



Displacement damage modelling with the FLUKA Monte Carlo code

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On behalf of the FLUKA.CERN Collaboration

RADSUM – Topical Workshop on RADiation effects in SUperconducting Magnets Jan 16, 2025 @ CERN



Outline

- Capabilities of the FLUKA particle transport code
- Condensed particle-history simulation
- Focus on radiation-damage-related quantities in FLUKA
- NIEL and DPA in FLUKA









An overview of the FLUKA particle transport code





The FLUKA particle transport code



https://fluka.cern

- Monte Carlo (MC) code for the <u>simulation</u> of coupled hadronic and electromagnetic particle showers in matter
- Born in the 1960s at CERN
- Actively developed and maintained by the FLUKA.CERN Collaboration (CERN + ELI ERIC)
- Standard tool at CERN for problems involving radiation-matter interaction in present and future colliders:
 - Targetry studies, beam intercepting devices, beam-loss assessments, radiation protection, radiation damage, radiation effects in electronics, etc.

- Serving a worldwide community of thousands of users working in:
 - Shielding, dosimetry, medical applications, space applications, etc
- User support and training:
 - <u>https://fluka-forum.web.cern.ch</u> <u>https://fluka.cern/support/courses-and-events</u>



https://doi.org/10.23732/CYRCP-2018-002.17 https://cds.cern.ch/record/1481554



FLUKA in a nutshell (overly simplified!)

• FLUKA handles the transport+interaction of:



 Rich physics engine with state-of-the-art modelling of all relevant radiation-matter interaction mechanisms:
 https://indico.cern.ch/event/1444491/timetable/#20241202 https://flukafiles.web.cern.ch/manual/chapters/guick_look.html



Photo- and lepto-nuclear interactions as well!

eli

E FLUKA

Secondary particle production (particle showers)

Radiation challenges for magnets in present and future colliders (HL-LHC, FCC, Muon Collider)	Anton Lechner
30/7-018 - Kjell Johnsen Auditorium, CERN	14:30 - 14:50

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MC workflow (1/3): geometry and material definition

- Combinatorial geometry, built from union/subtraction operations on basic geometrical bodies
- As of FLUKA v4-5.0 (Q1 2025), tetra-, penta-, and hexahedral unstructured meshes are supported
- <u>Materials in FLUKA are assumed</u> <u>homogeneous and isotropic</u>
- No coherent scattering effects in general
- (Ad-hoc account of molecular / crystalline binding environment for thermal neutrons, and channeling of positively charged particles in bent crystals)



See also the LineBuilder https://accelconf.web.cern.ch/ipac2012/papers/weppd071.pdf

MC workflow (2/3): source definition + particle history simulation

- Simulate a large ensemble of particle *random walks* according to the cross sections and mean free paths of all relevant interaction mechanisms (and decay where applicable)
- All particles are transported until they either exit the geometry, or their energy drops below a preset threshold

450 GeV/c proton beam loss







MC workflow (3/3): extract physical observables

- Every simulated particle history contributes to statistical estimators of relevant physical quantities requested by the user, featuring:
 - Particle fluences/currents in a volume or across a surface (differential in position, energy, angle, etc)
 - Energy deposition (heat, power, dose, ...)
 - Radionuclide inventories, including their time evolution in a single FLUKA run + associated protection quantities
 - <u>Damage-related quantities</u>: <u>NIEL</u>, Si 1-MeV-n equivalent fluence, <u>DPA-NRT, arc-DPA</u>
- NB: FLUKA contains built-in scoring capabilities for all of them, no coding involved, just an input-file option.
- <u>No on-line material degradation: every particle</u> <u>history sees the same new, pristine, ideal</u> <u>material</u>





FLUKA benchmarking and validation

https://doi.org/10.1051/epjconf/202328416006

EPJ Web of Conferences 284, 16006 (2023) ND2022

FLUKAVAL – A validation framework for the FLUKA radiation transport Monte Carlo code

Markus Widorski^{1,*}, Davide Bozzato^{1,2}, Robert Froeschl¹, and Vasiliki Kouskoura¹





- Dedicated workpackage (Code development support)
- Regular participation in code benchmarking campaigns, • among others within SATIF workshops



