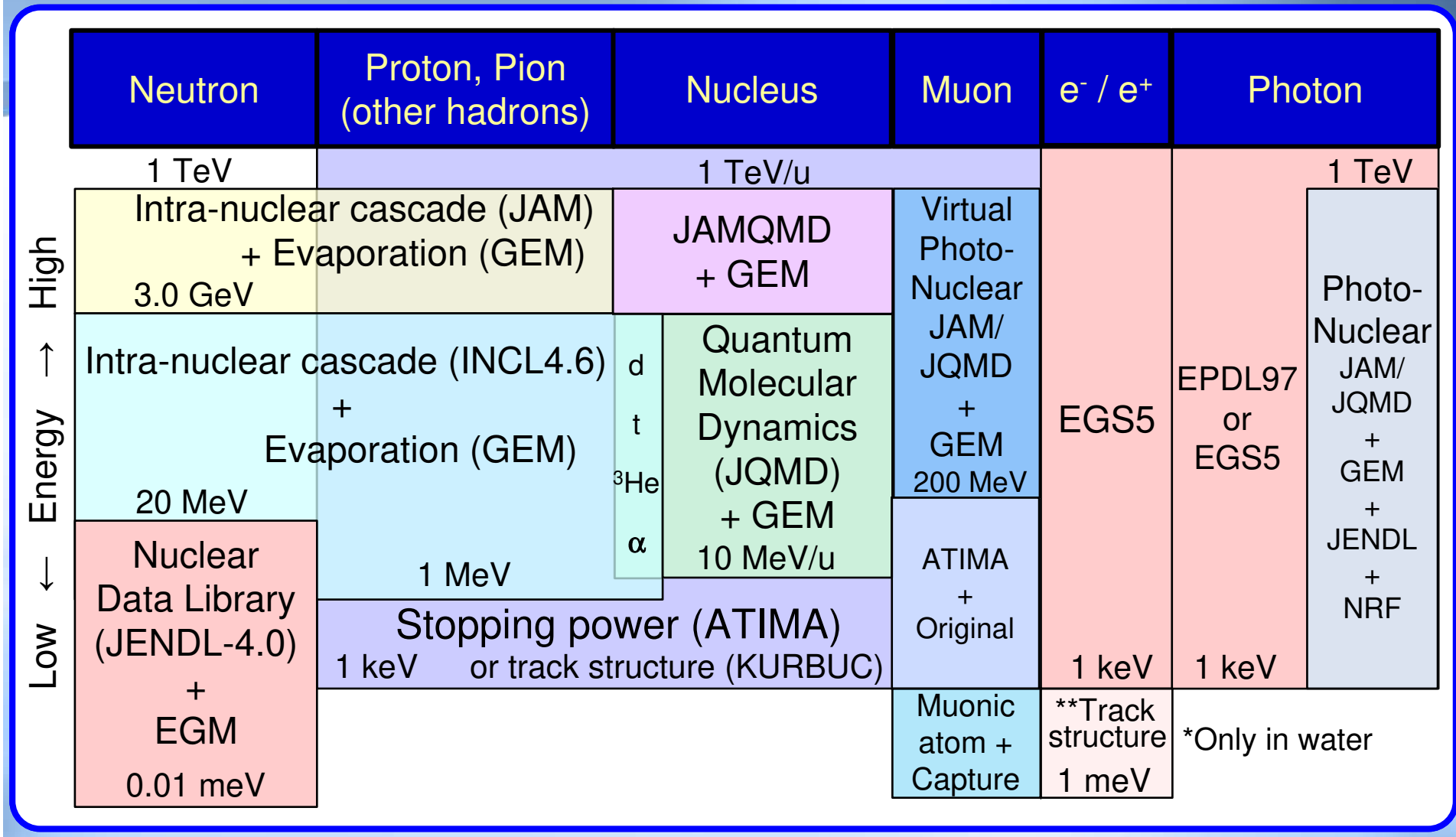
Features of PHITS3.20

PHITS development team, Mar. 2020

Map of Models Recommended to Use in PHITS



- ✓ Implement track structure mode for protons and ions based on KURBUC
- ✓ Implement reaction model for muon pair production by photon interaction

Major Upgraded Features in ver. 3.17

Upgrade patch to 3.17 was released in Nov. 2019

Upgraded Points from ver. 3.10

- ✓ A model for estimating DNA damage based on track-structure mode and [t-userdefined] is developed
- ✓ Surface-type source distribution (s-type=26) becomes available
- ✓ A function to draw the variance of statistical errors is implemented
- ✓ Initial “counter” value can be specified for each multi-source
- ✓ A function to consider the reduction of target material due to nuclear reactions is implemented in DCHAIN
- ✓ An option for excluding annihilation γ-ray from photon RI sources is introduced

