PHITS

Particle and Heavy Ion Transport code System

General Introduction

Last update 2022/03/25

Development Team Members

T. Sato[1], Y. Iwamoto[1], S. Hashimoto[1], T. Ogawa[1], T. Furuta[1], S. Abe[1], T. Kai[1], Y. Matsuya[1], N. Matsuda[1], Y. Hirata[1], Lan Yao[1],Pi-En Tsai[1*], H. Ratliff[1**], H. Iwase[2], Y. Sakaki[2], N. Shigyo[3], L. Sihver[4], K. Niita[5]

1. *Japan Atomic Energy Agency, JAEA, Japan*
2. *High Energy Accelerator Research Organization, KEK, Japan*
3. *Kyusyu University, Japan*
4. *Technische Universität Wien, Austria*
5. *Research Organization for Information Science and Technology, RIST, Japan*

Current affiliation: *LBL, USA; **HVL, Norway

Table of Contents

What is PHITS?

Particle and Heavy Ion Transport code System

Capability

Transport and collision of nearly all particles over wide energy range using Monte Carlo method

neutron, proton, ions, electron, photon etc

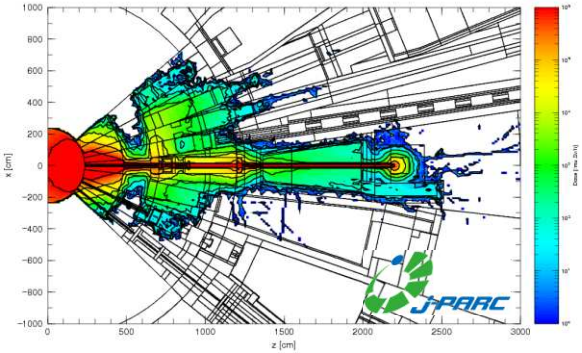
10^{-4} eV to 1 TeV/n

All-in-one-Package

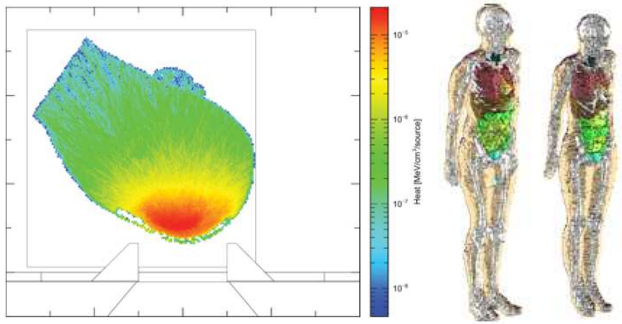
All contents of PHITS (source files, binary, data libraries, graphic utility etc.) are fully integrated in one package

