

New Features in PHITS3.37

PHITS development team, Aug. 2026

Recent Update History

2024 Apr. Register PHITS 3.34 to OECD/NEA Data bank
2025 Apr. Register PHITS 3.35 to OECD/NEA Data bank
2026 Apr. Register PHITS 3.36 to OECD/NEA Data bank
2026 Jun. AI agent workflow published on arXiv*
2026 Sep. Register PHITS 3.37 to OECD/NEA Data bank

**AI agent-driven autonomous execution version released off-cycle,
as an exception to the usual once-a-year release!**

*T. Sato et al., Toward AI-Agent-Driven Particle Transport Simulations: Implementation of AI-Assisted Workflows for PHITS, arXiv:2607.11309. <https://doi.org/10.48550/arXiv.2607.11309>

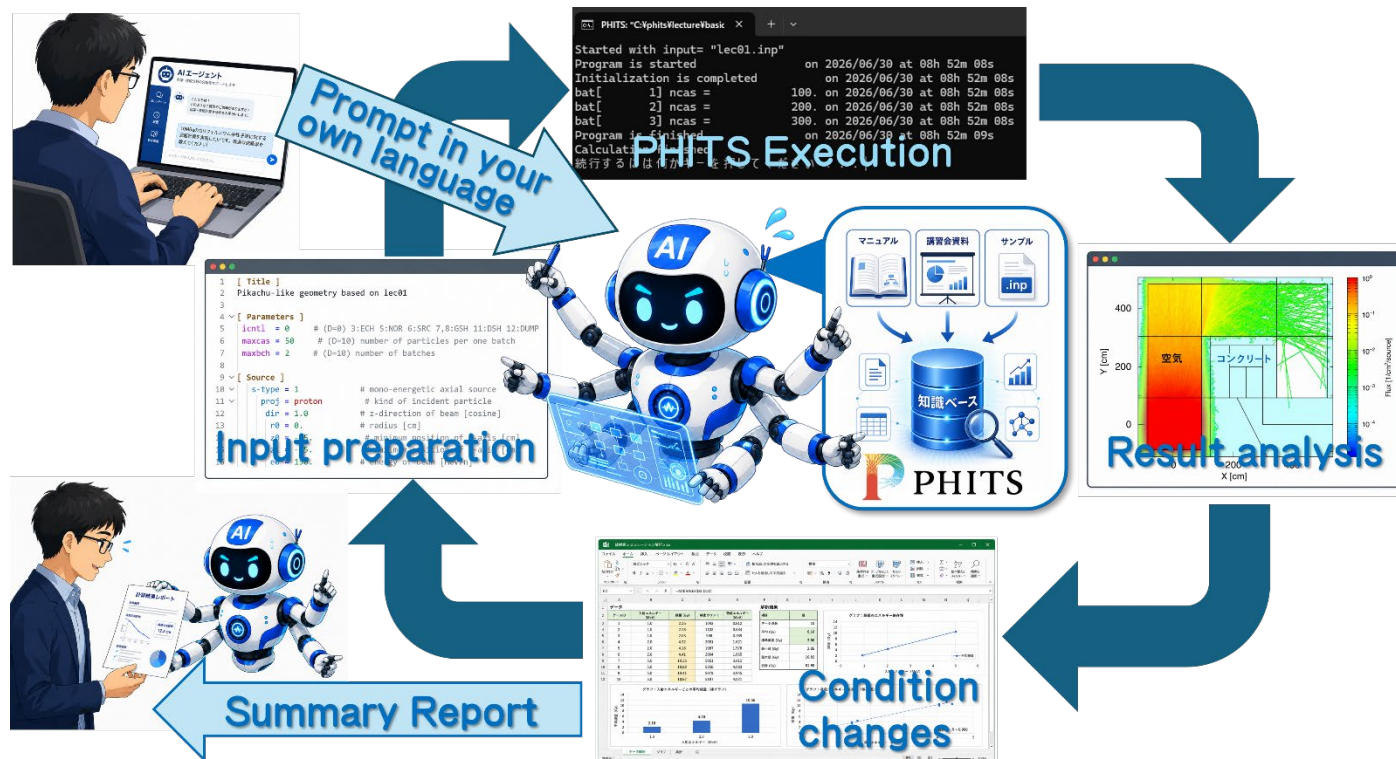
Major New Features in Version 3.37

- ✓ Introduction of AI agent-driven autonomous execution capability
- ✓ Introduction of the weight window (WW) auto-update function in [t-wwg]
- ✓ Introduction of the [expand hash-all] section for cases with many regions subtracted by #all
- ✓ Introduction of a new [material] definition method using pre-defined materials
- ✓ Introduction of reaction specification by identification number in [counter], [t-product] and [t-interact]
- ✓ Improvement of PHITS-Chem: temperature dependence
- ✓ Development of a function in [t-dchain] for calculating induced radioactivity from activation cross sections and fluence
- ✓ Completion of PHITS language support for PHITS-Pad, NotePad++, VS Code, etc.
- ✓ Reorganization of the recommendation, lecture, sample and utility folder structures
- ✓ Conversion of the DCHAIN-PHITS, ANGEL and PHIG-3D manuals to html format

Red items are described in detail in this document