Major Upgraded Features in ver. 3.20

PHITS 3.20 was released in Apr. 2020

Upgraded Points from ver. 3.17

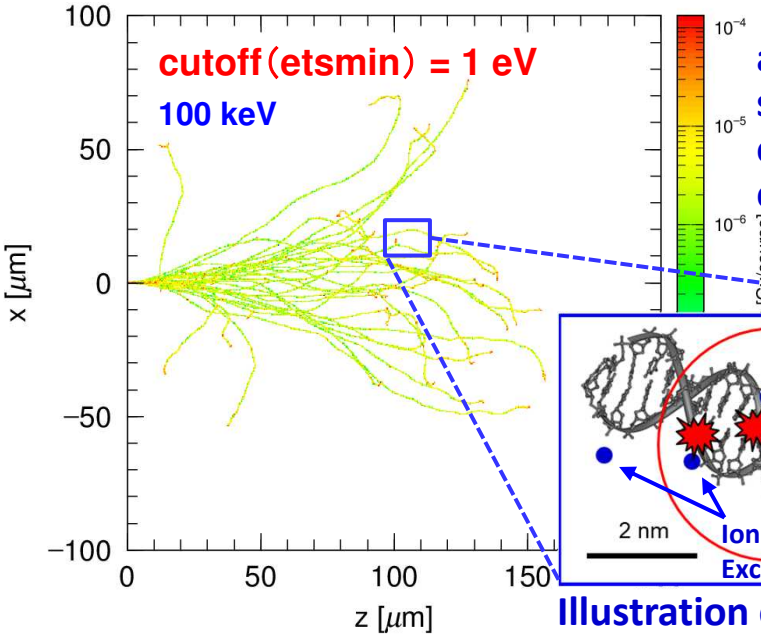
- ✓ A function to read the stopping power of each material from user-supplied table is implemented
- ✓ A new section [Repeated Collisions] is implemented to improve the statistics of rarely produced secondary particles[*1)]
- ✓ A pseudo random number generator based on xorshift64 is introduced
- ✓ Proton and carbon ion track structure code, KURBUC, is implemented[*2)]
- ✓ A function to estimate the systematic uncertainty based on ANOVA is developed
- ✓ Muon-pair production from photon interaction can be considered[*3)]
- ✓ DCHAIN is improved and their libraries are updated[*4)]
- ✓ A function to read electro-magnetic field maps is developed
- ✓ Group-wised cross section data are acceptable in [frag data] section

Under support of *1) Dr. H. Iwamoto of JAEA, *2) Prof. H. Nikjoo & Dr. T. Liamsuwan, *3) Dr. Y. Sakaki of KEK, and *4) C. Konno of JAEA

A model for estimating DNA damage

- ✓ DNA damage estimation based on track-structure mode and [t-userdefined]
- ✓ Output spatial patterns of interactions, analyze them, and obtain the yields
- ※ Damage type: Single-Strand Break (SSB)・Double-Strand Break (DSB)

[Output of interactions with etsmode]



analyzing the spatial patterns of ionization and excitation

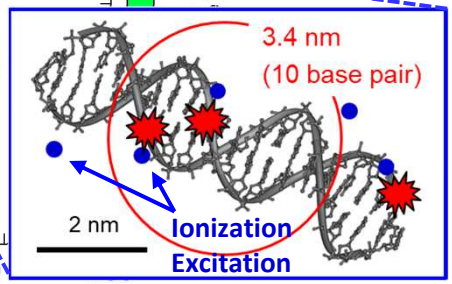
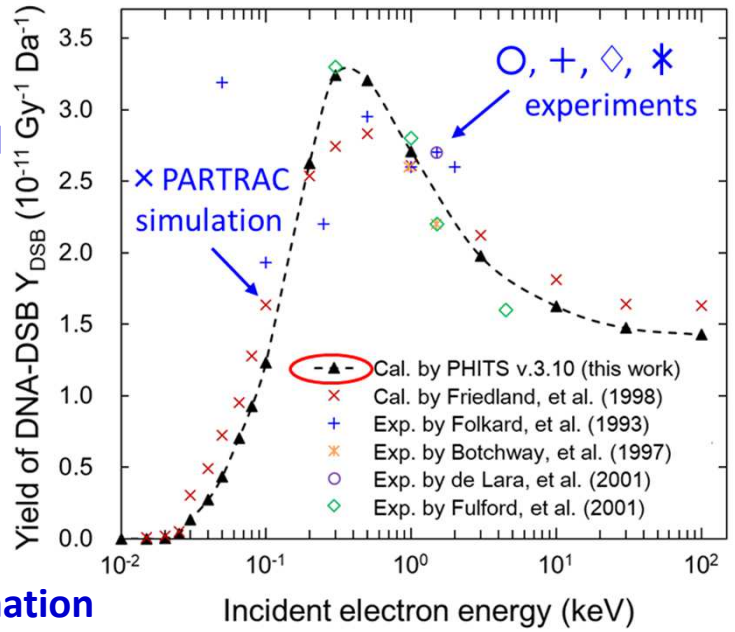