PHYSICAL REVIEW ACCELERATORS AND BEAMS 22, 071003 (2019)

Editors' Suggestion

Validation of energy deposition simulations for proton and heavy ion losses in the CERN Large Hadron Collider

A. Lechner,^{*} B. Auchmann,[†] T. Baer,[‡] C. Bahamonde Castro, R. Bruce, F. Cerutti, L. S. Esposito, et al.



FIG. 8. Geometry model of the LHC betatron cleaning insertion and the first superconducting magnets in the dispersion suppressors



Radiation hardness requirements for organic materials in magnets and radiation environments in muon colliders, FCC, ... Francesco Cerutti (tomorrow)



beam

20000

19950

19900

Flair – a one-stop shop for FLUKA simulations



https://flair.cern

- Advanced graphical user interface
- Allows users to edit/debug/render geometries, prepare the input file, set up the run (even in parallel / across cluster nodes), process results, plot physical observables
- FARM: Flair advanced render module





https://doi.org/10.1103/PhysRevAccelBeams.22.071003





https://indico.cern.ch/event/1444491/contributions/6234932/attachments/2977548/5241983/01 Introduction to FLUKA 2024 CERN.pdf



Displacement-damage modeling in FLUKA

FLUKA focuses not only on the description of radiation fields, but also on their effect in matter (within the approximations pointed out above)





Instantaneous effects and related quantities in FLUKA



Power density in Q2B magnet (mW/cm³)



- Power deposition (mW/cm³) \rightarrow local hot spots and SC magnet quench limits
- Total deposited energy \rightarrow Cryogenics constrains
- Accidental beam loss and consequences
- Single-event effects in electronics

•

See:





ISSI SRAM tester. Courtesy of G. Lerner.

Radiation challenges for magnets in present and future colliders (HL-LHC, FCC, Muon Collider)Anton Lechner30/7-018 - Kjell Johnsen Auditorium, CERN(yesterday)14:30 - 14:50





Cumulative effects

Total ionizing dose

- Affects chemical bonds
- Relevant for organic materials (insulators) TID [MGy]



Cylinders of alanine /polymer mixture $(\sim 4 \text{ cm length})$ From: M. Brugger

(see these talks tomorrow)

Daniele Calzolari

11:25 - 11:45

Magnet shielding design in present and future colliders	
30/7-018 - Kjell Johnsen Auditorium, CERN	

Radiation hardness requirements for organic materials in magnets and radiation environments in muon colliders. FCC... Francesco Cerutt

Gas production

- Production of H and He
- Correlated with production of "bubbles"/cracks in the material





- Primary knock-on atom (PKA) is transferred ٠ a recoil kinetic energy
- Cascade of ion-hole pairs ٠
- Recombination •
- Net displacement damage
- **Degradation of transport properties**



Fig. 1. T_c versus fluence for the same Nb₃Sn wires (#0904, PIT, Ta alloyed and #11976, RRP, Ti alloyed) after irradiation by high-energy protons (60 MeV and 24 GeV) [6] and neutrons (> 0.1 MeV) [4].



Fig. 2. T_c versus dpa, after replacing the fluence in Fig. 1 by the dpa values determined from the FLUKA code (see Table II).

http://dx.doi.org/10.1109/TASC.2016.2549858

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1.78

Relevant primary knock-on source: elastic scattering -

- Elastic scattering on the electrostatic potential:
 - Mostly small deflections, large cross section
 - Mean free paths O(nm-um)
- We can in general *not* afford to sample individual Coulomb scatterings in FLUKA*
- Instead, multiple Coulomb scattering theory (Molière) gives effective angular distribution after a macroscopic particle step
- Recoil: see next slide
- Elastic scattering on the **nuclear** potential:
 - Mostly large deflections, lower cross section
 - Mean free paths O(1-10) cm
 - Explicit recoil transport in FLUKA (if above threshold)



Computational Physics

Nuclear elastic scattering of protons below 250 MeV in FLUKA v4-4.0 and its role in single-event-upset production in electronics * https://doi.org/10.1016/i.cpc.2024.109276

