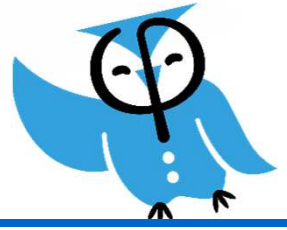
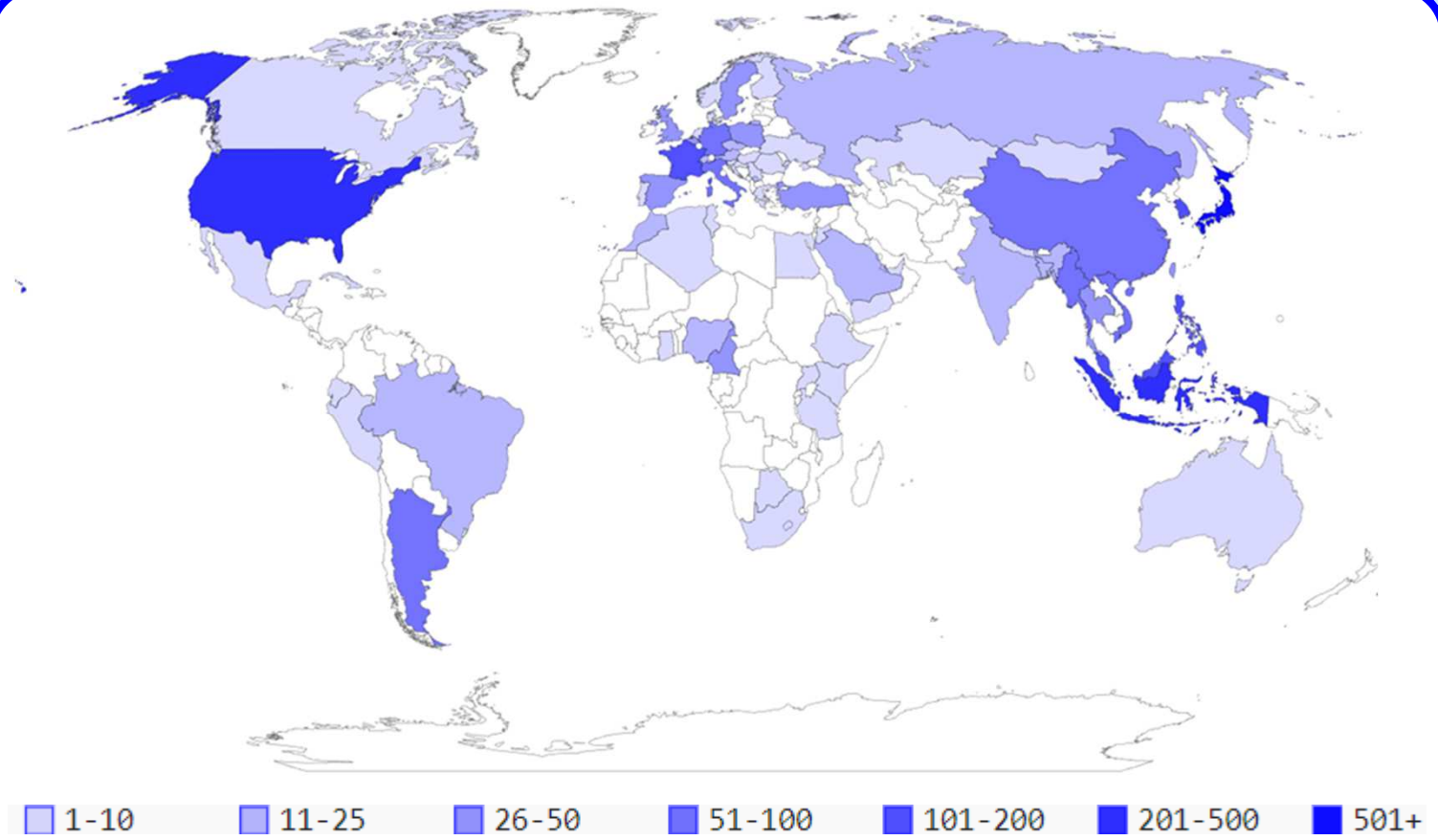


Features of PHITS3.34

PHITS development team, Apr. 2024

Number of PHITS users since 2019



Number of PHITS users in each country since 2019*

*@03/04/2024, based on the location of users' affiliation

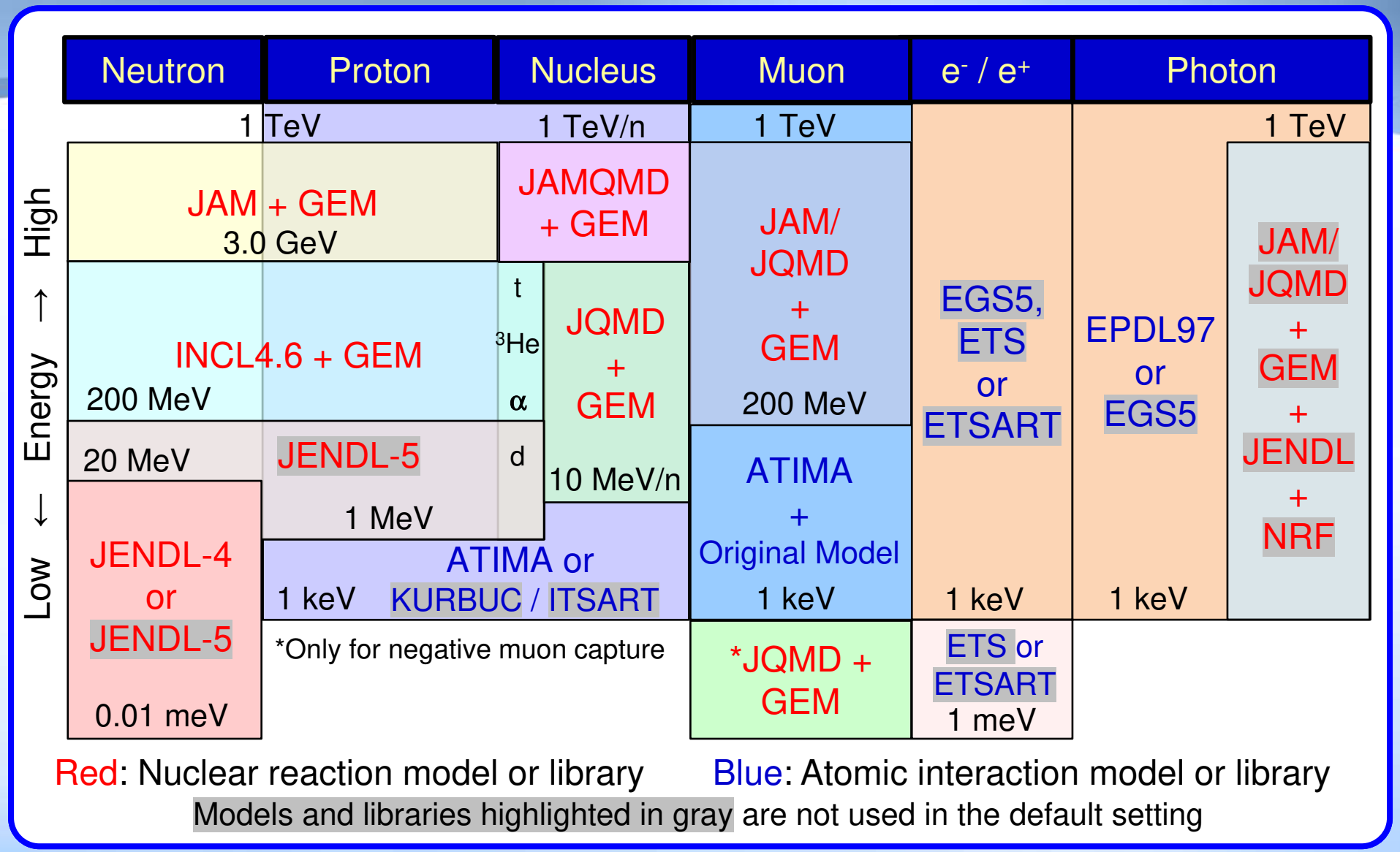
5,890 new users from 76 countries in five years!