Illustration of damage estimation

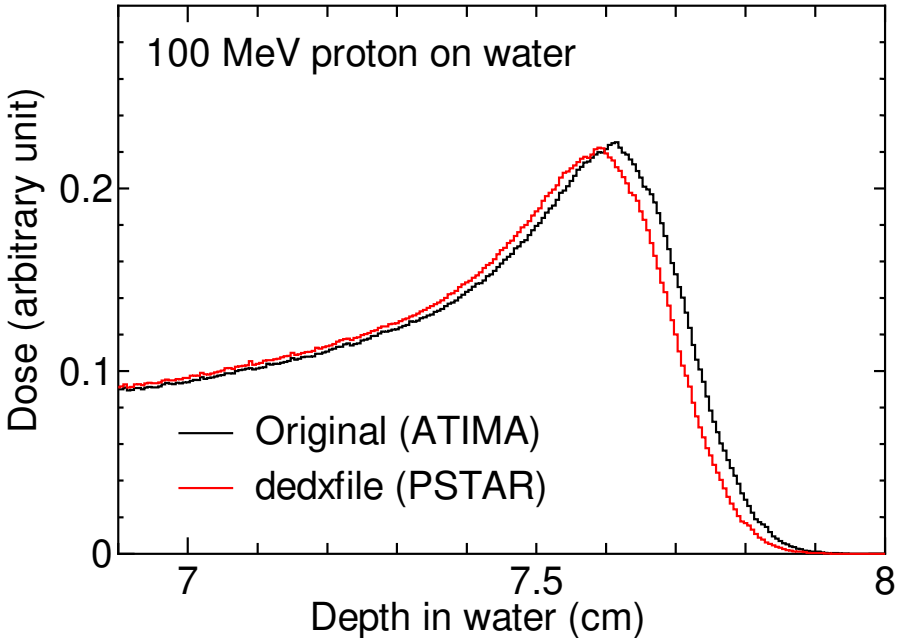
[Estimation of strand-break yields]



This simple model enables to reproduce *in vitro* experiments and other simulations

See phits/utility/usrtally/DNAdamage & Y. Matsuya et al., J. App. Phys. 126, 124701 (2019)

Function to Read Stopping Power Table



Depth-dose distributions calculated by ATIMA and stopping power table developed by PSTAR

(close-up view around Bragg Peak)

Outline of the function

- ✓ User can provide their own stopping power tables
- ✓ Stopping power tables developed by PSTAR and ASTAR* are included in the database folder *data/dedx*

How to use

Define *dedxfile* parameter in [material] section as written below

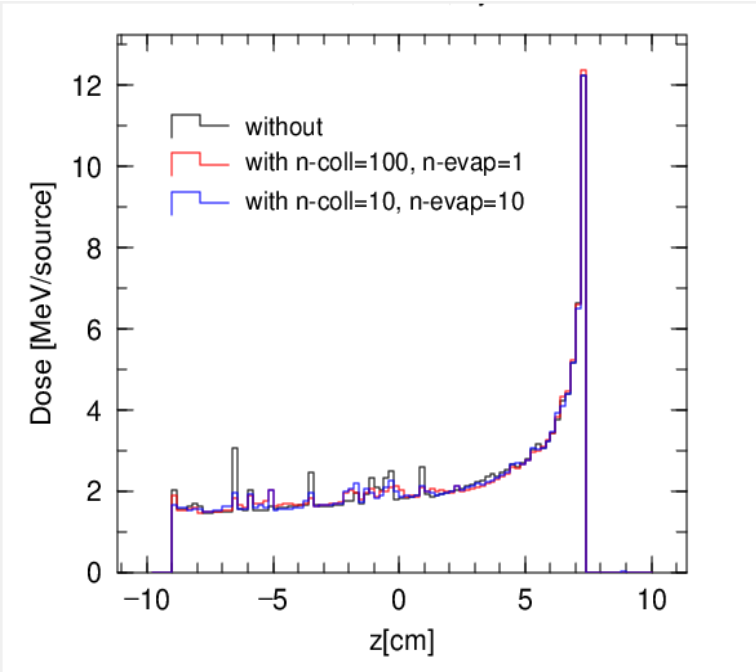
```
[material]
  m1   H  2.0   O  1.0
  dedxfile = water_liquid.txt
```