AI Agent-Driven Autonomous Execution

AI agents such as Codex, Claude Code, Antigravity, GitHub Copilot, and Qwen Code enable iterative PHITS workflows—from input preparation and execution to result analysis and condition changes—through prompts in your own language



Full-scale use requires a paid plan for the AI service you use, but free plans can also be used to a certain extent, so please give it a try. For setup instructions, see [phits/workbench/README.docx](https://github.com/keiichi-hara/phits/workbench/README.docx), and [phits/lecture/advanced/AI-agent](https://github.com/keiichi-hara/phits/lecture/advanced/AI-agent) for specific usage examples.

See <https://arxiv.org/abs/2607.11309> for details

Weight window (WW) auto-update function in [t-wwg]

Old method

- ✓ Set [t-wwg] and run PHITS once
- ✓ Import [t-wwg] result into PHITS input file and run PHITS multiple times to optimize the WW
- ✓ Run the main calculation with the optimized WW

Histories and runs needed to obtain the optimal WW should be decided based on users' experience

New method

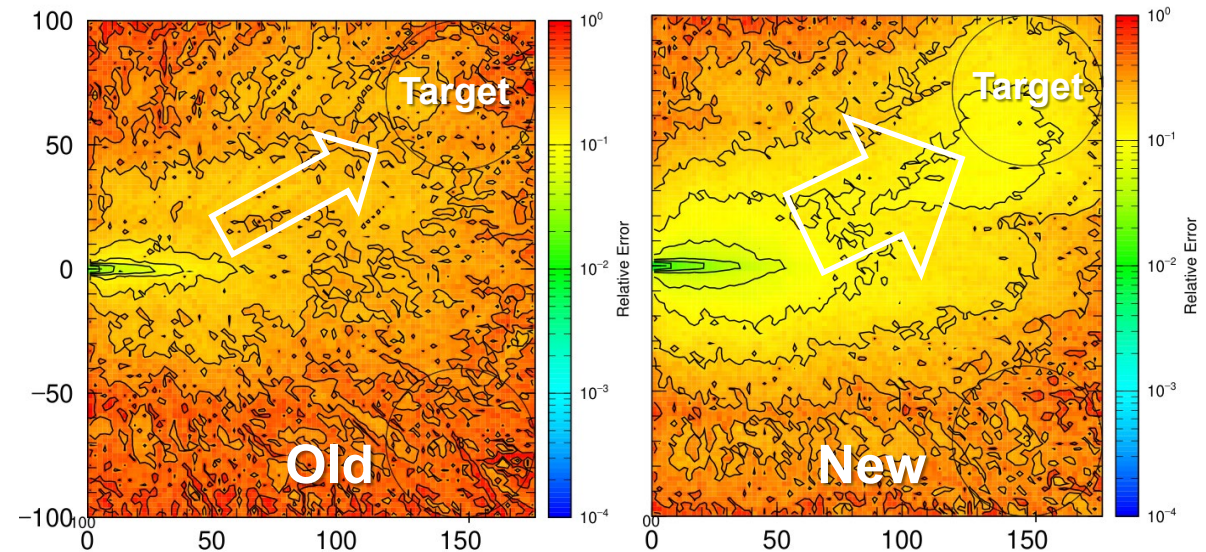
- ✓ Set [t-wwg] and run PHITS once
- ✓ Run the main calculation with the optimized WW

With upgraded [t-wwg], WW is updated every batch and the run stops automatically once results converge

Improvement of the particle navigation function

Old: **all tracks** of that history are emphasized

New: the track is back-analyzed and only **the tracks of the parent particles** are emphasized



Particle navigation is now much clearer

Introduction of the [expand hash-all] section

What is the [expand hash-all] section?

