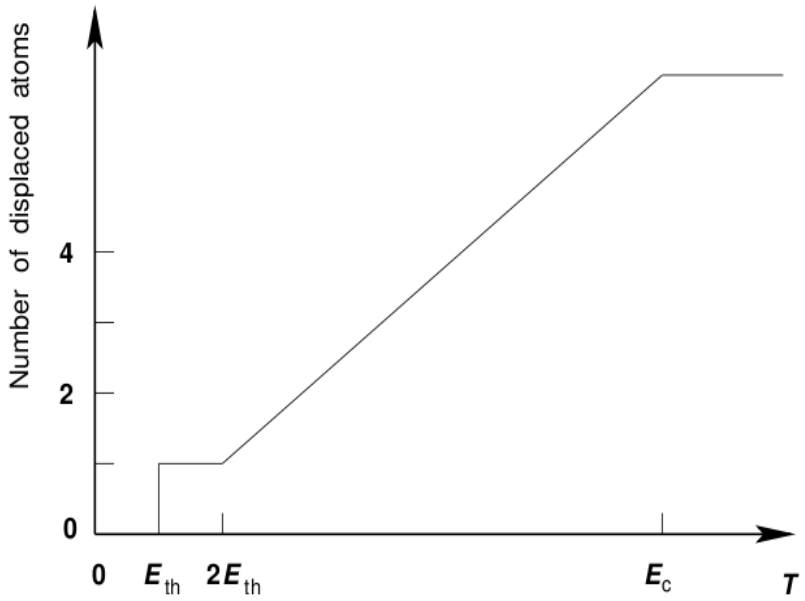
MAT-PROP *WHAT(1)* = E_{th} (eV)
WHAT(4,5,6) = Material range
SDUM = **DPA-ENER**

Factor of 2 (Kinchin & Pease)

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

- The cascade is created by a sequence of two-body elastic collisions between atoms
- In the collision process, the energy transferred to the lattice is zero
- For all energies $T < E_c$ electronic stopping is ignored and only atomic collisions take place. No additional displacement occur above the cut-off energy E_c
- The energy transfer cross section is given by the hard-sphere model.

$v(T)=0$ for $0<T< E_{th}$ (phonons)
$v(T)=1$ for $E_{th}<T<2E_{th}$
$v(T)=T/2E_{th}$ for $2E_{th}<T<E_c$
$v(T)=E_c/2E_{th}$ for $T > E_c$



Schematic relation between the number of displaced atoms in the cascade and the kinetic energy T of the primary knock-on atom

Energy is equally shared between two atoms after the first collision
Compensates for the energy lost to sub threshold reactions

κ displacement efficiency

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

- κ=0.8 value deviates from the hard sphere model (K&P), and compensates for the forward scattering in the displacement cascade
- The displacement efficiency κ can be considered as independent of T only in the range of T≤1–2 keV. At higher energies, the development of collision cascades results in defect migration and recombination of Frenkel pairs due to overlapping of different branches of a cascade which translates into a decrease of κ(T).
- From molecular dynamics (MD) simulations of the primary cascade the number of surviving displacements, N_{MD}, normalized to the number of those from NRT model, N_{NRT}, decreases down to the values about 0.2–0.3 at T≈20–100 keV. The efficiency in question only slightly depends on atomic number Z and the temperature. N_{MD}/N_{NRT} = 0.3–1.3

$$N_{MD} / N_{NRT} = 0.3\text{–}1.3\left(-\frac{9.57}{X}+\frac{17.1}{X^{4/3}}-\frac{8.81}{X^{5/3}}\right)$$

where X ≡ 20 T (in keV).

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

Lindhard partition function ξ [1/3]

- The partition function gives the fraction of stopping power S that goes to NIEL

$$\xi(T) = \frac{S_n}{S} \quad \text{where} \quad S = \frac{dE}{dx} = \frac{dE_n}{dx} + \frac{dE_e}{dx} = S_n + S_e$$

- Lindhard, Robinson assumption:

  The incident particle has energy E, and due to the interactions during the slowing down the energy is transferred to atoms E_n and to electrons E_e $\qquad E = E_e + E_n$

The equation that has to be satisfied is

$$\int d\sigma_{ne} \left[E_n\left(E - T_n - \sum_i T_{ei} \right) - E_n(E) + E_n(T_n - U) + \sum_i E_{ne}(T_{ei} - I_i) \right] = 0$$

where $d\sigma_{n,e}$ are the differential cross-sections corresponding to particle scattering on nuclei and electrons, $T_n(T_{ei})$ energy transfer to nuclei (electrons), U energy in atomic(lattice) binding, I_i ionization energies