Stopping power tables calculated by other codes can be used in PHITS

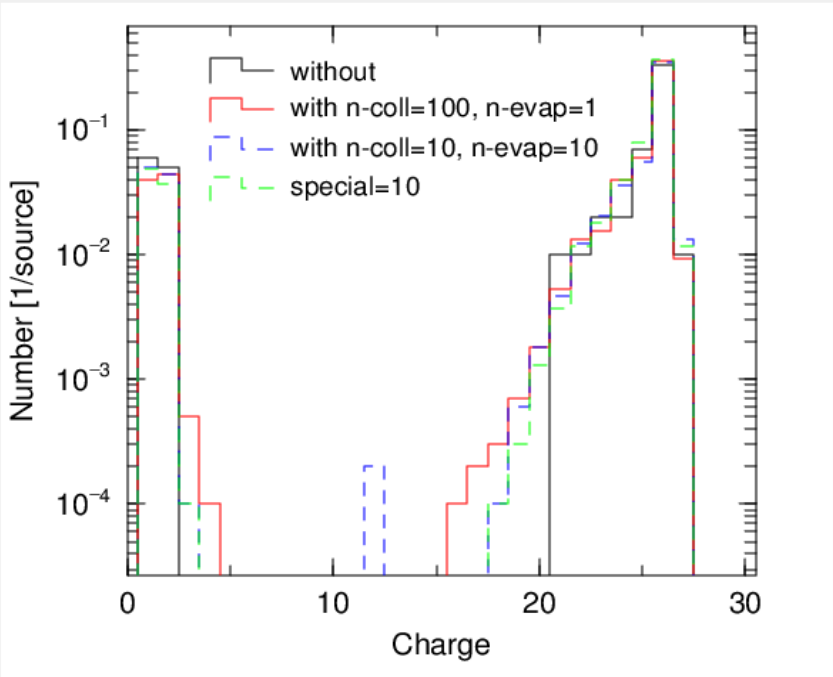
* https://www.nist.gov/pml/stopping-power-range-tables-electrons-protons-and-helium-ions

Repeated Collisions

- ✓ [Repeated Collisions] is introduced → Similar to *special* in [t-yield]
- ✓ Repeat only nuclear reaction simulations to improve the statistical errors
- ✓ Numbers of iterations can be separately specified for direct and evaporation processes



Example for [t-deposit]



Example for [t-product]

Effective when low-probability but high-impact nuclear reaction channels such as nuclear fission exist