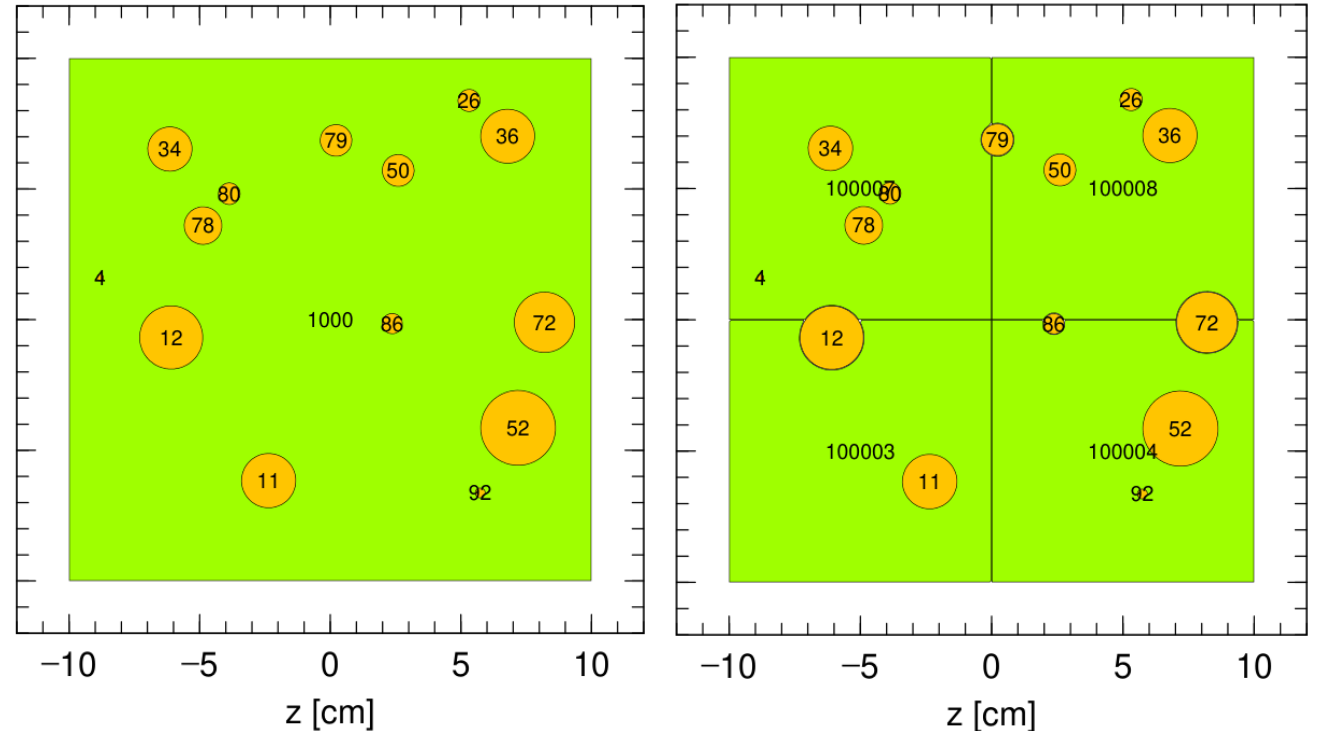
A preprocessing function that automatically divides cells containing #all and then expands them.

When should it be used?

It should be used when the number of cells subtracted by #all is large or complex, causing insufficient memory or a delay in computation time.

How should it be used?

1. Define the [expand hash-all] section, set icntl=18, and run PHITS → **The Bounding box of each region is calculated, and from that information, #all is expanded, and [cell] and [surface] are output.**
2. Include the output files with the infl command, comment out the regions where #all was defined, and then run PHITS



Results when 100 water-vapor bubbles are randomly placed in water, using #all (left) and expanding with [expand hash-all] (right)

See phits/sample/misc/expand_hash-all for details

Introduction of Pre-defined Materials

New material definition method using pre-defined materials

- ✓ In [material], select a pre-defined material* from data/predefined_material.dat
- ✓ Define each pre-defined material by enclosing its Alias name in @ (e.g., **m1 @WATER@**)
- ✓ In [cell], define it by enclosing the Alias name in % and set the density to 0.0 (e.g., **1 %WATER% 0.0 -1**)