Lindhard partition function ξ [2/3]

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

- Approximations used: Electrons do not produce recoil nuclei with appreciable energy, lattice binding energy is neglected, etc...

$$(S_n + S_e)E_n'(E) = \int E_n(T)\frac{d\sigma_n}{dT}dT$$

where

$$S_{n\ell}(E) = \int T_{n\ell}\, d\sigma_{n\ell}$$

- approximated to

$$\xi(T) = \frac{1}{1 + F_L \cdot \left(3.4008 \cdot \varepsilon(T)^{1/6} + 0.40244 \cdot \varepsilon(T)^{3/4} + \varepsilon(T)\right)}$$

$$F_L = 30.724 \cdot Z_1 \cdot Z_2 \sqrt{Z_1^{2/3} + Z_2^{2/3}}$$

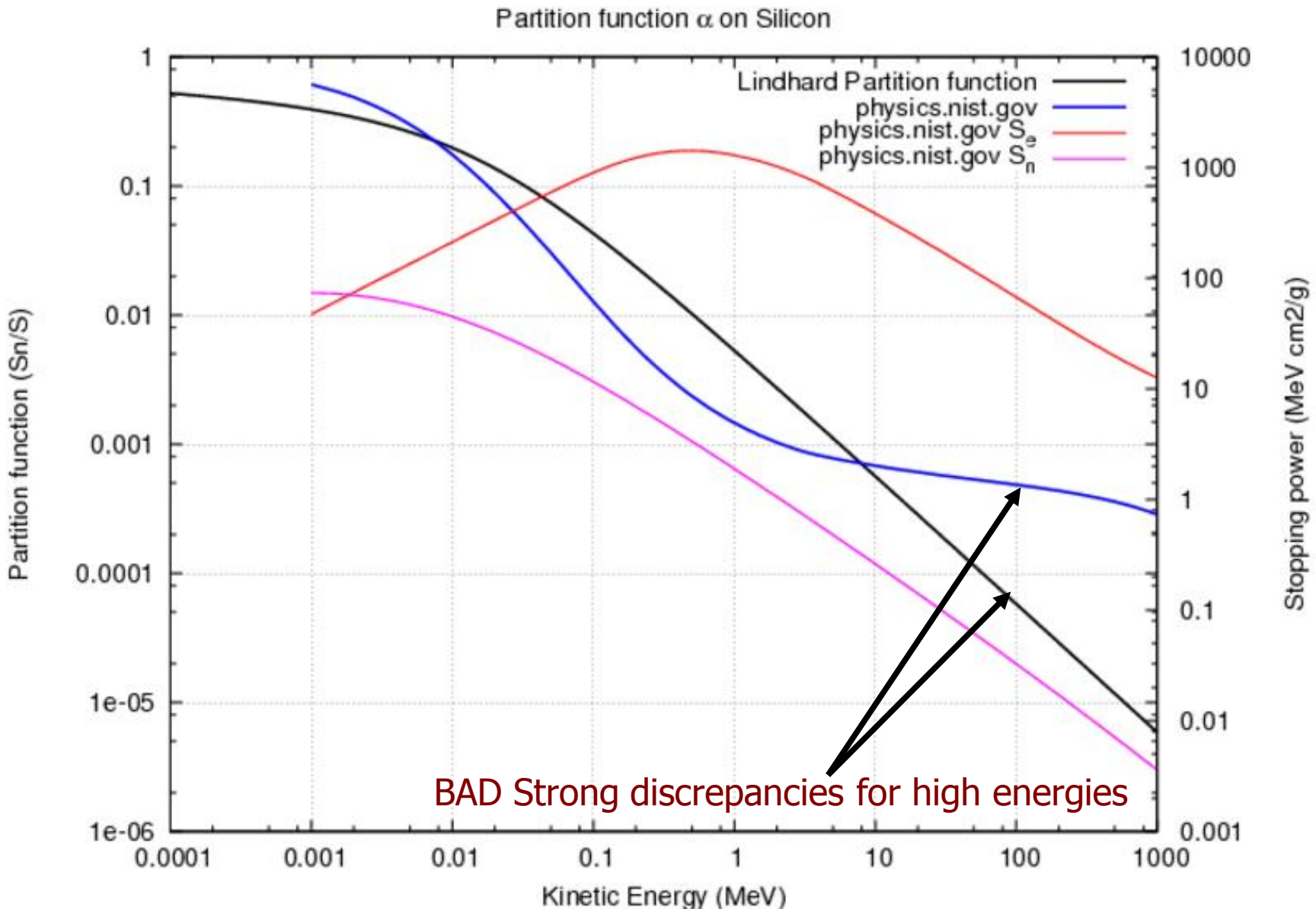
$$\varepsilon(T) = \frac{T}{0.0793 \frac{Z_1^{2/3} \cdot \sqrt{Z_2}}{\left(Z_1^{2/3} + Z_2^{2/3}\right)^{3/4}} \cdot \frac{(A_1 + A_2)^{3/2}}{A_1^{3/2}\sqrt{A_2}}}$$