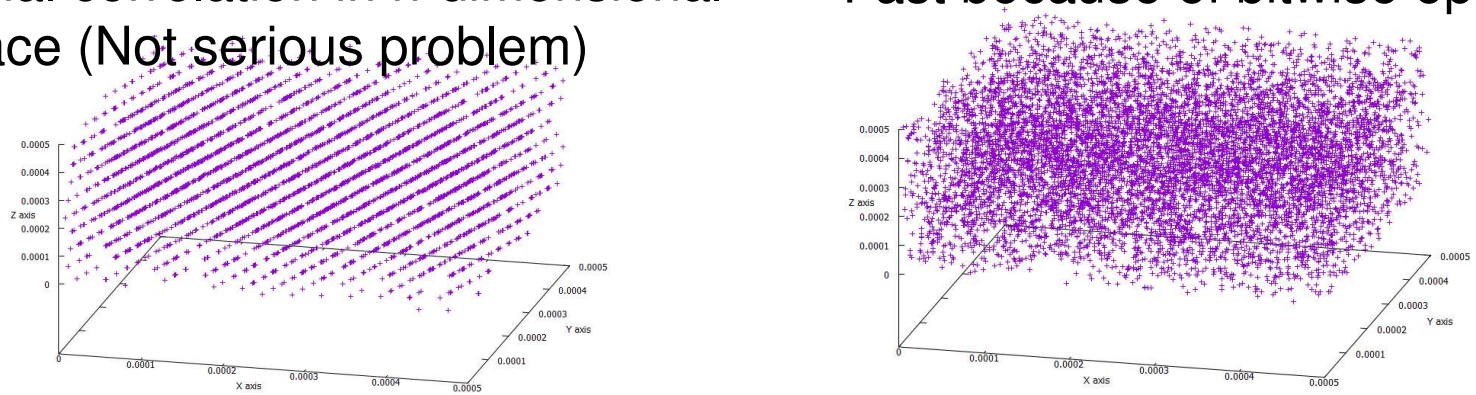
New pseudo-random number generator

Xorshift64 was implemented to obtain pseudo-random numbers used in Monte Carlo calculations

Linear congruential generator (former) ➡ **xorshift64** (new)

- Recurrence relation: $X_{n+1}=A*X_n \bmod M$
- Period length: 2^{46}
- Serial correlation in n-dimensional space (Not serious problem)

- Shift-register generator $\boldsymbol{X}_{n+1}=(\boldsymbol{I}+\boldsymbol{L}_a)(\boldsymbol{I}+\boldsymbol{R}_b)(\boldsymbol{I}+\boldsymbol{L}_c)\boldsymbol{X}_n$
- Period length: 2^{64}-1
- Fast because of bitwise operation