Top 10 countries

Country	#users
Japan	2873
Indonesia	410
United States	333
South Korea	249
Philippines	211
China	165
France	148
Argentina	129
Spain	114
Malaysia	113

https://phits.jaea.go.jp/usermap/PHITS_map_userbase.html

Map of Models Recommended to Use in PHITS



Red: Nuclear reaction model or library Blue: Atomic interaction model or library

Models and libraries highlighted in gray are not used in the default setting

JENDL-5 is recommended to use for neutrons, protons, and deuterons if available

Major Upgraded Features in ver. 3.34

Since version 3.31

- ✓ A function for calculating extended statistical indicators has been implemented
- ✓ A new program for analyzing the chemical reactions (PHITS-Chem) has been developed
- ✓ An electron track-structure model applicable to arbitrary target (ETSART) has been developed
- ✓ [weight window] and [t-wwg] have been improved in various aspects
- ✓ [Forced collisions] has become applicable to thick targets for charged particle irradiation*1)
- ✓ An adjoint mode applicable to charged particles has been implemented
- ✓ An automatic download and setup program for JENDL-5 has been developed*2)
- ✓ A text editor specialized for making PHITS input file (PHITS-Pad) has been developed*3)
- ✓ A function to visualize 4-dimensional (x,y,z,t) particle trajectory has been implemented in PHIG-3D*4)

*1) Under the support of RIST
*2) Under the support of AdvanceSoft Corporation
*3) Under the support of CCCE of JAEA
*4) Under the support of National Maritime Research Institute

Major Upgraded Features in ver. 3.34

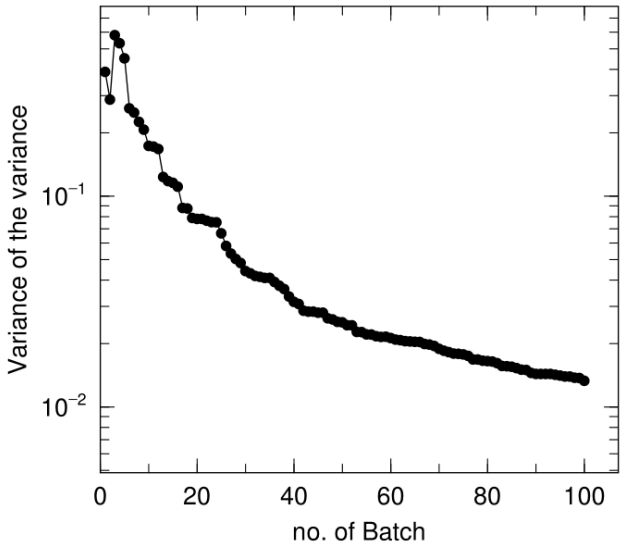
Since version 3.31

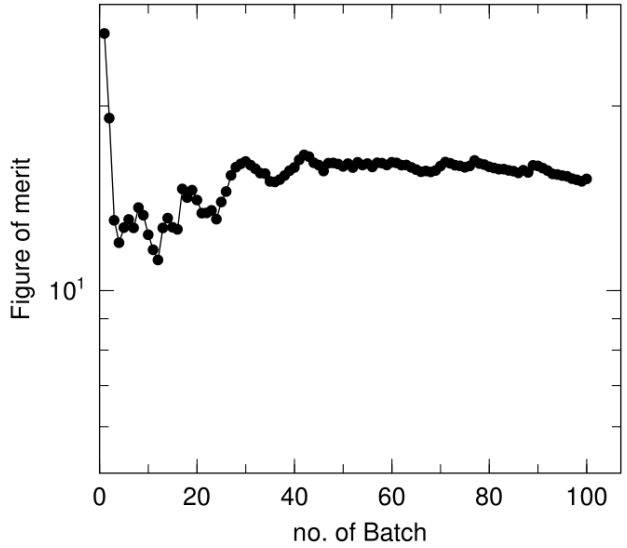
- ✓ JENDL-4.0/HE and JENDL/DEU-2020 were replaced by JENDL-5[*1)]
- ✓ A new function to output the multiplier values has been implemented[*2)]
- ✓ The installer for Windows has been updated[*3)]
- ✓ A new function to scale the maximum tally output value to a certain value has been implemented[*4)]
- ✓ A function to consider the detector resolutions has been implemented in [t-deposit2]
- ✓ A function to read neutron libraries for meta-stable nuclides has been implemented
- ✓ The algorithm of ITSART has been improved
- ✓ Weighting factors defined in [multiplier] as a function of LET can be considered in [t-deposit]
- ✓ [User-Defined Interaction] and [User Defined Particle] have been developed
- ✓ Categories of reaction channels for track-structure modes in [t-interact] have been re-organized

*1) Under support of Dr. Konno, Dr. Tada, Dr. Nakayama, Dr. Iwamoto of JAEA
*2) Under support of RIST
*3) Under the support of AdvanceSoft Corporation
*4) Under the support of CCCE of JAEA

Extended statistical indicators

1. Output function of new statistical indicators for tally results: variance of the variance (VOV), figure of merit (FOM), and probability density function.
2. Statistical check sheet to confirm convergence of statistical indicators.