Available in free of charge by submitting application form via PHITS website

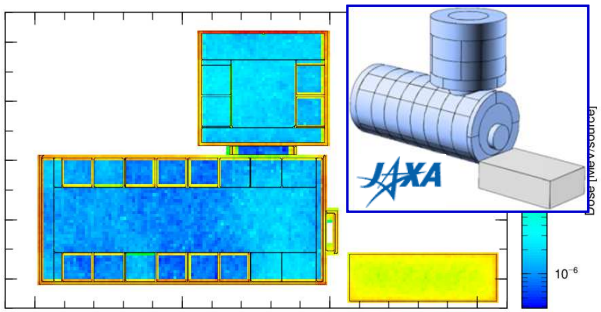
Applications



Accelerator Design



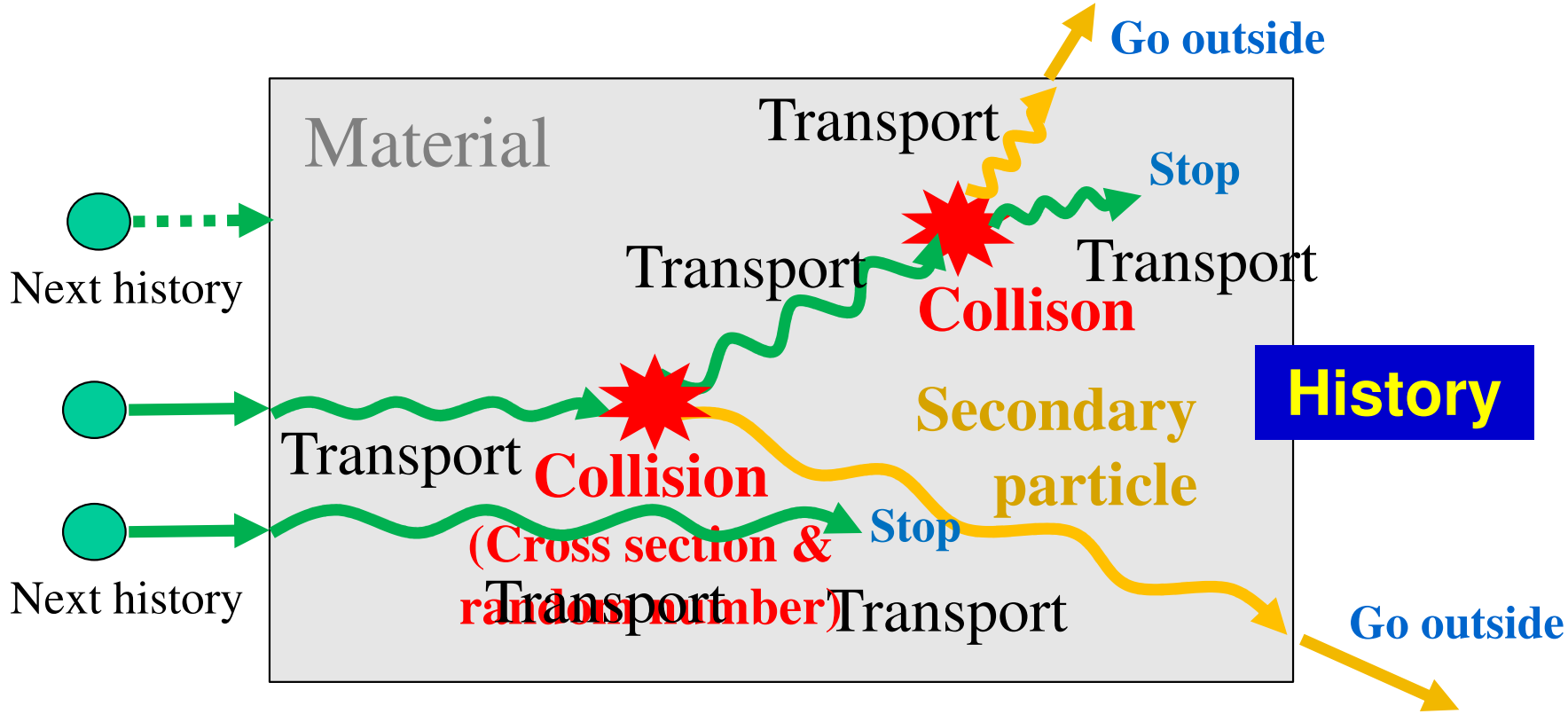
Radiation Therapy & Protection



Space & Geoscience

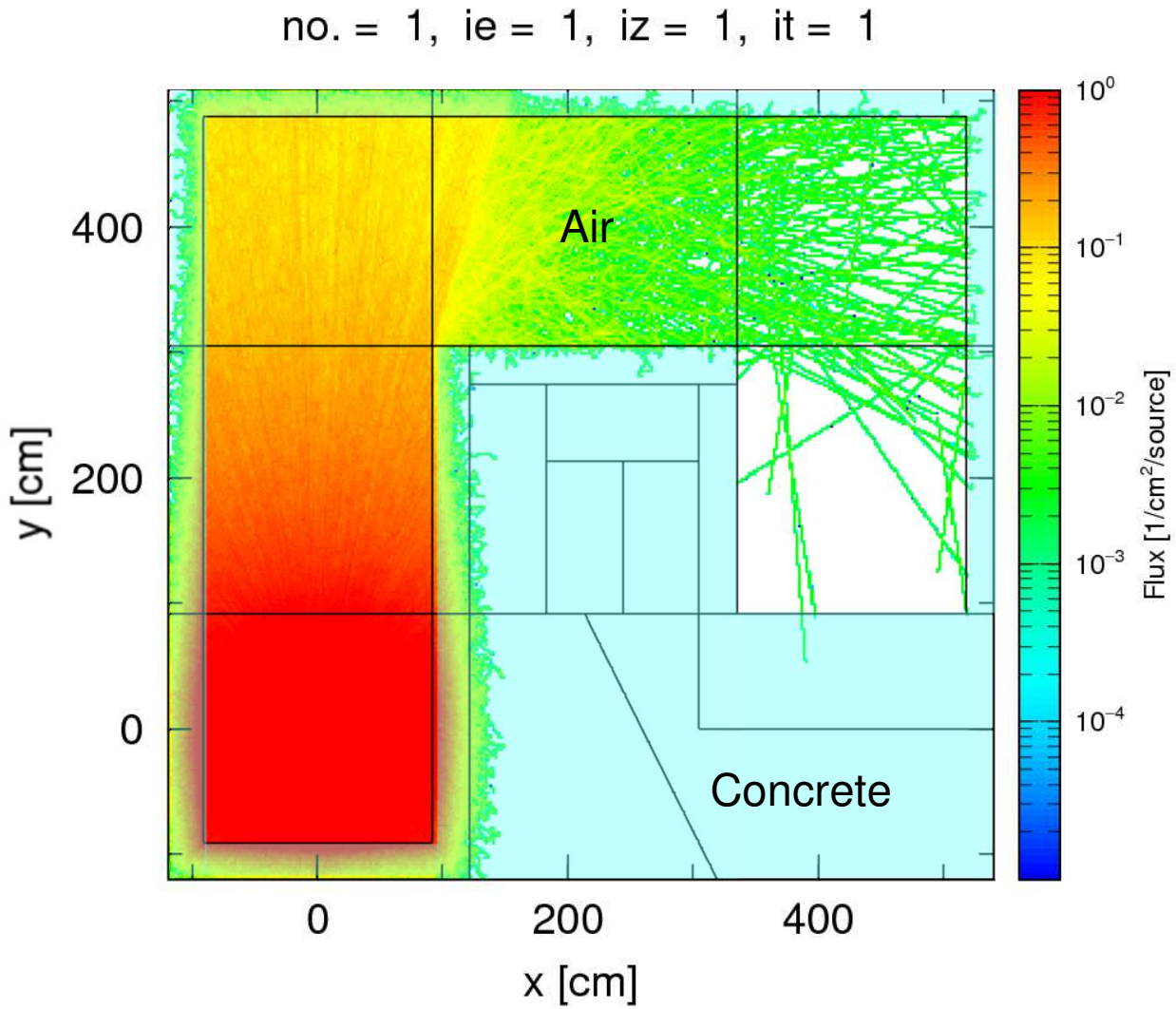
What is Monte Carlo method?

Trace each particle motion using random number, and estimate their average behavior by iterating the simulation



- ✓ Behavior of each particle is highly stochastic issue
- ✓ Average behavior is getting closer to the realistic
- ✓ Monte Carlo method is time consuming, but accurate!