Alexandra-Gabriela Şerban ^{a,b,c,*}, Andrea Coronetti ^a, Rubén García Alía ^a, Francesc Salvat Puiol ^a on behalf of the FLUKA-CERN Collaboration



• One-to-one correspondence between $\theta_{\rm CM}$ and recoil energy transfer T:

$$T = \frac{p_{CM}^2(1 - \cos \theta_{CM})}{m_t} \qquad \qquad \frac{d\sigma}{d\Omega} \to \frac{d\sigma}{dT}$$



Nuclear stopping power

- With a condensed-history approach, one loses the possiblity of an event-by-event explicit production of primary knock-on atoms (PKAs) from Coulomb scattering
- FLUKA accounts for the specific energy transfer to the material as a result of Coulomb scattering via the <u>nuclear stopping power</u>, (average energy loss per unit path length due to Coulomb scattering) for every charged particle species:



Not every T dislodges atoms: damage threshold energy

 Only recoil energies above the damage threshold E_d

(typically 10s of eV) dislodge the target ion from its lattice site (PKA)



<u>Considerable variation of *E_d* as a function of</u> lattice site, momentum-transfer direction, etc

Estimate	doi.org/10.10	<u>("A")</u> <i>E</i> _{dmin}	values in eV.	007		Estimate ues in e	d and adopted (' V.	'A'') averag	ed displacement	threshold e	energy E _d val-
3 Li	9 ± 7	39 Y	15 ± 3 A	69 Tm	$16 \pm 3 \text{ A}$	3 Li	19 + 4	37 Rh	17 + 4	65 Th	36 + 7
4 Be	15 ± 5	40 Zr	$22\pm5~\mathrm{A}$	70 Yb	$9 \pm 2 A$	4 Be	31 ± 6	38 Sr	24 ± 5	66 Dv	30 ± 7 34 ± 7
5 B	19 ± 5	41 Nb	$32 \pm 6 \text{ A}$	71 Lu	$17 \pm 3 \text{ A}$	5 B	46 ± 9	39 Y	36 ± 7	67 Ho	36 ± 7
6 C	$25 \pm 5 \text{ A}$	42 Mo	$34 \pm 7 A$	72 Hf	27 ± 5	6 C	69 ± 14	40 Zr	40 ± 8 A	68 Er	30 ± 7 37 ± 7
11 Na	7 ± 4	43 Tc	32 ± 6	73 Ta	$32 \pm 6 \text{ A}$	11 Na	17 ± 4	41 Nb	78 ± 16 A	69 Tm	36 ± 7
12 Mg	$10 \pm 2 \text{ A}$	44 Ru	34 ± 7	74 W	$41 \pm 8 \text{ A}$	12 Mg	20 ± 4 A	42 Mo	65 ± 13 A	70 Yh	27 ± 5
13 Al	$16 \pm 3 \text{ A}$	45 Rh	33 ± 7	75 Re	$44 \pm 9 A$	13 Al	27 ± 5 A	43 Tc	58 ± 12	71 Lu	$\frac{1}{44} + 9$
14 Si	$13 \pm 3 \text{ A}$	46 Pd	$34 \pm 7 A$	76 Os	46 ± 9	14 Si	37 ± 7	44 Ru	60 ± 12 60 ± 12	72 Hf	61 ± 12
15 P	10 ± 4	47 Ag	$25\pm5~\mathrm{A}$	77 Ir	$46 \pm 9 \text{ A}$	15 P	20 ± 5	45 Rh	51 ± 10	73 Ta	90 ± 18 A