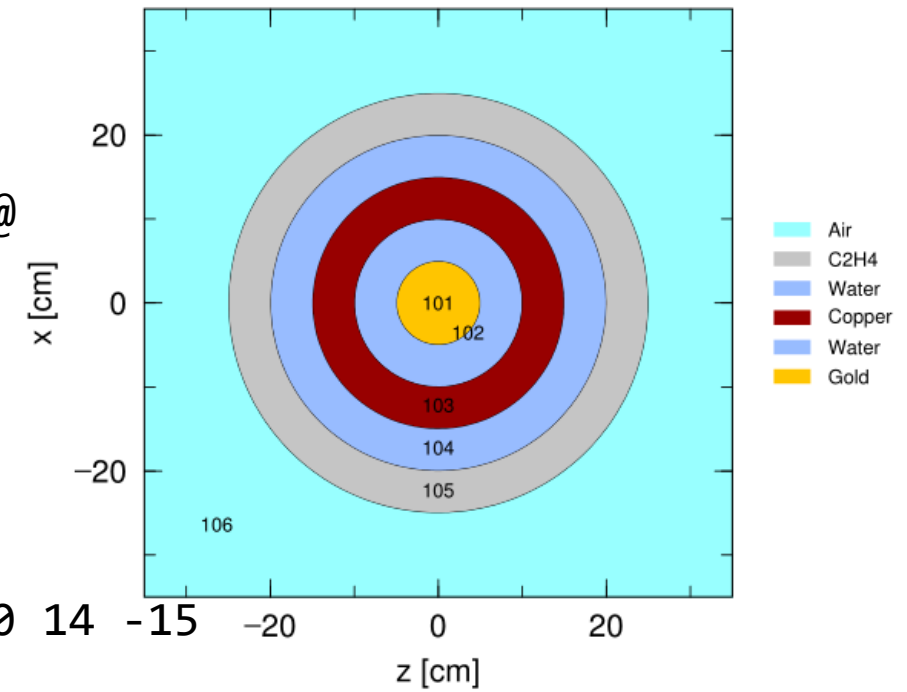
```
[ Material ]
mat[1]      Au 1
mat[2]      H 2 0 1
mat[3]      Cu 1
mat[5]      C 2 H 4
mat[6]      N 8 0 2
```

```
[ Cell ]
100 -1      10
101 1 -19.32 -11
102 2 -1.00  11 -12
103 3 -8.93  12 -13
104 2 -1.00  13 -14
105 5 -0.90  14 -15
106 6 -0.0012 15 -10
```



```
[ Material ]
mat[1]      @GOLD@
mat[2]      @WATER@
mat[3]      @COPPER@
mat[5]      @POLYETHYLENE(0.94)@
mat[6]      @AIR_DRY@
```

```
[ Cell ]
100 -1      10
101 %GOLD% 0 -11
102 %WATER% 0 11 -12
103 %COPPER% 0 12 -13
104 %WATER% 0 13 -14
105 %POLYETHYLENE(0.94)% 0 14 -15
106 %AIR_DRY% 0 15 -10
```



Onion geometry using the old and new definition methods ([phits/lecture/basic/lec03/onion.inp](https://phits.jp/lecture/basic/lec03/onion.inp))

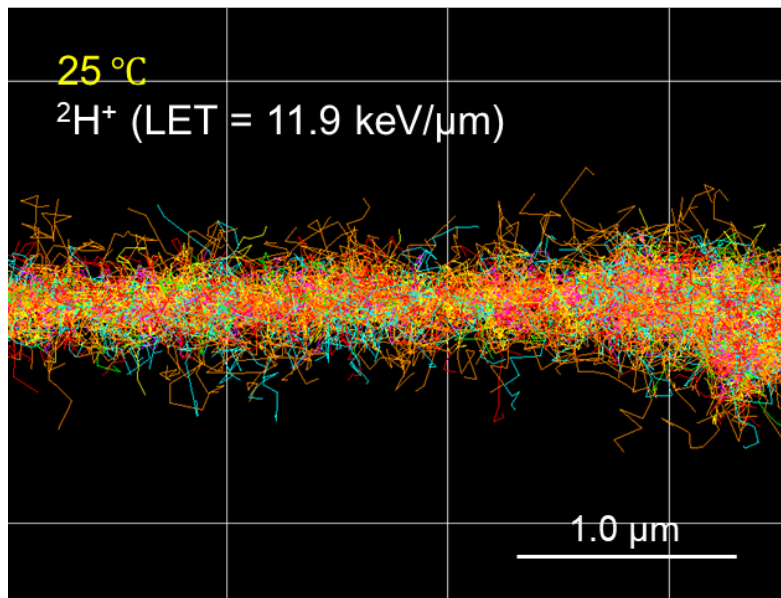
*The database registers the pre-defined materials from Flair, 641 materials in total, plus 3 types of Japanese and US concrete.