Z,A	charge and mass
1	projectile
2	medium
T	recoil energy (eV)

Nice feature: It can handle any projectile Z_1,A_1 whichever charged particle

Lindhard partition function ξ [3/3]

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$



Restricted Nuclear Stopping Power

- Lindhard approximation uses the unrestricted NIEL. Including all the energy losses also those below the threshold E_{th}
- FLUKA is using a more accurate way by employing the restricted nuclear losses

$$S(E,E_{th}) = N\int_{E_{th}}^{\gamma E} T\left(\frac{d\sigma}{dT}\right)dT$$

where:

$S(E,E_{th})$	is the restricted energy loss
N	atomic density
T	energy transfer during ion-solid interaction
$d\sigma/dT$	differential scattering cross section

$$\gamma = \frac{4M_1M_2}{(M_1+M_2)^2}$$ maximum fraction of energy transfer during collision

FLUKA Implementation [1/2]

Charged particles and heavy ions

- **During Interactions**
  - ✔ For all charged particles and Heavy Ions, calculate the recoil. Use recoil as a normal particle

- **During transport**
  - ✔ Calculate the restricted and unrestricted nuclear stopping power for the average energy at the middle of the step with calls to DEDXNU and SNRDFR and add it to TKNIEL and TKEDPA global variables
  - ✘ For electrons Bremsstrahlung, sample randomly a recoil energy from the distribution of the recoils (uncorrelated with the event) Treat the recoil as a normal particle (*work on progress*)

- ✔ **Below threshold**
  - Calculate the TKNIEL(=TKEDPA) by using the Lindhard partition function

FLUKA Implementation [2/2]

Neutrons

- **High energy E_n>20 MeV**
  - ✔ Like CP, calculate the recoil.
    Treat recoil as a normal particle

- **Low energy E_n≤20 MeV (group-wise)**
  - ✔ Calculate the NIEL from NJOY, then add it to TKNIEL and TKEDPA global variables

- **Low energy E_n≤20 MeV (point-wise, where available)**
  - ✔ Calculate the recoil if possible
    Treat the recoil as a normal particle

Photons

- ✘ Pair production, sample randomly a recoil for a distribution (uncorrelated with the event) Treat the recoil as a normal particle

dpa: Recipe

FLUKA is using a more accurate treatment during the particle transport. While below the transport threshold is employing the Lindhard approximation with the NRT model, it is strongly advisable to use as low thresholds as possible:

Thresholds:

- All Hadrons 1 keV
- Neutrons down to thermal (10^{-14} GeV)
- Leptons 50-100 keV would be ok

Material Damage:

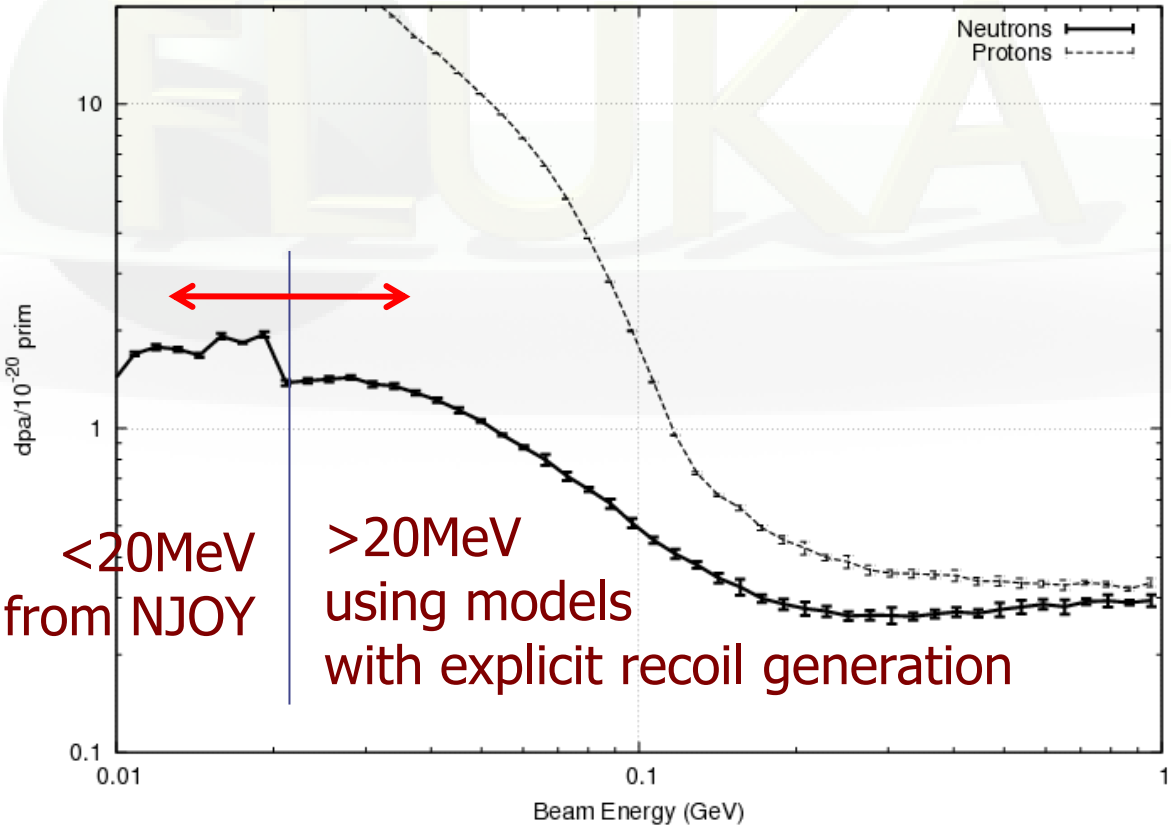
Set with MAT-PROP the damage threshold for all materials under consideration. All other will use the default of 30 eV!!!!

Scoring:

Use USRBIN with DPA-SCO or NIEL

dpa: Limitations

- Due to the group treatment of low-energy neutrons, there is no direct way to calculate individual recoils at each interaction.
- Therefore the evaluation is based on the NIEL factors calculated by NJOY, which in turn is based on the Unrestricted Nuclear losses from using the NRT model.



<20MeV
using NRT from NJOY

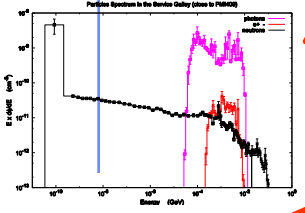
>20MeV
using models
with explicit recoil generation

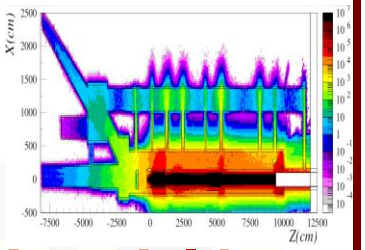
Main Radiation Effects on Electronics

Category		Effect
Single Event effects (Random in time)	***Single Event Upset (SEU)***	Memory bit flip (soft error) Temporary functional failure
	Single Event Latchup (SEL)	Abnormal high current state Permanent/destructive if not protected
Cumulative effects (Long term)	***Total Ionizing Dose (TID)***	Charge build-up in oxide Threshold shift & increased leakage current Ultimately destructive
	Displacement damage	Atomic displacements Degradation over time Ultimately destructive

Radiation Physics/Effects/Monitoring

nuclear cascade





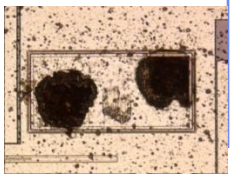
h > 20 MeV

Radiation Field

h, e,.. > 100 KeV

EM cascade

radiation damage in semiconductors



Single Events

Effect in the Device

Displacement

Dose

radiation monitor

SEU counter

Measurement

PIN Diodes

Radfet

Corresponding FLUKA Estimators

Category		Scales with simulated/measured quantity
Single Event effects (Random in time)	***Single Event Upset (SEU)***	High-energy hadron fluence (>20 MeV)* [cm-2]
	Single Event Latchup (SEL)	High-energy hadron fluence (>20 MeV)** [cm-2]
Cumulative effects (Long term)	***Total Ionizing Dose (TID)***	Ionizing Dose [GeV/g]
	Displacement damage	1 MeV neutron equivalent [cm-2] {NIEL}