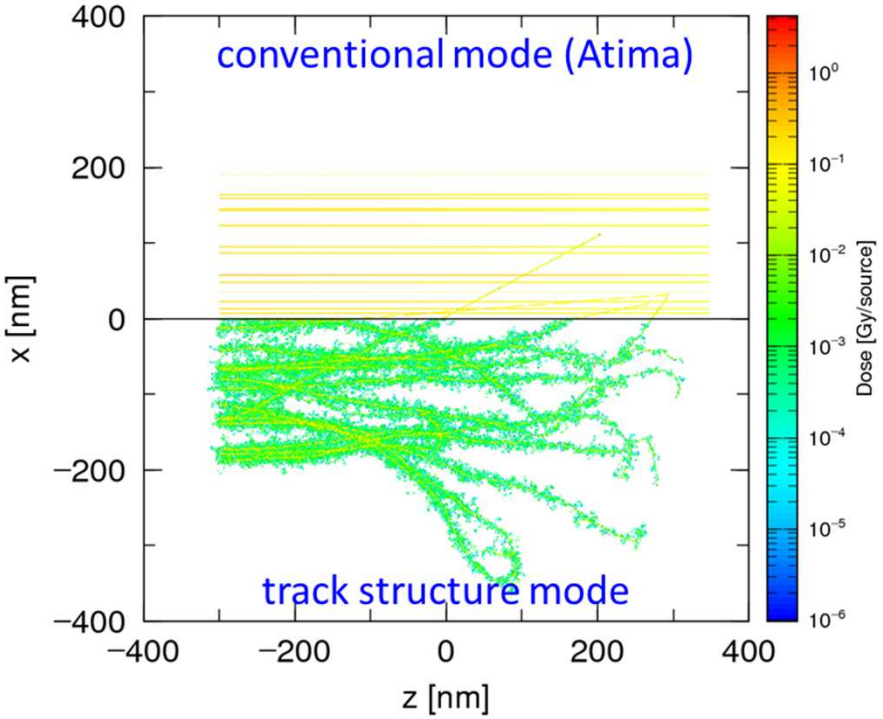


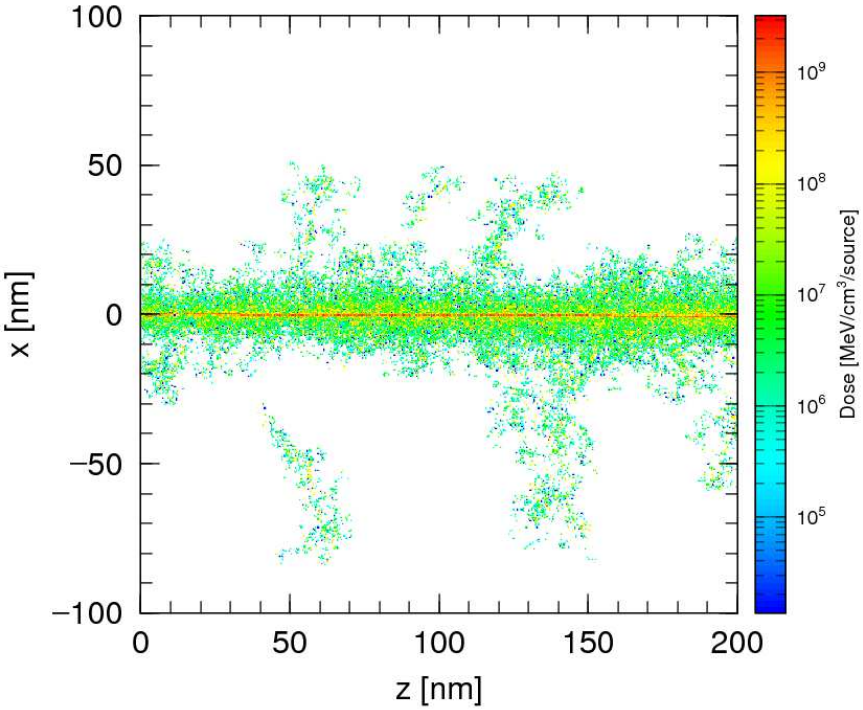
Figures of local coordinate spaces [0<x,y,z<10^{-5}] with the points defined as (x,y,z)=(r_1,r_2,r_3),(r_2,r_3,r_4),… by using random numbers r_i: linear congruential generator makes multi-planes (left panel).

- ✓ Xorshift64 is default (after 3.18). Old method is used by nrandgen=0
- ✓ Initial seed is changed by rseed= positive or negative real number
- ✓ Time dependent initial seed is used by setting itimrand=1

Proton and Carbon Ion Track Structure Mode

Implementation of KURBUC





30 keV proton trajectories calculated by ATIMA (up) and TS mode (down)

1 MeV/n Carbon ion trajectory calculated by TS mode

- ✓ Activate by setting *tsmax* parameter
- ✓ Applicable only to proton (E < 300 MeV) and carbon ion (E < 10 MeV/n)
- ✓ Source code of KURBUC is not included in the package

Under support of Prof. Hooshang Nikjoo & Dr. Thiansin Liamsuwan

ANOVA(analysis of variance)

Estimation of systematic uncertainty based on ANOVA

Effects caused by errors of PHITS input information can be estimated

$$u_{\mathrm{tot}}^2 = u_{\mathrm{syst}}^2 + \frac{1}{N} u_{\mathrm{stat}}^2$$

Total uncertainty

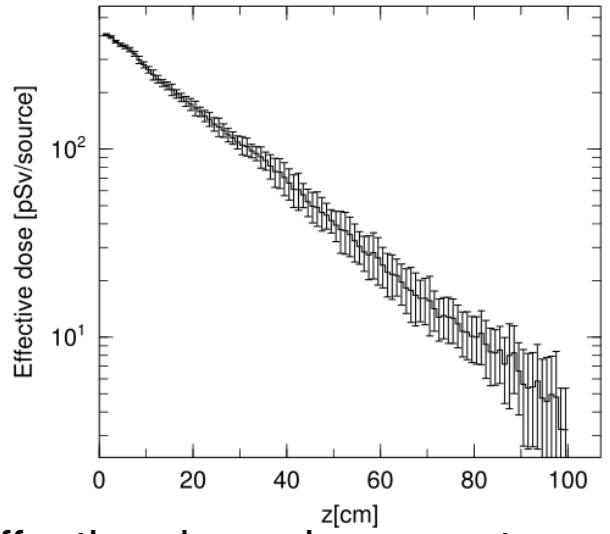
Systematic uncertainty

Statistical error

1. Make a PHITS input file that a value with errors is specified by ci. (icntl=16 is set)
2. Make an input file for the script, where information on variation of ci is written.
3. Execution of the script autorun outputs total uncertainties, systematic uncertainties, and statistical errors.

Ex. case that density of water has error
→specify the density value by ci in [cell]

100 MeV neutron ➡ Concrete + water



Effective doses in concrete material (error bars: total uncertainties)