Improvement of PHITS-Chem: temperature dependence

New features

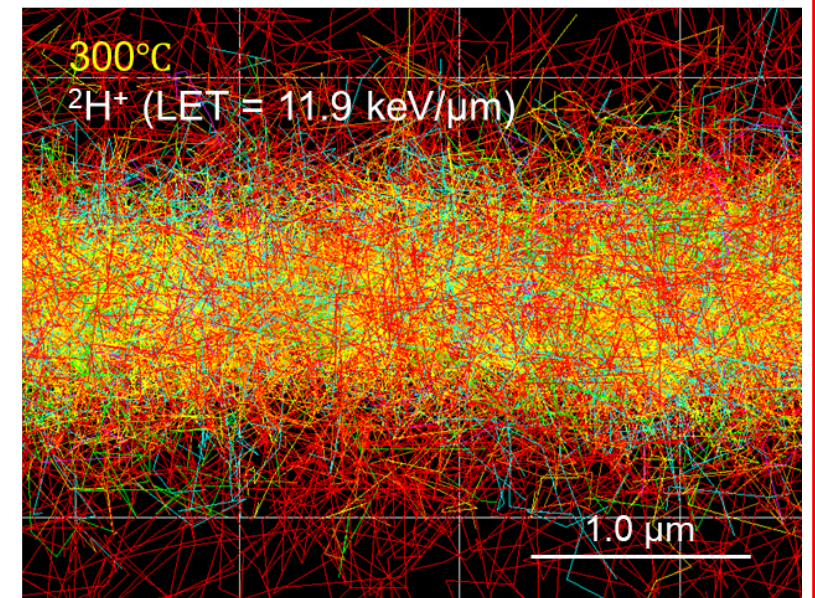
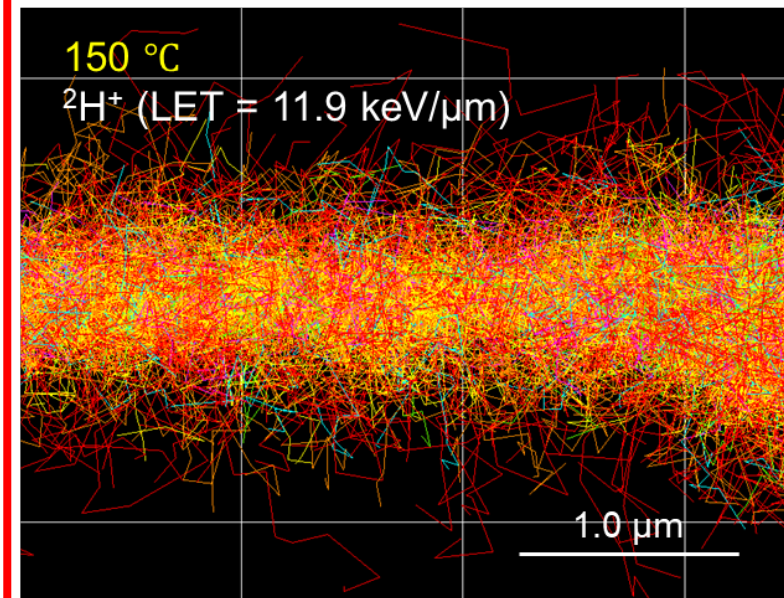
- ✓ Newly implemented temperature dependence of diffusion coefficients and chemical reaction rate constants for water radiolysis products in aqueous solution
- ✓ PHITS-Chem extends the calculation temperature range from the conventional 25 °C to 0–350 °C.

Conventional temperature (25 °C)



NEW

Expanded to a temperature range of 0–350 °C!