* Reality is more complicated (*e.g.*, contribution of thermal neutrons)

** Energy threshold for inducing SEL is often other than 20 MeV (*e.g.*, 5-20MeV, see scoring lecture and discussion on future scoring possibility)

Main Sources of Radiation at Accelerators

Losses

- Collimators and collimator like objects , Dumps
- Scales with beam intensity

Collisions

- In experimental areas
- Scales with luminosity (collision rate)

Beam-gas

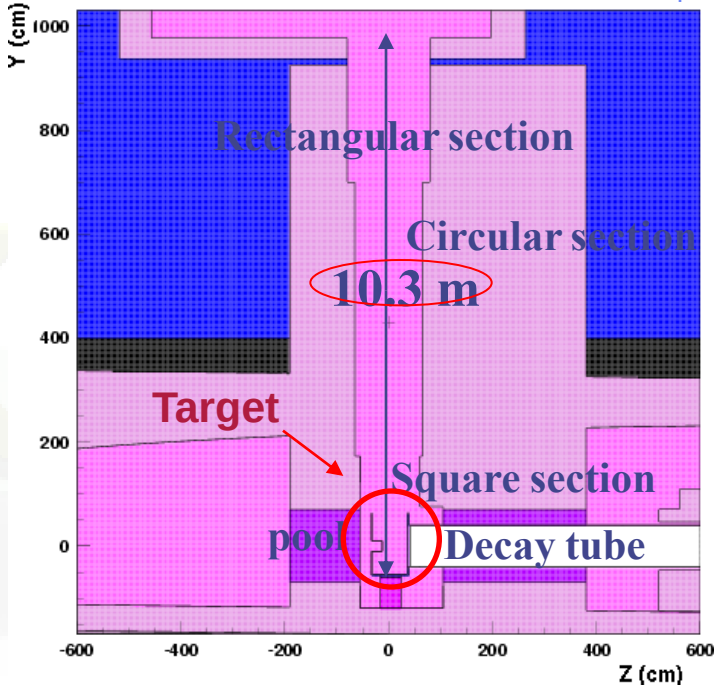
- All areas along the accelerator
- Scales with both intensity and residual gas density

n_ToF (old) target: Dose Rate Survey

Neutron Time-of-Flight facility at CERN-PS. It is underwent a major upgrade, including a new target.

Old target: 4 years of operation (≈$5 \cdot 10^{19}$ @ 20 GeV), 3 years of cooling. Checked for activation and results compared with simulations

Inside the pit: using a laser attached to the crane to control the position of the remote detector (attached to the hook)



Around the target: same method, starting at 3 meters distance & going towards the target surface.

(fully remote, thus possibility to wait & get enough statistics while performing continuous measurements)