Transition of VOV (left panel) and FOM (right panel) as the total history number increases.

- VOV, variance of statistical error, decreases by 1/*N*.
- FOM, computational efficiency over time, converges to a constant value.

Statistical check sheet at batch 100

no. = 1, reg = 11

Quantity	Output	Value	Desired	Pass
Mean	Current value	7.8418E-07	Constant	yes
Mean	History dep. (rel. slope)	-0.0162	= 0.00	
Relative error	Current value	0.0769	< 0.05	no
Relative error	History dep. (p in N^p)	-0.5053	= -0.50	yes
Variance of the variance	Current value	0.0133	< 0.10	yes
Variance of the variance	History dep. (p in N^p)	-1.0189	= -1.00	yes
Figure of Merit	Current value	1.5221E+01	Constant	yes
Figure of Merit	History dep. (rel. slope)	-0.0169	= 0.00	

Statistical check sheet

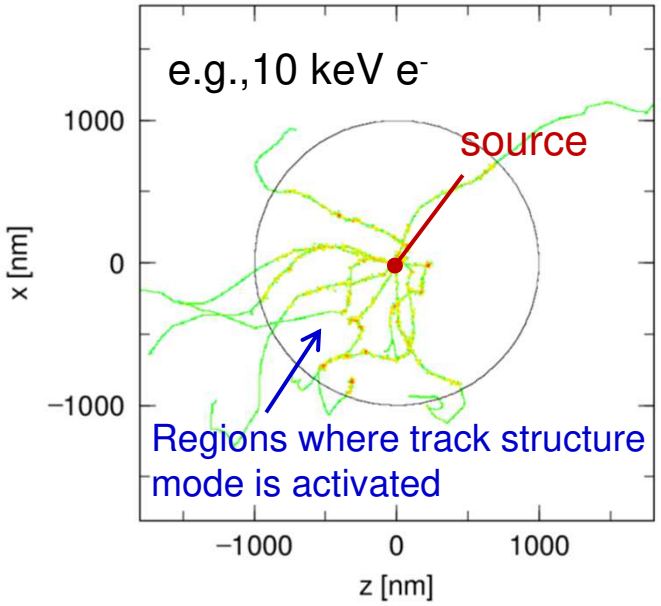
See Sec. 6.10 of PHITS manual (sample input in phits/sample/itall3)

Development of chemical code in PHITS

✓ Estimate of G values resulting from water radiolysis using track-structure mode
✓ Considering the generation, diffusion, and reaction of 13 types of chemical products
※ Chemical species : $^{\bullet}OH$, e_{aq}^{-}, $^{\bullet}H$, H_3O^{+}, H_2, H_2O_2, HO_2, O_2,OH^{-}, O_2^{-}, HO_2^{-}, $^{\bullet}O^{\bullet}$, O^{-}

[Track-structure mode (PHITS-ETS)]

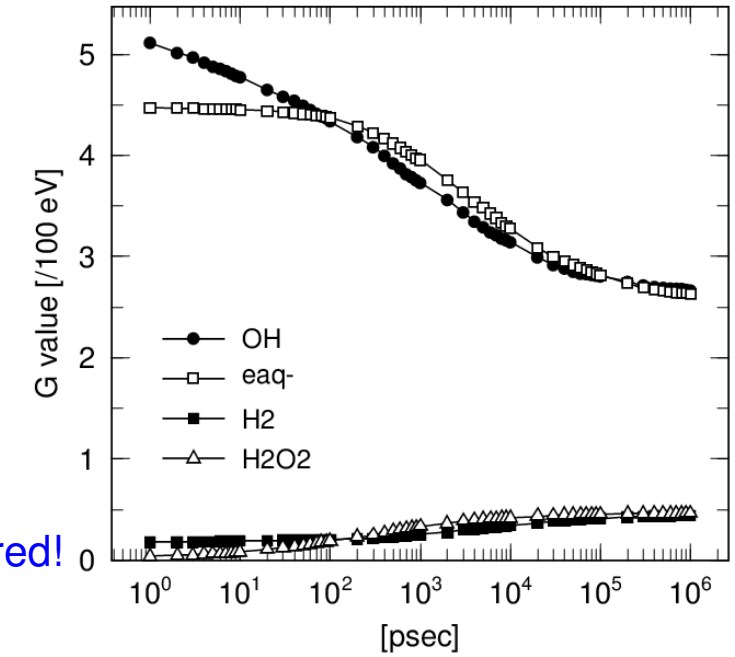
Output of the atomic interaction



Consideration of generation, diffusion, and reaction of 13 chemical products

$^{\bullet}OH$ radical scavenger of (Tris, DMSO) can be considered!

[Developed code（PHITS-Chem code)]

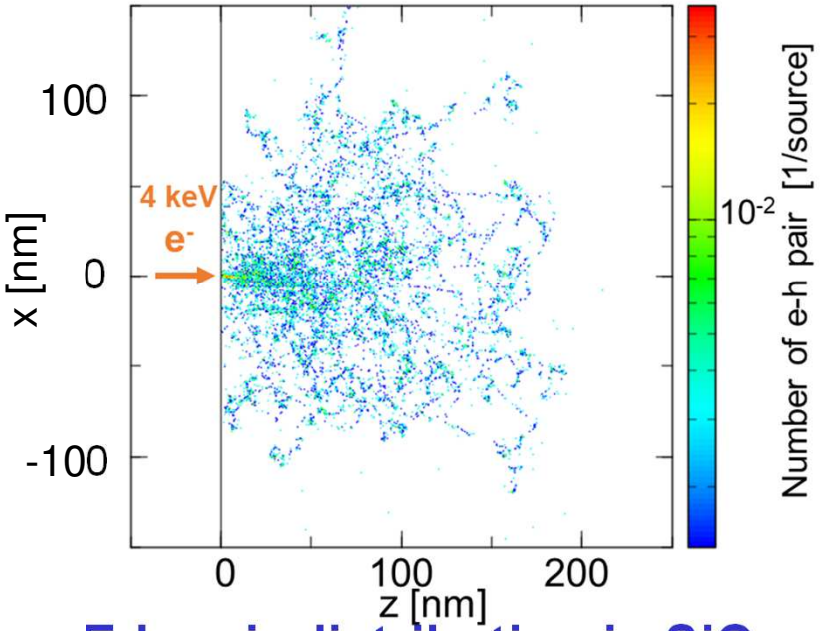


Succeeded in developing a chemical code for PHITS that can reproduce experimental values and other simulation codes!