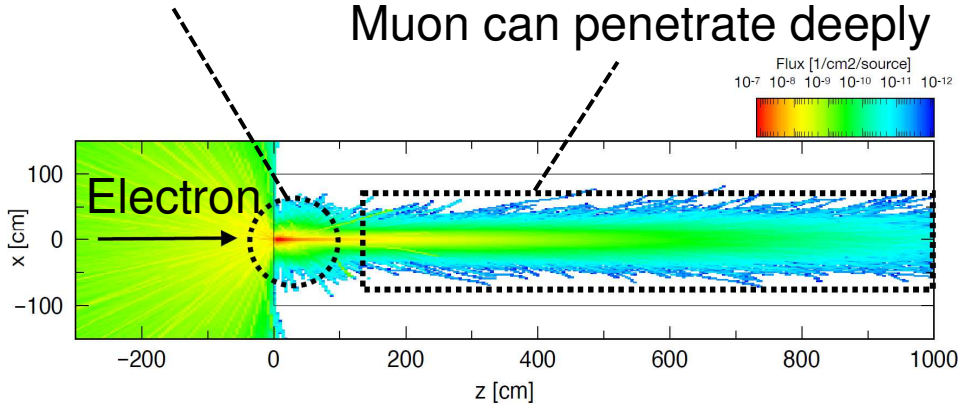
phits/utility/autorun; S. Hashimoto and T. Sato, J. Nucl. Sci. Technol. 56, 345 (2019)

Photon-Induced Muon Pair Production

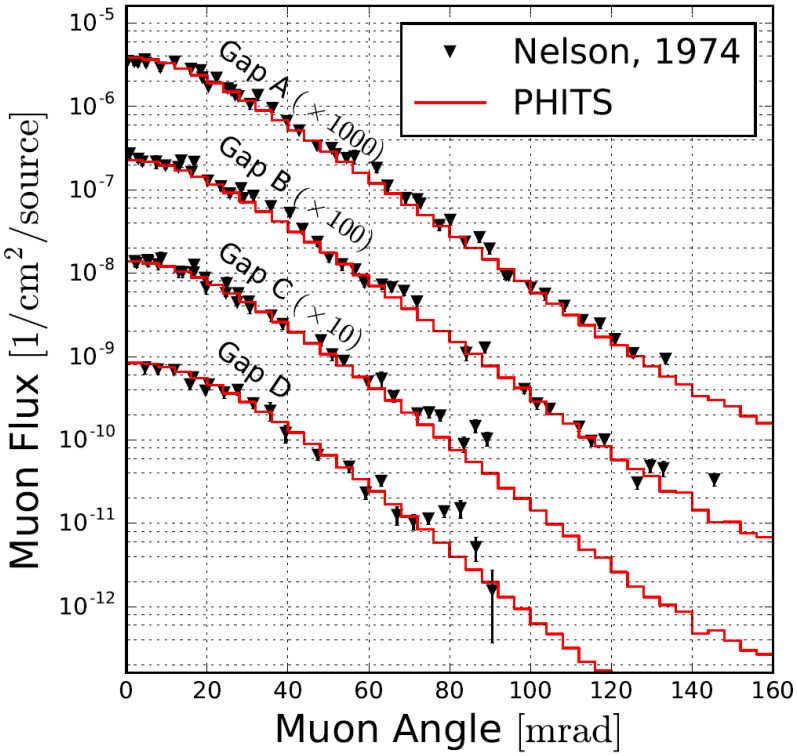
- ✓ Activate the model by setting *igmuppd* = 1 in [parameters]
- ✓ Effective for shielding calculation for high-energy electron accelerators

Secondary photon generates muon pair

Muon can penetrate deeply



Muon fluence behind Fe target irradiated by 18 GeV electrons



Model verification (angular distributions of muon flux)

Ref.) W. R. Nelson et al., Nucl. Instr. Meth., **120**, 413 (1974).

Implemented model can reproduce the experimental data well

Under the support of Dr. Y. Sakaki of KEK

Improvements of DCHAIN & its Libraries

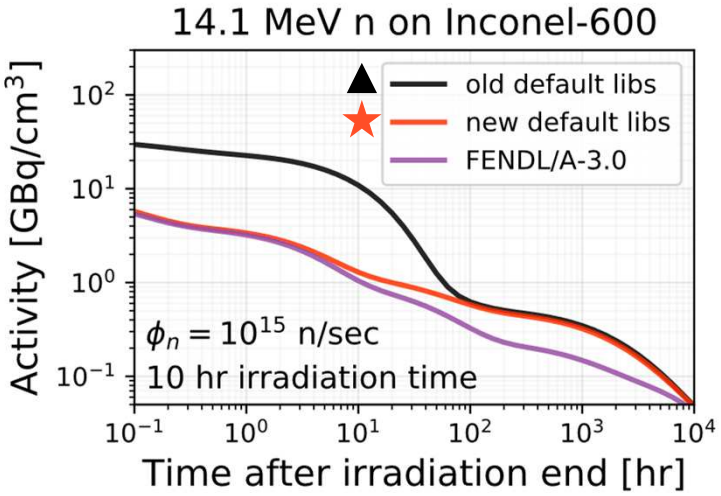
Rebranded from "DCHAIN-SP" to "DCHAIN-PHITS"