Example of PHITS Calculation



Motion of 100,000 photons produced from ^{137}Cs simulated by PHITS

Average of all particle behaviors → mean particle fluence → shielding ability

Basic Features of PHITS

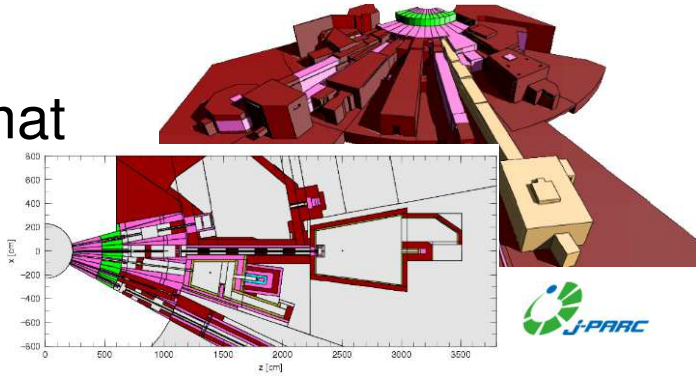
✓ **Source code:** Fortran (Intel Fortran, gfortran)

✓ **Input file:** PHITS original language in free-format text

You do not have to write Fortran program nor compile PHITS

✓ **Geometry**

- General Geometry (GG) format
- Graphic utilities
- Support software:
  (ParaVIEW*, SuperMC**)



ANGEL output (2D & 3D)

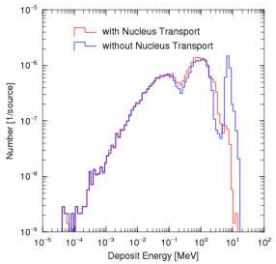
PHIG-3D (GUI)