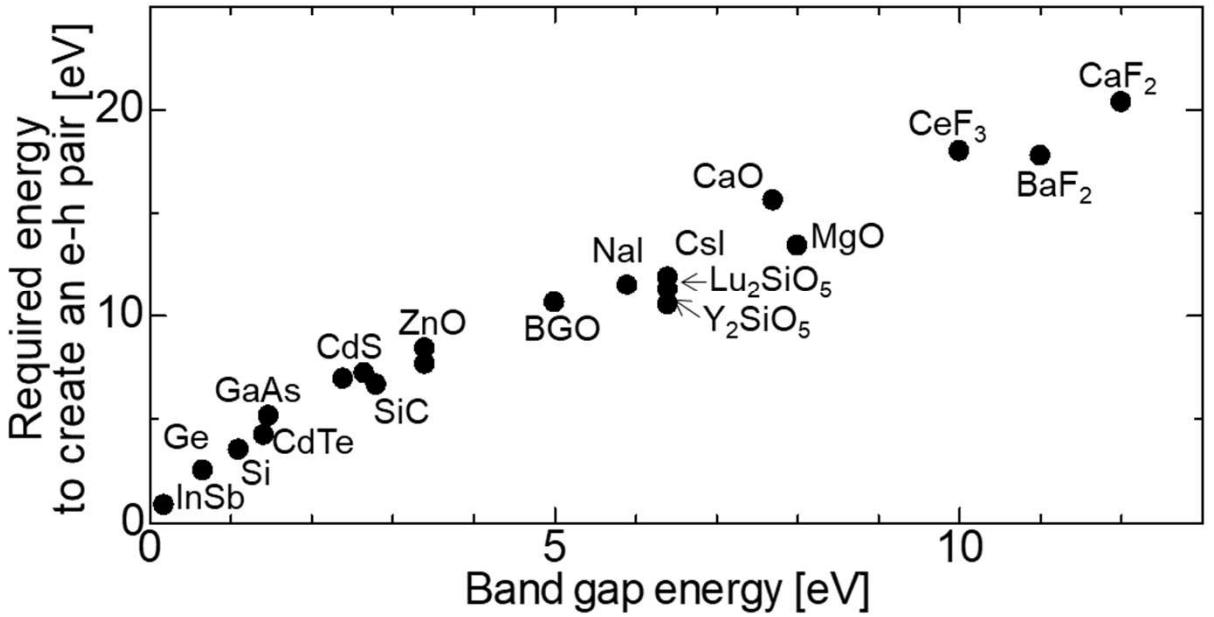
See phits/utility/usrtally/ChemCode & Y. Matsuya et al. *Phys. Med. Biol.* 69, 035005 (2024)

Electron Track Structure for ARbitrary Target (ETSART)

- ✓ ETSART is a function to simulate the behavior of electrons in arbitrary materials down to energies as low as a few eV. (only the model for solids is implemented in ver.3.34.)
- ✓ The bandgap energy can be input to simulate electronic excitations in solids.



E-h pair distribution in SiO_2



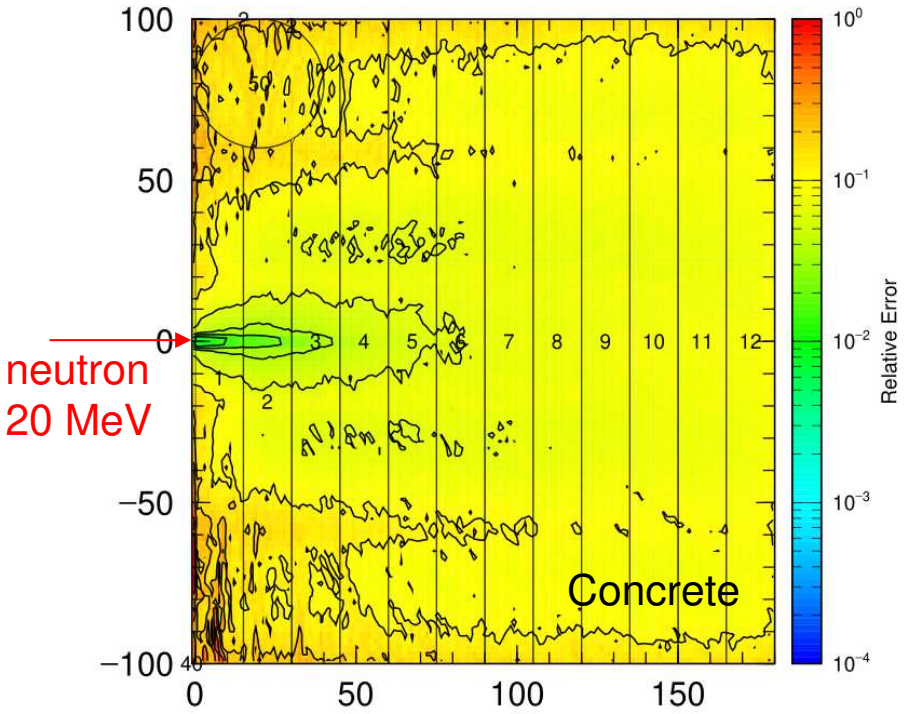
The ε values of semiconductor and phosphors

ETSART can compute the production distribution of electron-hole (e-h) pairs on the order of nanometers (left figure) and the required energy to create an e-h pair (ε value), which is important for evaluating the response of the output device (right figure).