16 S	10 ± 3	48 Cd	$19 \pm 4 \text{ A}$	78 Pt	$34 \pm 7 \text{ A}$	16 S	20 ± 4	46 Pd	$41 \pm 8 \text{ A}$	74 W	$90 \pm 18 \text{ A}$
19 K	7 ± 5	49 In	$10 \pm 2 \text{ A}$	79 Au	$34 \pm 7 \text{ A}$	19 K	16 ± 4	47 Ag	$39 \pm 8 \text{ A}$	75 Re	$60 \pm 12 \text{ A}$
20 Ca	10 ± 3	50 Sn	$22 \pm 4 \text{ A}$	80 Hg	14 ± 5	20 Ca	23 ± 5	48 Cd	$30 \pm 6 \text{ A}$	76 Os	69 ± 14
21 Sc	$14 \pm 3 \text{ A}$	51 Sb	18 ± 4	81 TI	16 ± 3	21 Sc	33 ± 7	49 In	$12 \pm 2 A$	77 Ir	58 ± 12
22 Ti	$19 \pm 4 \text{ A}$	52 Te	15 ± 3	82 Pb	$14 \pm 3 \text{ A}$	22 Ti	$30 \pm 6 \text{ A}$	50 Sn	20 ± 10	78 Pt	$44 \pm 9 A$
23 V	$26 \pm 5 \text{ A}$	53 I	11 ± 3	83 Bi	$13 \pm 3 \text{ A}$	23 V	$57 \pm 11 \text{ A}$	51 Sb	22 ± 6	79 Au	43 ± 9 A
24 Cr	$28 \pm 6 \text{ A}$	55 Cs	7 ± 4	84 Po	13 ± 3	24 Cr	$40 \pm 8 \text{ A}$	52 Te	20 ± 5	80 Hg	20 ± 5
25 Mn	18 ± 4	56 Ba	11 ± 2	85 At	16 ± 4	25 Mn	33 ± 7	53 I	16 ± 4	81 TI	24 ± 5
26 Fe	$17 \pm 3 \text{ A}$	57 La	15 ± 3	87 Fr	21 ± 6	26 Fe	$40 \pm 8 \text{ A}$	55 Cs	15 ± 4	82 Pb	$25 \pm 5 A$
27 Co	$22 \pm 4 \text{ A}$	58 Ce	14 ± 3	88 Ra	14 ± 3	27 Co	$36 \pm 7 \text{ A}$	56 Ba	22 ± 4	83 Bi	23 ± 5
28 Ni	$23 \pm 5 \text{ A}$	59 Pr	$10 \pm 2 \text{ A}$	89 Ac	24 ± 5	28 Ni	$33 \pm 7 \text{ A}$	57 La	29 ± 6	84 Po	22 ± 4
29 Cu	$20 \pm 4 \text{ A}$	60 Nd	$9 \pm 2 A$	90 Th	$35 \pm 7 \text{ A}$	29 Cu	$30 \pm 6 \text{ A}$	58 Ce	28 ± 6	85 At	22 ± 4
30 Zn	$14 \pm 3 \text{ A}$	61 Pm	13 ± 4	91 Pa	33 ± 9	30 Zn	$29 \pm 6 \text{ A}$	59 Pr	27 ± 5	87 Fr	34 ± 6
31 Ga	$12 \pm 2 A$	62 Sm	$10 \pm 2 \text{ A}$	92 U	36 ± 8	31 Ga	23 ± 5	60 Nd	28 ± 6	88 Ra	24 ± 5
32 Ge	$15 \pm 3 \text{ A}$	63 Eu	$8 \pm 2 A$			32 Ge	35 ± 7	61 Pm	30 ± 5	89 Ac	33 ± 7
33 As	15 ± 3	64 Gd	$14 \pm 3 \text{ A}$			33 As	31 ± 6	62 Sm	27 ± 5	90 Th	$44 \pm 9 A$
34 Se	12 ± 2	65 Tb	$15 \pm 3 \text{ A}$			34 Se	23 ± 5	63 Eu	24 ± 5	91 Pa	43 ± 7
35 Br	9 ± 3	66 Dy	15 ± Thr	Threshold Displacement Energies of Ovugan in VE22Cu2O7: A Multi Dhusies Analysis							Ashlev Dickson
37 Rb	7 ± 4	67 Ho	$15 \pm$	Theonord Displacement Energies of Oxygen in Thazeddor. A mulli-Fnysics Analysis							loney Dickson
38 Sr	10 + 3	68 Er	$16 \pm \frac{30/7}{30}$	30/7-018 - Kjell Johnsen Auditorium, CERN							11:00 - 11:20

 FLUKA asks user for average displacement threshold (user-input or 30 eV by default)