•OH e_{aq}^- $\text{H}^\bullet$ H_3O^+ H_2 H_2O_2

Y. Matsuya et al. Sci. Rep. 16, 21477 (2026)

See [phits/sample/UserDefined/usrtally/ChemCode](https://phits.sample/UserDefined/usrtally/ChemCode)

This improvement was performed under the support of Dr. Yuji Yoshii (Hokkaido University of Science)

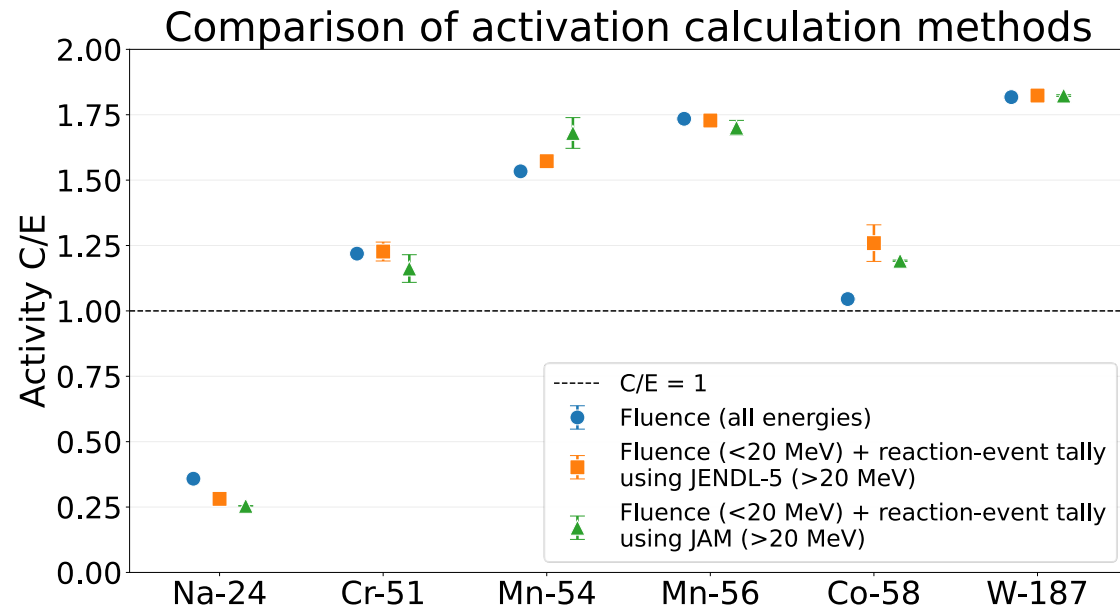
Fluence-based activation calculation in [T-Dchain]

New idyldmode option in [T-Dchain]

Nuclide production is calculated from particle fluence rather than tallied only when reaction events occur, thereby improving statistical precision.

Method	Neutrons below 20 MeV	Particles with JENDL-5*	Others
idyldmode=0 (old)	JENDL-5 (fluence)	JENDL-5 (reaction events)	Nuclear reaction models
idyldmode=1 (new)	JENDL-5 (fluence)		Not included

*n ($20 < E < 200$ MeV), p ($E < 200$ MeV), d ($E < 100$ MeV/n), α ($E < 3.75$ MeV/n), γ ($E < 150$ MeV)



Statistical error for the same history number:
Old method: 3% avg → New method: 0.2% avg
Substantially improved statistical precision

Activation of Eurofer-97 by secondary neutrons produced by 67 MeV protons incident on a D₂O target

Important bug fixes in Ver. 3.37

- ✓ A bug that causes an abnormal termination due to insufficient EXS array length when reading electron cross-section data with `nucdata = 0`.
- ✓ A bug in which the automatically generated constant names are not output correctly when more than 20 energy groups are defined in `[t-wwg]` (changed to use the parameters from `c100` onward).
- ✓ A bug in which `autorun.sh` terminates abnormally due to too many arguments when many `*.out` files, or files with long names, exist on Linux and macOS.
- ✓ A bug in which the initial random number does not change according to the calculation start time in an MPI environment even when `itimrand = 1` is specified.
- ✓ A bug in which the computation time increases significantly in `[t-deposit2]` due to unnecessary array initialization and array allocation for each history.
- ✓ A bug in which the progress information given by `ihistout` is not output in ascending order in an OpenMP environment.
- ✓ A bug in which the results differ between the single version, the OpenMP version and the MPI version when reading a dump source.

Please refer “1.1 Recent Improvements” of PHITS manual for more details

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

➤ Develop user support functions

- ✓ Output of various tallies in HDF5 format
- ✓ CAD-to-PHITS geometry simple conversion function
- ✓ AI agent-driven operation of PHIG-3D

➤ Improve accuracy and nuclear reaction model

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