Y. Hirata, et. al., Jpn. J. Appl. Phys., 62, 106001 (2023)

Improvements of [weight window] and [t-wwg]

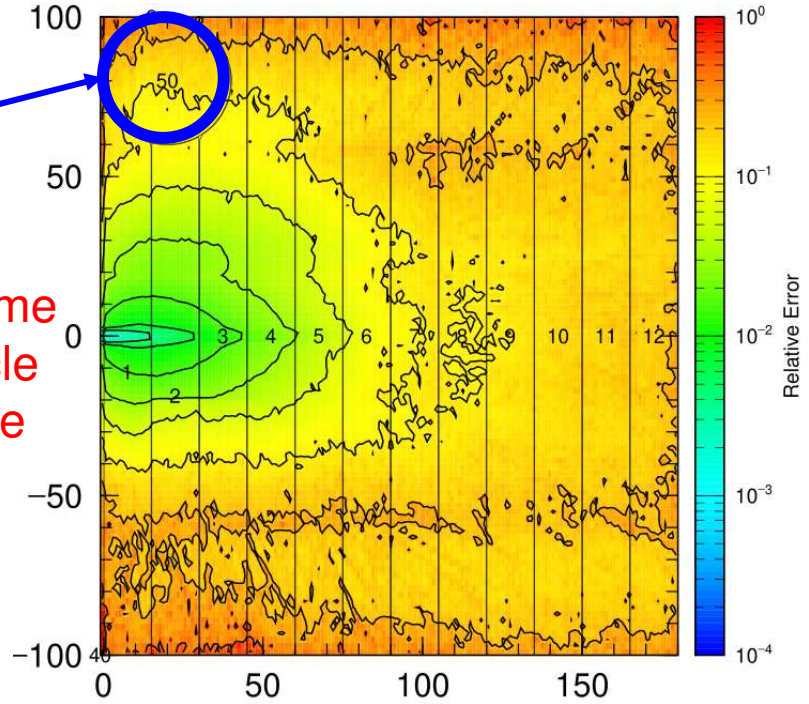
- ✓ A function to navigate particles to regions of interest was developed in [t-wwg] using history counter
- ✓ A function to prevent particles from too-much splitting was introduced in [weight window]
- ✓ A function to automatically fine-tune min & max values of xyz-mesh was introduced



Conventional [t-wwg]

History counter was set in this region

Statistical uncertainties around this region become smaller due to the particle navigation function, while those in other regions become higher



[t-wwg] with particle navigation

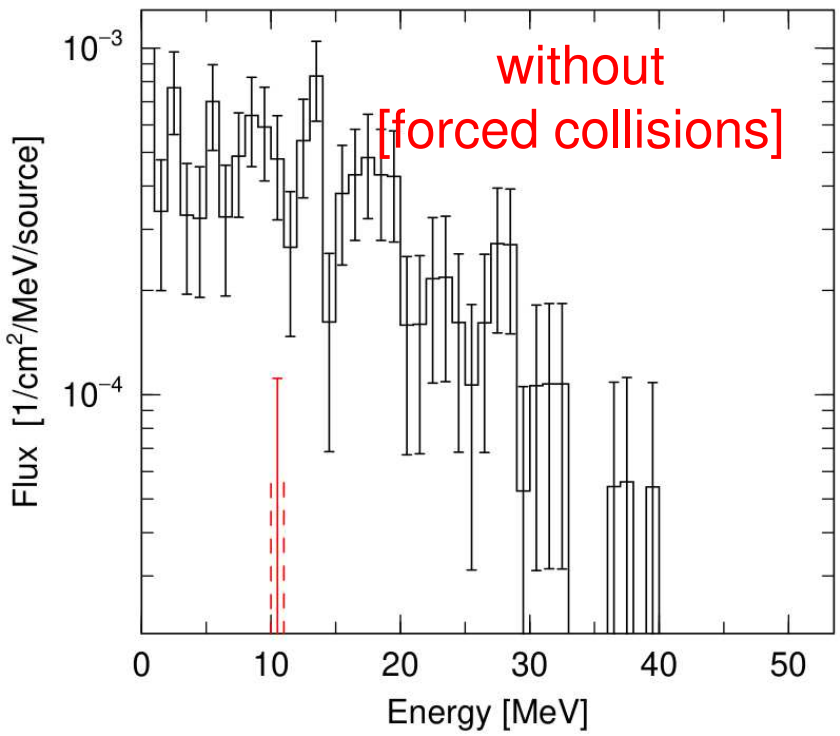
Statistical uncertainties of the effective doses calculated with [weight window] created by different [t-wwg] with the same computational time

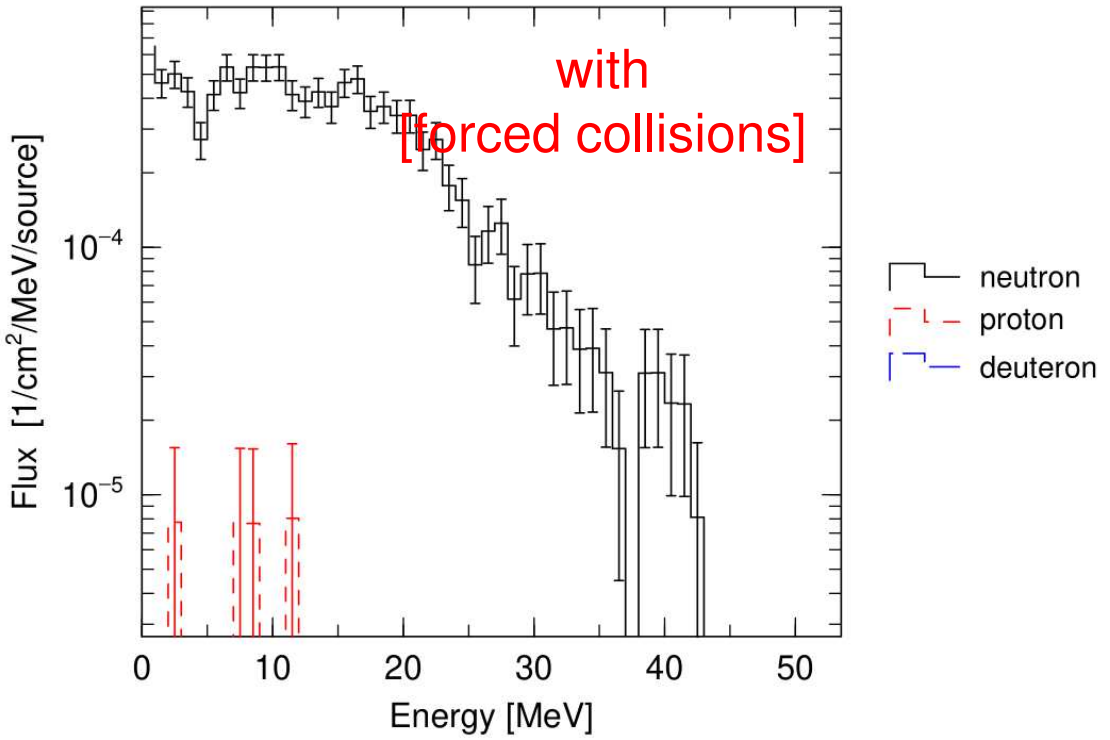
See phits/lecture/advanced/weightB in detail