- ✓ A lot of selections in activation cross section and nuclear decay libraries
- ✓ Nuclide yield statistical uncertainties are now propagated to results
- ✓ Reduction of target nuclides can be considered → (default since ver. 3.20)

Upgrade of Libraries

Under support of C. Konno of JAEA

← Neutron activation XS	↓ Nuclear decay data
▲JEFF-3.1A (2007)	▲Various 1990s evaluations
★JENDL/AD-2017	JENDL/DDF-2015
★JENDL-4.0 (2010)	ENDF/B-VIII.0 (2016)
★ENDF/B-VIII.0 (2018)	★JENDL + ENDF + '90s
ENDF/B-VII.1 (2011)	ENDF + JENDL + '90s
★JEFF-3.3 (2017)	
★FENDL/A-3.0 (2012)	
EAF-2010	
BROND-3.1 (2016)	
CENDL-3.1 (2009)	
TENDL-2017	



Comparison with new & old libraries

- ✓ Reaction library controlled with **`inxslib`** (+ **`hnxslib`**)
- ✓ Decay library controlled with **`idcylib`**

Bug Fix & Default Changes in PHITS 3.17

Upgrade patch to 3.17 was released in Nov. 2019

Important changes since ver. 3.10

- ✓ Bug in EGS5 mode when it is combined with lattice or tetrahedral structures is fixed（Only related to versions 3.08 ~ 3.14)
- ✓ Bug in the [t-deposit] calculation using EGS5 is fixed (Only related to versions 3.13 ~ 3.16)
- ✓ The default cut off energies of pions, muons and ions are decreased from 1 MeV (or 1 MeV/n) to 1 keV (or 1 keV/n)
- ✓ The maximum number of multi-sources that can be written in a PHITS input file is increased from 200 to 500
- ✓ Bug in reading ionization potential in water, *ih2o* parameter, is fixed
- ✓ Bug that *stdcut* does not work in MPI version is fixed
- ✓ Bug that tetrahedral geometry cannot be read in MPI version is fixed

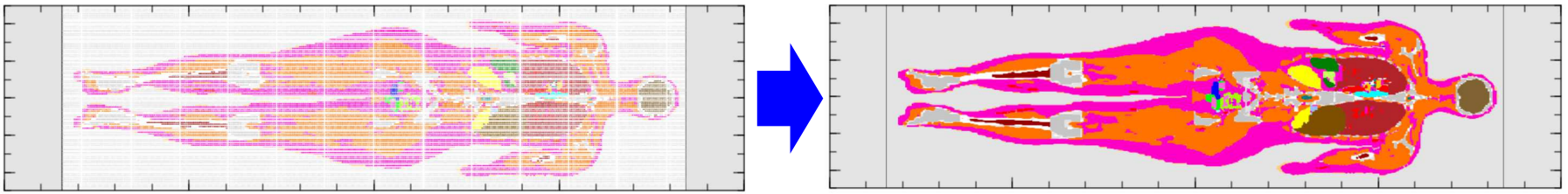
Bug Fix & Default Changes in PHITS 3.20

PHITS 3.20 was released in Apr. 2020

Important changes since ver. 3.17

- ✓ Bug of providing particle energy in MeV/n instead of MeV/u with ATIMA is fixed
- ✓ Bug in generating the Maxwellian energy-spectrum source (e-type=3 & 7) is fixed
- ✓ 2-dimensional geometry drawing function, gshow, has been improved to properly depict complicated geometry defined by voxel or tetrahedron*
- ✓ The default cut off energy of proton is decreased down to 1 keV

***ICRP voxel phantom depicted by gshow using PHITS 3.17 and 3.20**



PHITS 3.17 PHITS 3.20

Upcoming Futures

We are planning to …

- ✓ **Improve nuclear reaction model and data library**
  - ✓ Full set of JENDL-4.0/HE
  - ✓ Adoption to the latest data format
  - ✓ Fission & intral-nuclear cascade models
- ✓ **Implement new functions**
  - ✓ track-structure mode to other ions & targets
  - ✓ xyz-mesh for [t-dchain]
  - ✓ Estimation of systematic uncertainties
- ✓ **Improve user support functions**
  - ✓ Special editor for making PHITS input file