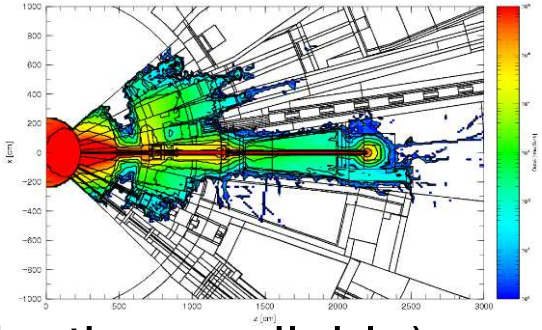
✓ **Tally functions**

Particle fluence, absorbed dose, number of interaction, nuclide yield etc.

✓ **Output Data**

Text data, histograms, contour maps





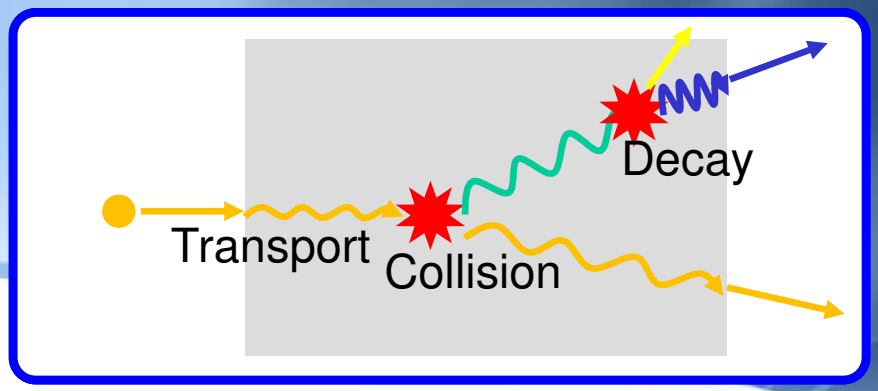
✓ **Platforms**

Windows, Mac and Linux (MPI & OpenMP parallelization available)

*Visualize PHITS geometry & tally results **Convert CAD geometry to PHITS input format