[Forced collisions] in thick target

1. Divide the target into 50 segments* and calculate the collision probabilities in each segment
2. Determine the collision point using the probabilities
3. Reproduce nuclear reaction using either nuclear reaction model or nuclear data library

*Number of segments can be controlled by *nfcseg* parameter in [parameters]





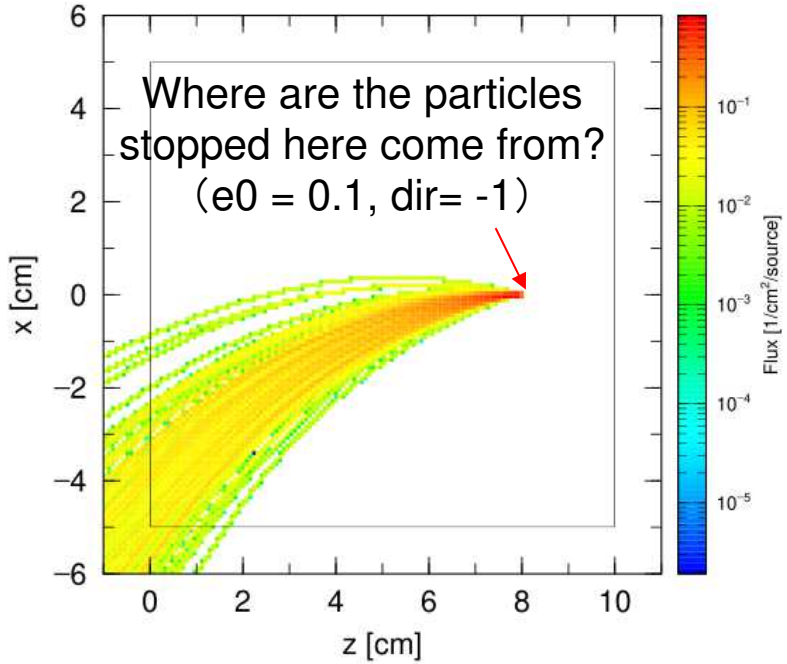
Fluences of outgoing particles from thick Be target (0.9 cm) irradiated with 20 MeV/n deuteron

See phits/recommendation/neutronsource

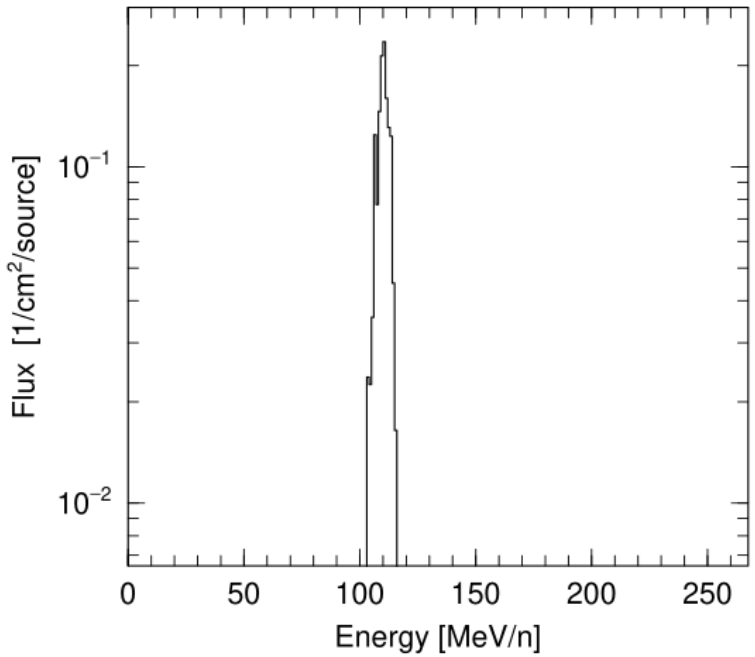
Adjoint mode for charged particles

What is adjoint mode?

- Time-inverse particle transport simulation
- Useful when you want to know the origin of the particle arrived at a certain location
- Used to be applicable only to photon, but a new modality for charged particles has been implemented
- Only stopping power and magnetic field can be considered (no nuclear reaction)