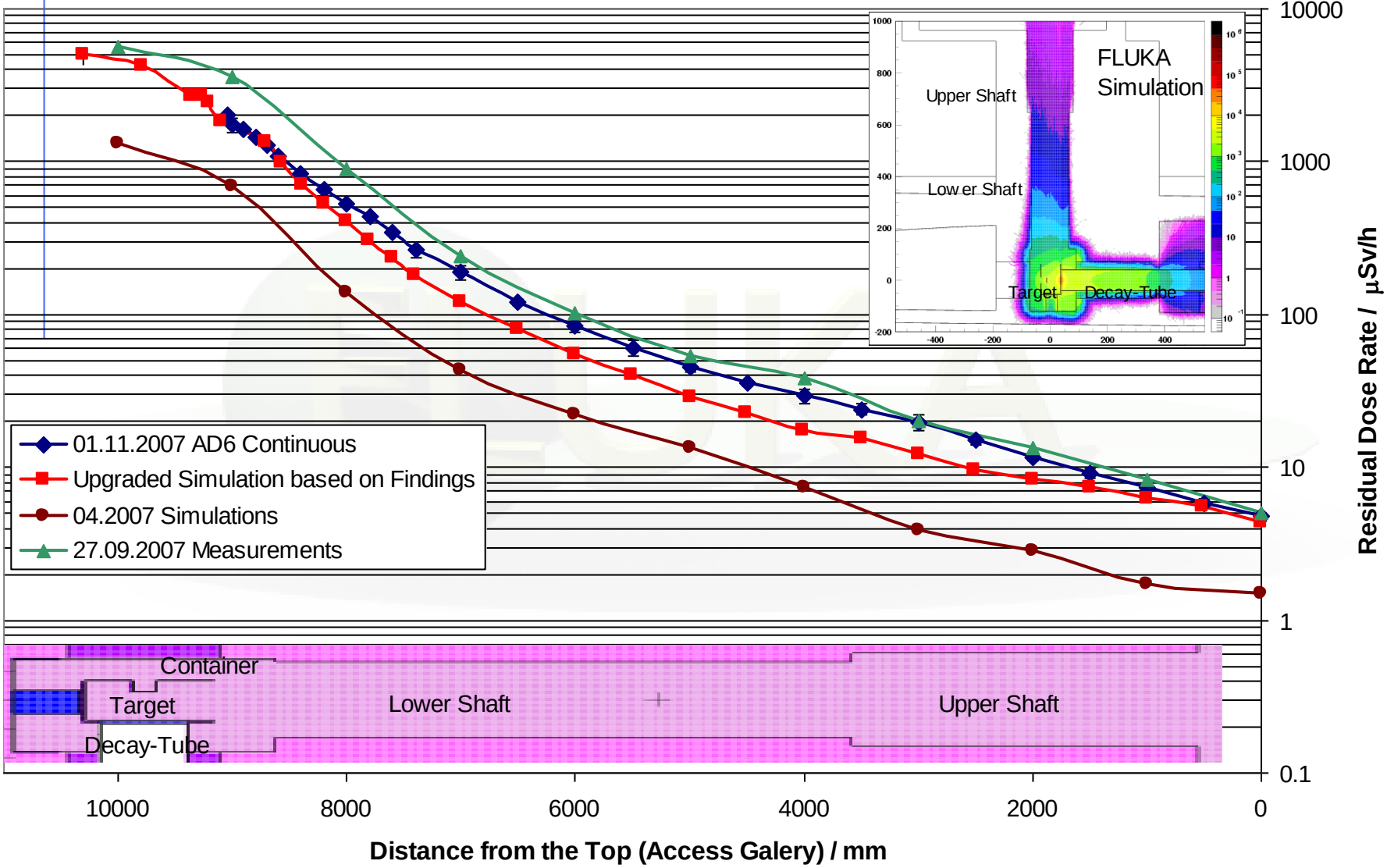
N_ToF target: Findings & Changes wrt the initial (dismaying) comparisons

- **Pit & Target**
  - update of geometry (container, support, 30cm, steel faces), in summary extra steel parts originally not included
- **Pit**
  - chemical composition of concrete and aluminium (open)
  - new survey with special dose rate meter and laser controlled distance $\Rightarrow$ more accurate measurements (and proof that contamination is a negligible contribution to residual dose rates)
- **Target**
  - detailed survey with ***special dose rate meter*** (up to a factor 2 difference with the initial measurements done in a hurry)
  - chemical composition ***stainless steel – cobalt content***
    - important influence on residual dose rate distribution (up to a factor of ***25*** in the possible concentration range)
    - a cobalt content of 0.1% results in a very good agreement with simulations (this concentration value is confirmed by existing steels at CERN)