Table of Contents

Physical Processes included in PHITS



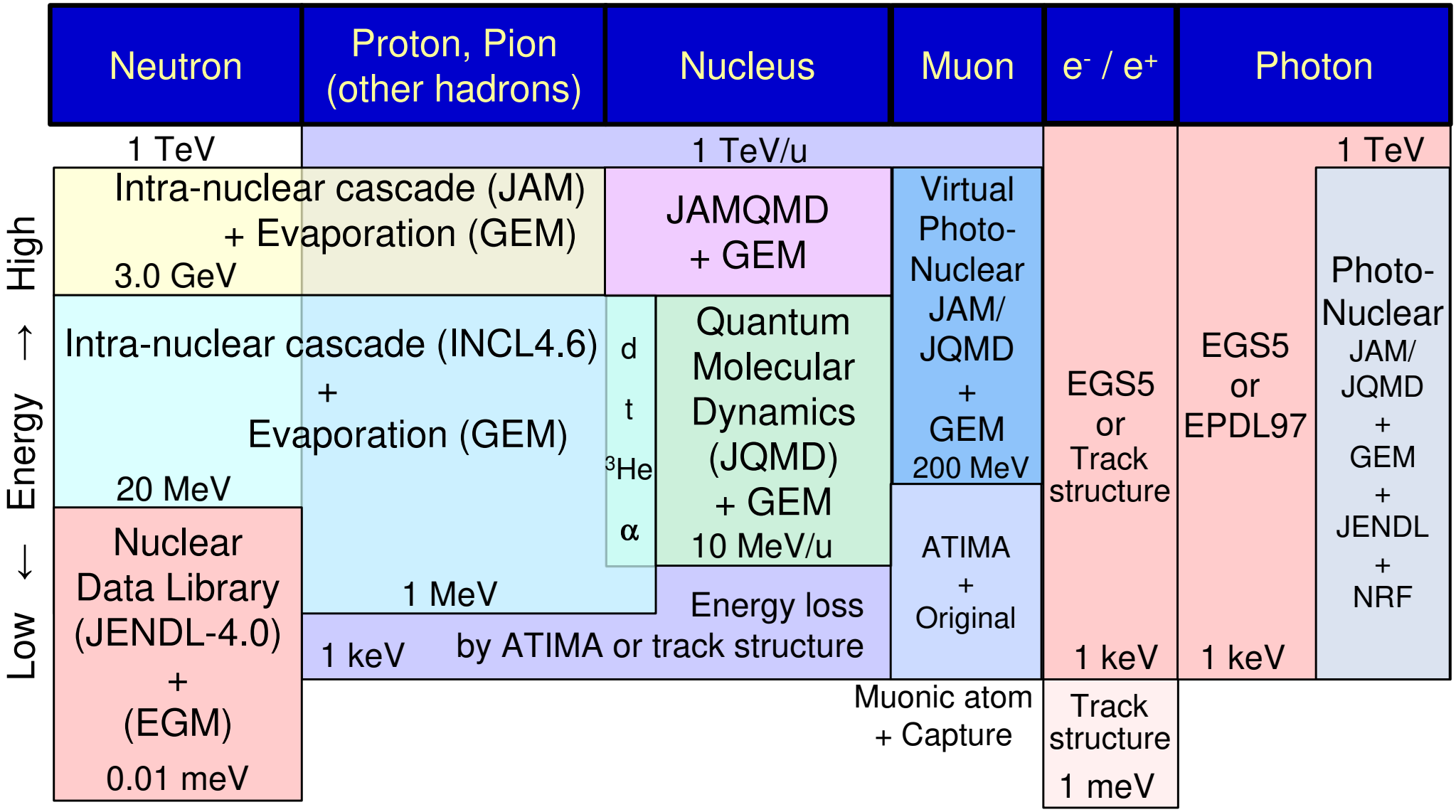
Collision & decay processes

- **Nuclear interaction**
  - High-energy spallation reaction
  - Photon and muon-induced reaction
  - Absorption, resonance, fission reaction
- **Atomic interaction**
  - Photo-electric, Compton, pair production
  - Møller/Bhabha scattering, Annihilation
  - Bremsstrahlung
  - Knock-out electron (δ-ray) production
  - Ionization/excitation (track structure mode)
- **Particle decay**
  - Decay with lifetime (neutron, μ, π etc.)

Transport process

- **Ionization / excitation**
  - Continuous slowing down approximation
  - Energy & angular struggling
- **External field / reflection**
  - Electric / magnetic field
  - Gravity
  - Reflection (super mirror etc.)