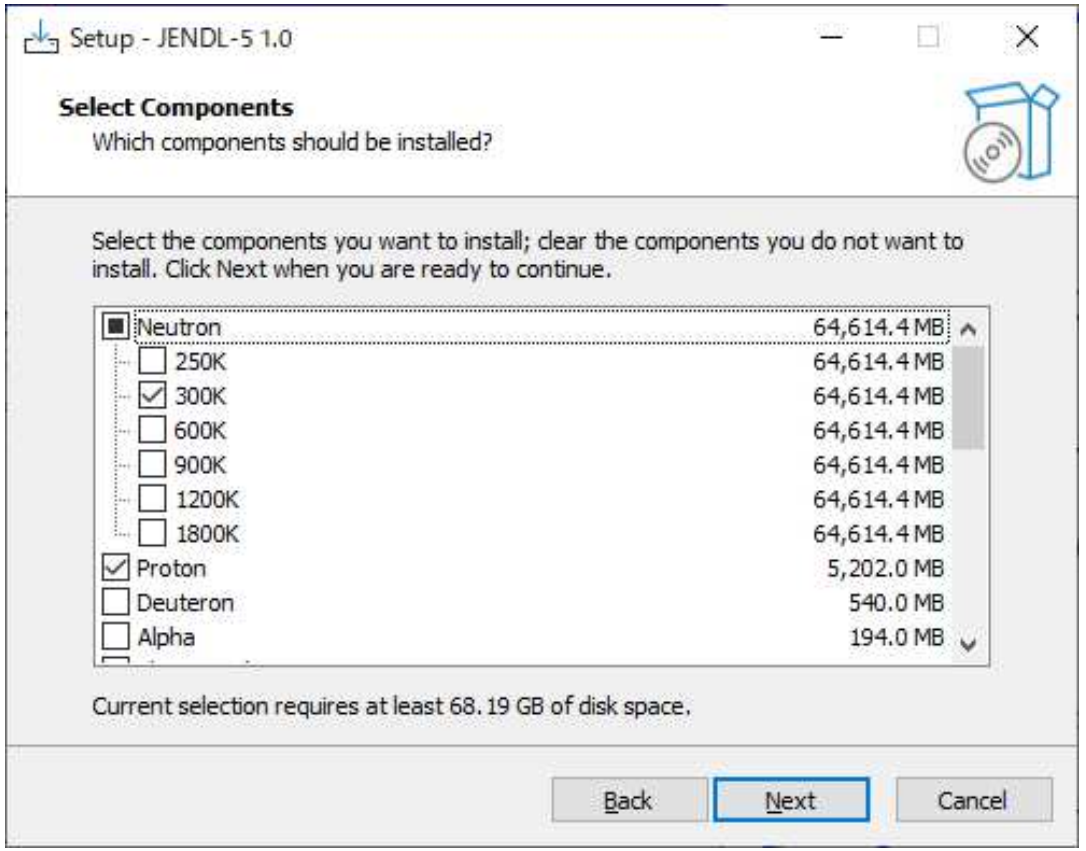
Proton trajectory in water with magnetic field



Energy distribution of protons when they go out

See /phits/utility/adjoint/charged in more detail

Automatic download and setup program for JENDL-5



Library Selection Window

Setup Procedures

1. Select the libraries* to be set up
2. Automatically download and extract the selected libraries
3. Copy address information given in xsdir in the downloaded library to that used in PHITS**
4. Change the natural abundance database used in material expansion according to JENDL-5 neutron libraries

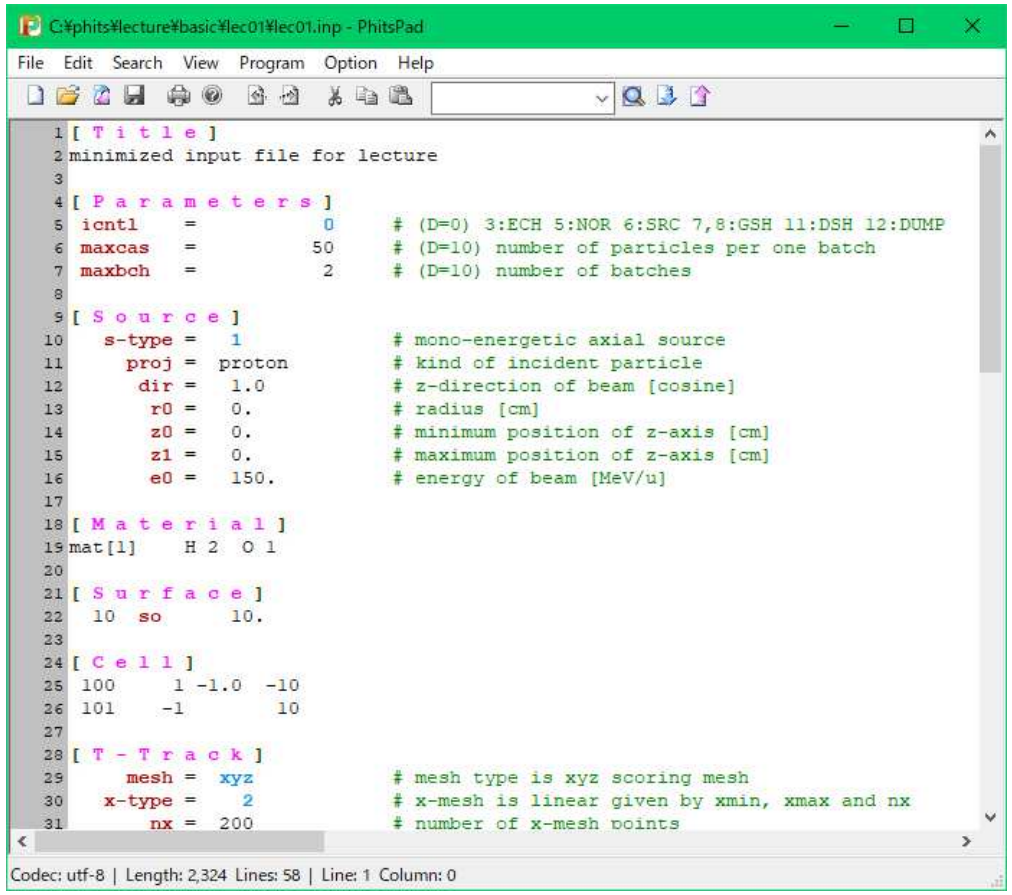
*Neutron for various temperatures, proton, deuteron, alpha particle, photo-atomic and photo-nuclear libraries as well as thermal neutron scattering kernels are available

**Neutron library will give priority to the last downloaded data. Thus, please be careful when you selected the neutron data library with temperature other than 300 K.