Not all of *T* goes into atomic collisions: the partition function

- The PKA kinetic energy T will be lost to ionization (no displacement damage) and Coulomb scattering (displacement damage).
- One needs an effective way to "discount" the fraction of T which would be spent on ionization: enter the Lindhard partition function
- In FLUKA we rely on a parametrized function based on <u>https://doi.org/10.1109/23.907581</u>:

$$L(T) = \frac{1}{1 + F_L(3.4008\varepsilon^{1/6} + 0.40244\varepsilon^{3/4} + \varepsilon)} \qquad \varepsilon = \frac{T}{E_L}$$

(L: lattice atom) (R: recoil atom)

$$E_L = 30.724Z_R Z_L (Z_R^{2/3} + Z_L^{2/3})^{1/2} \frac{A_R + A_R}{A_R}$$
$$F_L = \frac{0.0793Z_R^{2/3} Z_L^{1/2} (A_R + A_L)^{3/2}}{(Z_R^{2/3} + Z_L^{2/3})^{3/4} A_R^{3/2} A_L^{1/2}}.$$

- Approximations:
 - Recoil energy << Projectile kinetic energy
 - Electronic stopping << Nuclear stopping



Considerable differences wrt Sn/(Sn+Se) at high energies.

 To minimize their impact, it's best to lower FLUKA ion transport cuts to lowest limit (~250 eV/u)



Non-ionizing energy loss (NIEL) in FLUKA

 The NIEL is a basic quantity accounting for both the damage threshold and the partition function:

$$\text{NIEL}(E) = \frac{N_A \rho}{A_w} \int_{E_d}^{T_{\text{max}}} \mathrm{d}T \ T \frac{\mathrm{d}\sigma(E)}{\mathrm{d}T} L(T) \qquad \text{(GeV/cm)}$$

- Tabulated in FLUKA at initialization as a function of energy, apportioned among particle steps runtime.
- NIEL: quantifies the fraction of energy transferred to the material which might produce displacement damage.
- Although still in use, it is not the end of the story. <u>Not all</u> of the NIEL goes into displacement damage: some is dissipated as heat (phonons)
- <u>NIEL does not make any prediction of defect</u> <u>cascades</u>

Particularly useful for Si as target material, i.e. for electronics

Conveniently recast in terms of a damage function D(E)

$$NIEL = \frac{N_A \rho}{A_W} \int dE D(E) \frac{d\Phi(E)}{dE} \quad (\text{GeV/cm}^3)$$

https://doi.org/10.1016/S0168-9002(98)01462-4



Estimating displacement damage: DPA in FLUKA*

- The quantity displacements per atom (DPA) goes beyond the NIEL, in that it converts the energy available for displacement into a number of ion-hole (Frenkel) pairs
- Two variants available in FLUKA, both treated as "stopping-powerlike" quantities, apportioned over macroscopic particle steps:
 - Norgett-Robinson-Torrens displacements per atom (DPA)*:



http://dx.doi.org/10.15496/publikation-20433

$$DPA-NRT(E) \sim \frac{N_A \rho}{A_w} \int_{E_d}^{T_{\text{max}}} dT \, \frac{d\sigma(E)}{dT} N_{\text{NRT}}(T_d), \qquad T_d = L(T)T, \qquad N_{\text{NRT}}(T_d) = \begin{cases} 0 & \text{if } 0 < T_d < E_d, \\ 1 & \text{if } E_d < T_d < \frac{2E_d}{0.8} \\ \frac{0.8T_d}{2E_d} & \text{if } \frac{2E_d}{0.8} < T_d \end{cases}$$
(1/cm)

Ref: Nordlund K. et al., Nat. Commun. 9 1084 (2018)

"The binary collision simulations used as the basis of the NRT-dpa model focused on the collisional phase of the displacement cascade and did not consider the dynamics of cascade evolution as atomic velocities fell" (Overestimation of displacement damage)

*See however the following paper+slides for second-level sub-cascade treatment:

http://dx.doi.org/10.15669/pnst.2.769

https://indico.cern.ch/event/769192/contributions/3287282/attachments/1794339/2924300/RadiationEffectsLHCexperiments.pdf