Map of Models Recommended to Use in PHITS

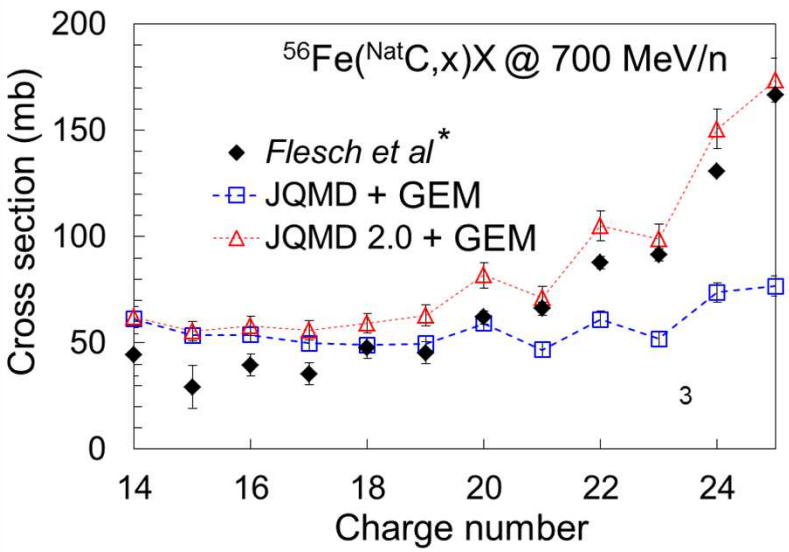


Physics models of PHITS and their switching energies

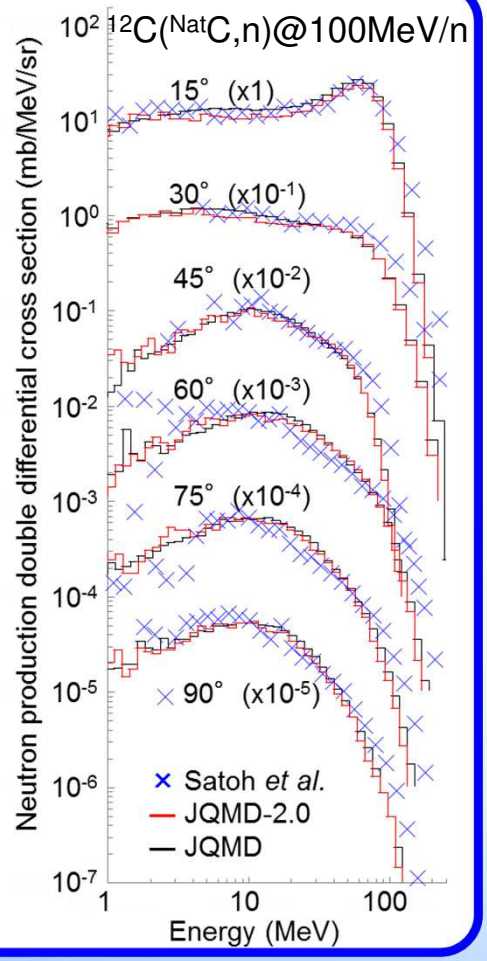
Switching energies can be changed by input file of PHITS

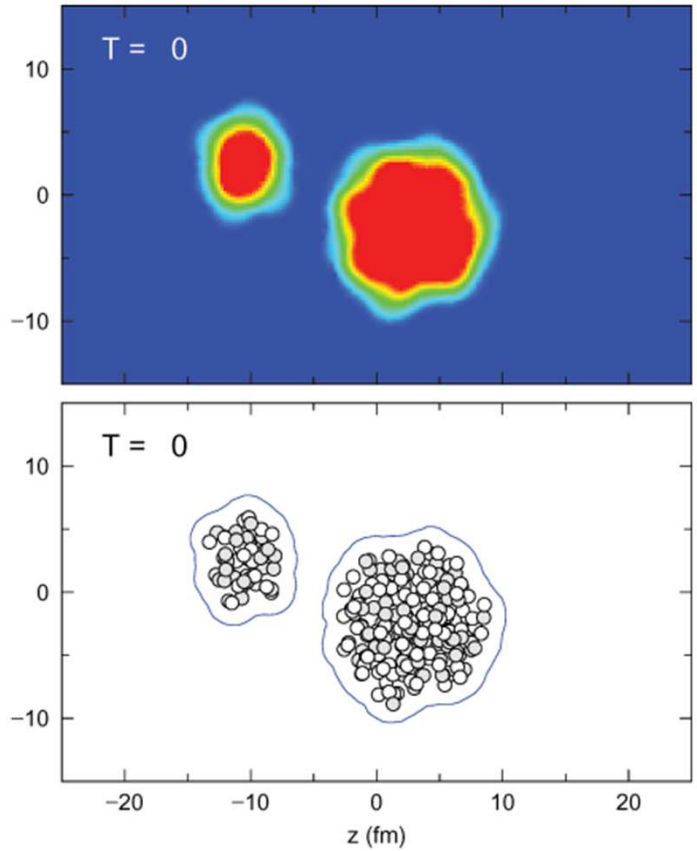
JQMD (JAERI Quantum Molecular Dynamics) Model

- ***JQMD*** can dynamically simulate the time evolution of nuclear reactions, considering the correlations between *every combination of nucleons*.
- Dedicated to simulation of ion-induced nuclear reactions



Precisely reproduce residual nuclide yields (↑) and secondary neutron productions (→)