PRELIMINARY

New FLUKA Comparison after Detailed Pit Survey Measurments 01.11.2007

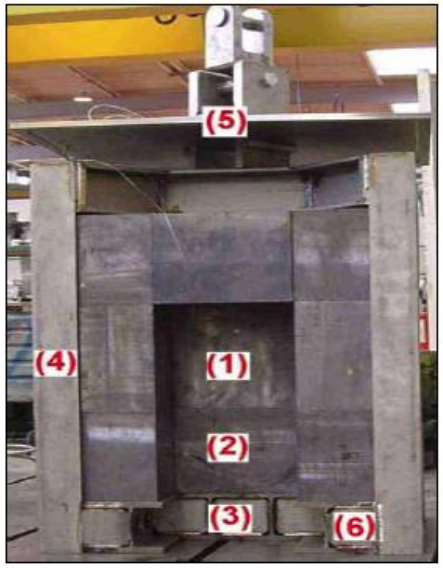
PRELIMINARY



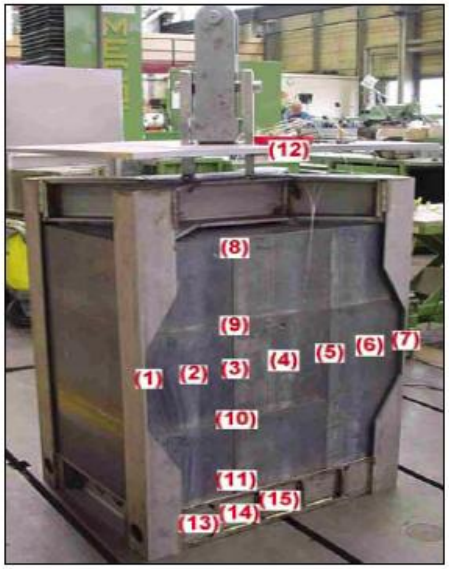
Residual Dose Rates at ~10cm

Location		1st FLUKA Simulations 04. 2007 [mSv/h]	Upgraded Simulations [mSv/h]		Measurement 27.09.2007 [mSv/h]	Ratio Measurement/FLUKA			
@ 10 cm	Point	Co1 [0.01%]	Co1 [0.01%]	Co4 [0.1%]	Oct. 2007	First	Co1 [0.01%]	Co4 [0.1%]	Main Material
Entrance	(1)	6.7	5.9	7.3	11	1.6	1.9	1.5	Pb
	(3)	3.6	5.8	51.8	52	14.4	9.0	1.0	SS
	(4)	2.1	1.7	14.8	21	10.0	12.4	1.4	SS/Pb
Exit	(3)	4.4	3.5	8.6	16	3.6	4.6	1.9	Pb/SS
	(14)	4.7	4.0	39.5	40	8.5	10.0	1.0	SS/Pb
Right	(1)	1.7	1.3	11.3	20	11.8	15.4	1.8	Pb -> SS!
	(5)	3.3	4.2	44.8	33	10.0	7.9	0.7	SS
Left	(1)	1.1	0.8	7.8	10	9.1	12.5	1.3	Pb -> SS!
	(3)	2.5	3.1	33.5	42	16.8	13.5	1.3	SS

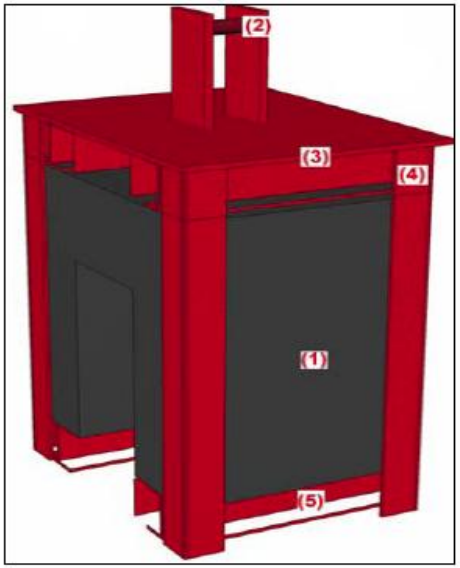
Entrance



Exit



Right



Left

Examples of steels used at CERN

- Cast No E33408, Nippon Steel, Inspection Certificate (F.Bertinelli, used for LHC)
- Density 7.252 g/cm^3