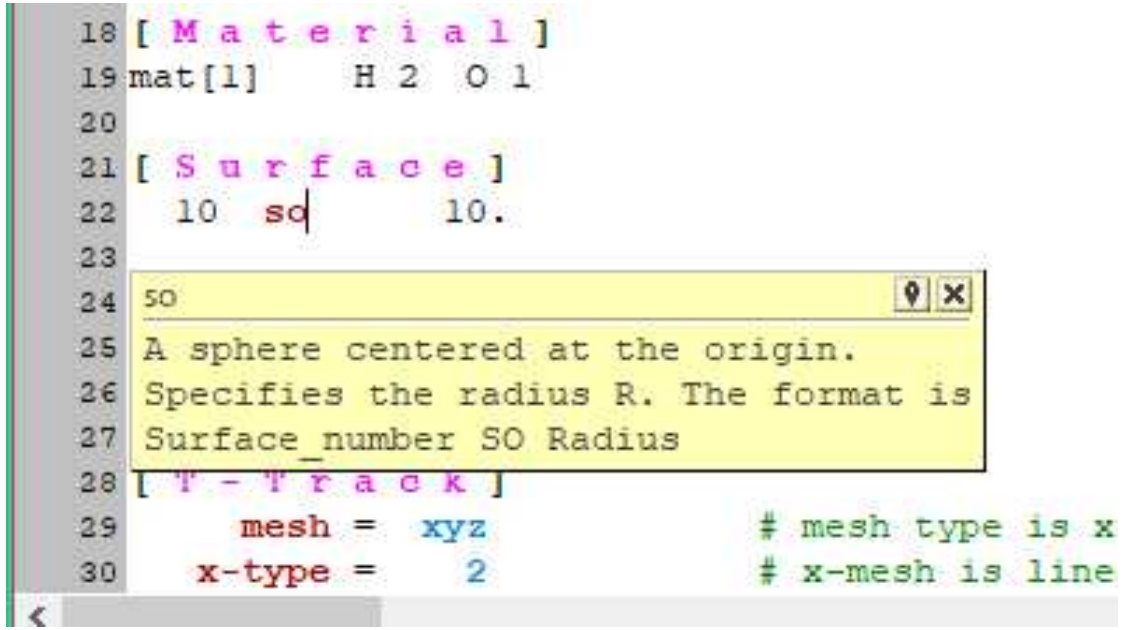
Setup program is included in phits/XS folder

Original text editor PHITS-Pad

1. Color highlighting of PHITS-specific parameters and input values.
2. Hint function to assist in making input files.



PHITS-Pad window

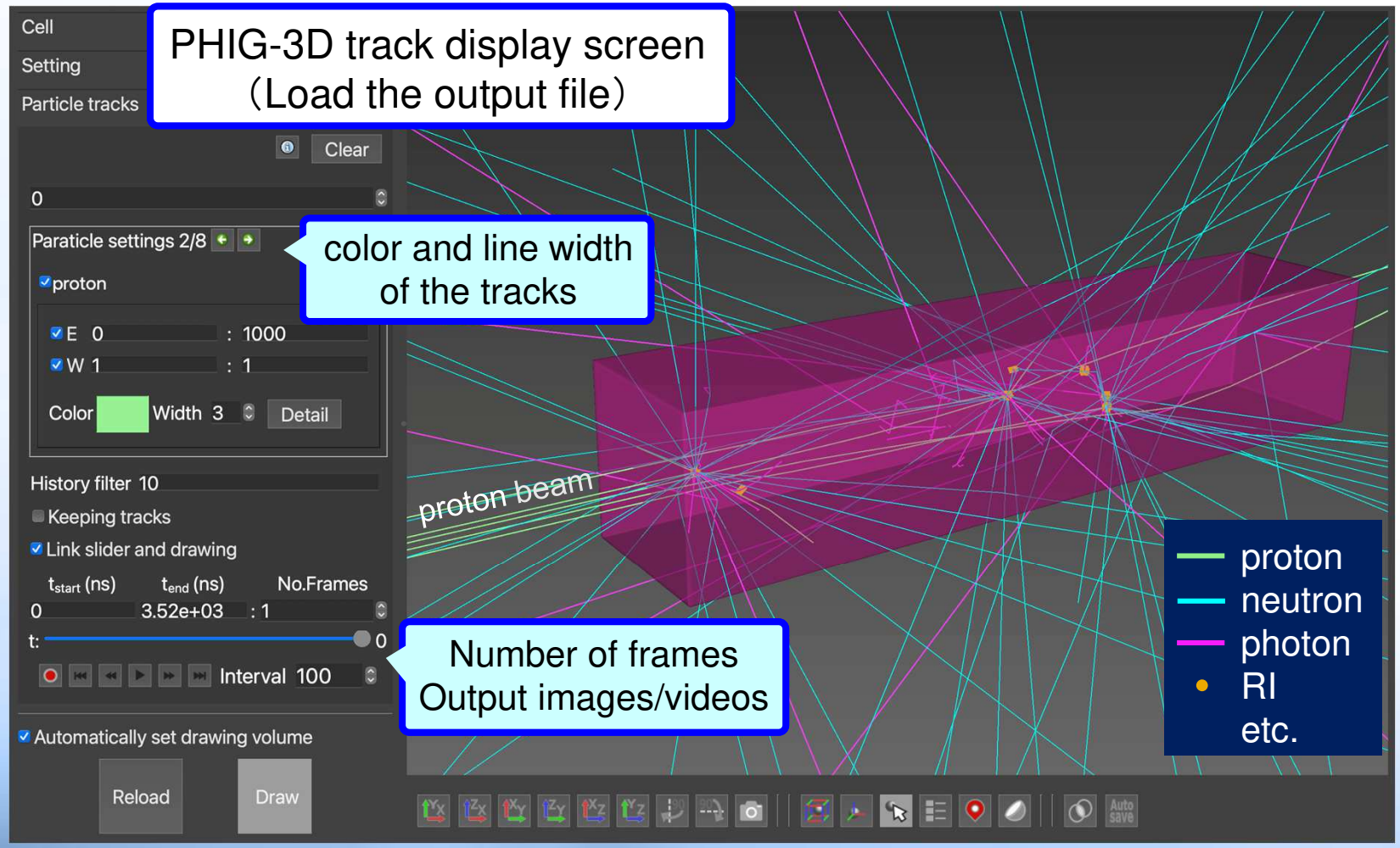


Hint window
（This can be moved by dragging）

See phits/phitspad/manual

Visualization of 4D (x,y,z,t) tracks in PHIG-3D

1. Create particle track files using [t-4Dtrack] section.
2. Render the track files with PHIG-3D.
   - ✓ Capable of creating images and videos.



Example of the section
[t-4Dtrack]
file = track.out

So Simple!!

Upcoming Futures

We are planning to …

➢ Improve the track structure mode

- ✓ Extension of the precise mode applicable to other elements/compounds
- ✓ Improvement of coupling modules connecting to material & life sciences

➢ Improve affinity to nuclear data library

- ✓ Enables dose calculation and event-generate mode using JENDL-5.0

➢ Develop user support functions

- ✓ Improvement of PHITS-Pad (help function)
- ✓ Improvement of RT-PHITS

➢ Improve accuracy and nuclear reaction model

- ✓ Improvement of JQMD ver. 2.0 to be faster and more accurate
- ✓ Improvement in the evaluation methods for both statistical & systematic uncertainty
- ✓ Comprehensive V&V