Ref: Norgett M.J. et al., Nucl Eng Des 33 50-54 (1975) https://doi.org/10.1016/0029-5493(75)90035-7

Legacy binary collision model

The factor of 0.8 accounts for more realistic atomic potential instead of hard sphere scattering of original Kinchin-Pease calculations + crude recombination efficiency

d,

Estimating displacement damage: DPA in FLUKA*

• Athermal-recombination-corrected DPA*:

Ref: Nordlund K. et al., Nat. Commun. 9 1084 (2018)

$$\operatorname{ARC-DPA}(E) \sim \frac{N_A \rho}{A_w} \int_{E_d}^{T_{\max}} dT \frac{d\sigma(E)}{dT} N_{\operatorname{arcDPA}}(T), \quad T_d = L(T)T, \quad N_{\operatorname{arcDPA}}(T_d) = \begin{cases} 0 & \text{if } 0 < T_d < E_d, \\ 1 & \text{if } E_d < T_d < \frac{2E_d}{0.8T_d} \\ \frac{0.8T_d}{2E_d} \\ \frac{1}{2E_d} \\ \frac{1}$$

*See however the following paper+slides for second-level sub-cascade treatment: For elementary materials... Scoring of arc-DPA is available in FLUKA

http://dx.doi.org/10.15669/pnst.2.769

https://indico.cern.ch/event/769192/contributions/3287282/attachments/1794339/2924300/RadiationEffectsLHCexperiments.pdf



RADSUM

since v4-3.0 (Sep 2022)

DPA of all particles scored on equal footing in FLUKA

Charged particles:

- a) Transport step (condensed history): restricted NIEL/DPA over the step
- **b)** Below transport threshold: estimate NIEL/DPA as integral over nuclear stopping power x L(T).

Recoils from nuclear elastic scattering (n,p, π ,K) / residuals from nuclear reactions:

• Go to a) if its kinetic energy is above transport threshold, go to b) if below

NB: as of newly included point-wise treatment of neutron interactions below 20 MeV in FLUKA v4-4.0 (Feb 2024), their* contribution to NIEL/DPA is treated coherently with the rest of particles





• See this talk tomorrow for more consequent examples relevant for Muon Collider studies:



 See also SATIF15 code intercomparison for MC simulation of displacement damage <u>https://www.oecd-nea.org/upload/docs/application/pdf/2024-05/satif15-session-7-and-8.pdf#page=25</u>



Radiation to Muon-Collider ring magnets





eli

Cumulative dose and DPA in coils of arc dipoles after 5 yrs (with **3 cm thick tungsten shielding**):



Dose in coils \rightarrow mostly due to e-/ γ DPA in coils \rightarrow mostly due to neutrons

Assuming 5 years with 140 days of operation per year



Summary

- General overview of FLUKA
- Displacement damage modelling in FLUKA: NIEL and DPA
- Advantages and limitations
 - Coherent treatment across all particle species
 - Built-in scoring of NIEL, DPA-NRT, arc-DPA
 - Use of average damage thresholds
 - No on-line simulation of material degradation
- Still, effective DPA scoring as a probe of displacement damage
- Feel free to register and download FLUKA!
- If interested, consider attending one of our trainings!





Courses and events

FLUKA/Flair courses are typically organized once or twice a year. Future courses will be announced below. Presentations, demos and exercises from previous courses can be accessed on the respective course websites listed below under "Past events" (see links).

Upcoming/ongoing events:

Past events:

2024 FLUKA.CERN Beginner's course, <u>Course website</u> CERN, Geneva, Switzerland 02 - 05 December 2024, FLUKA beginner's course

2024 FLUKA.CERN Topical course, <u>Course website</u> CERN, Geneva, Switzerland 25 - 27 November 2024, FLUKA user workshop

2024 FLUKA.CERN Beginner's course, Course website National Institute for Aerospatial Technologies, Madrid, Spain 15 - 19 April 2024, FLUKA beginner's course

2023 FLUKA.CERN Beginner's course, <u>Course website</u> NEA, Boulogne-Billancourt, Paris, France 05-10 November 2023, <mark>FLUKA beginner's course</mark>