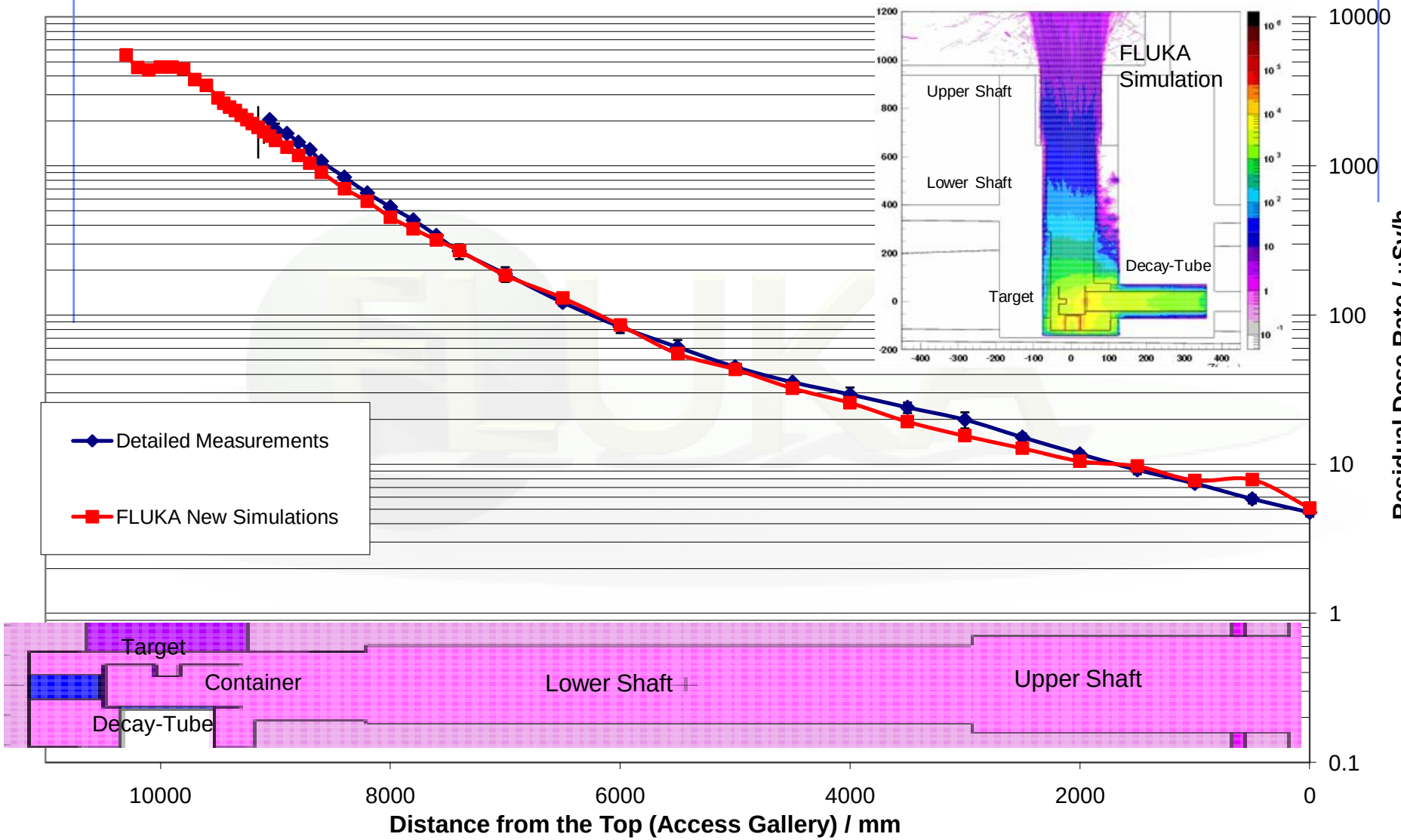
Isotope	CERN-Spec	EA	EMPA
Fe	63.31	63.96	62.823
C	0.09	0.1	0.094
Cr	17.82	17.54	18
Mn	11.4	11.28	11.6
N	0.3	0.32	nb
Ni	6.58	6.23	6.7
P	0.02	0.016	0.022
Si	0.38	0.37	0.39
Mo	0.1	0.09	0.08
S	-	0.001	< 0.001
Cu	-	0.09	0.08
O	-	0.002	nb
Ti	-	-	< 0.01
V	-	-	0.07
Co	-	-	0.11
Nb	-	-	0.01
W	-	-	0.01

- CERN store 44.57.10.420.4 SCEM: 44.57.10.420.4, INOX RNDS.304L
- Density 7.908 g/cm^3

Isotope	CERN-Spec	EIG
Fe		69.1924
Cr	17-20	18.62
Ni	10-12.5	8.32
C	< 0.03	-
Si	< 1	0.648
Mn	< 2	1.52
P	< 0.045	0.0302
S	< 0.03	0.037
Mo		0.567
Cu		0.393
Al		0.277
Co		0.172
V		0.0704
W		0.0407
Ca		0.0368
Na		0.033
Mg		0.0166
Sn		0.0147
Nb		0.0083
As		0.0029

EA: ICP-AES (AES=Atomic Emission Spectrometry)
EMPA: WD-XRF (wavelength-dispersive X-ray fluorescence spectrometry)
EIG: XRF

Measurement/FLUKA Comparison
after Detailed Pit Survey Measurements 01.11.2007



Oct 13th, 2008