^{56}Fe 800 MeV/u on ^{208}Pb

K. Niita et al, Phys. Rev. C52 (1995) 2620, T. Ogawa *et al.*, Phys. Rev. C92 (2015) 024614

Nuclear Data Library

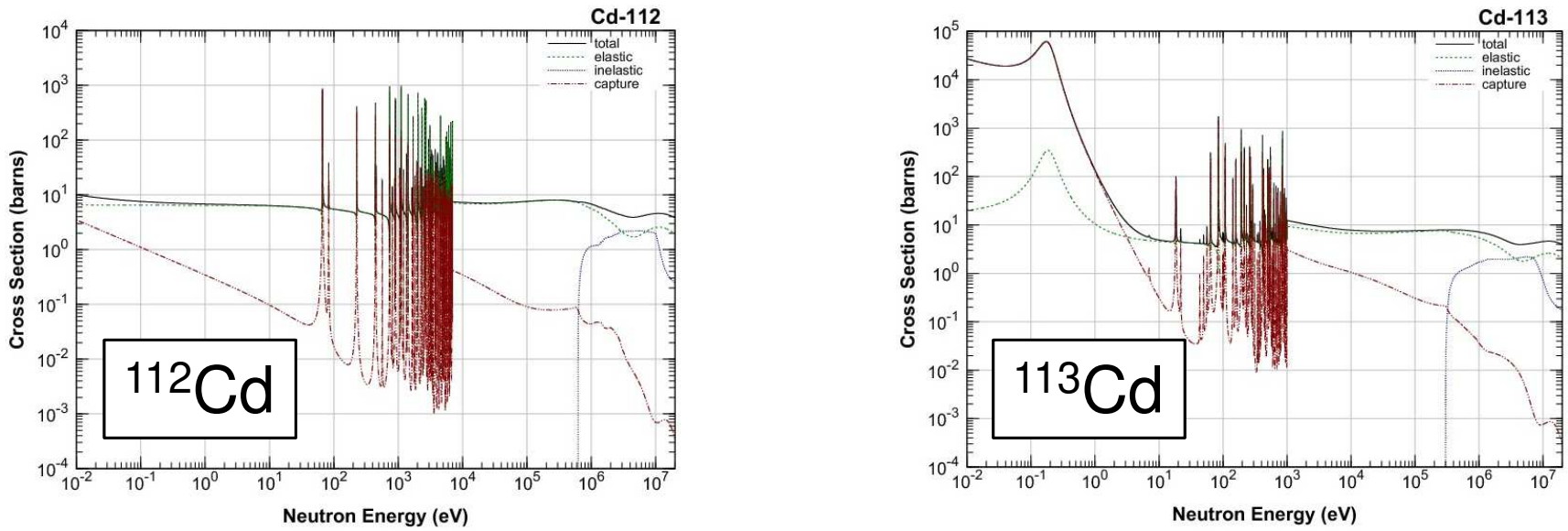
Cross sections for low energy neutrons strongly depend on nuclear structure

▼

Physics models are inadequate because they cannot consider the structure

▼

Nuclear data library evaluated based on experimental data is necessary



Neutron reaction cross sections of ^{112}Cd and ^{113}Cd taken from JENDL-4.0

- ✓ JENDL-4.0: Neutron cross sections below 20 MeV for 407 isotopes
- ✓ JENDL-4.0/HE: Neutron and proton cross sections below 200 MeV for 25 isotopes

http://wwwndc.jaea.go.jp/jendl/j40/J40_J.html
https://rpg.jaea.go.jp/main/en/ACE-J40HE/index.htm

Event Generator Mode

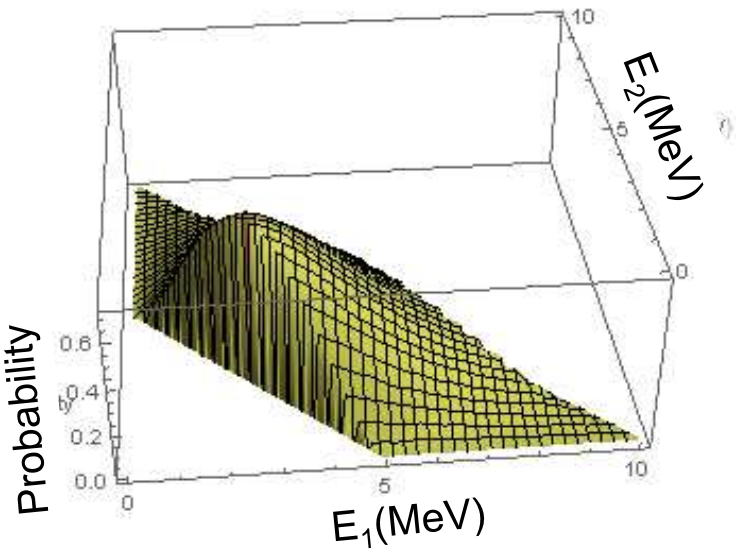
What is event generator mode (EGM)?

Original sampling method of secondary particles using nuclear data library

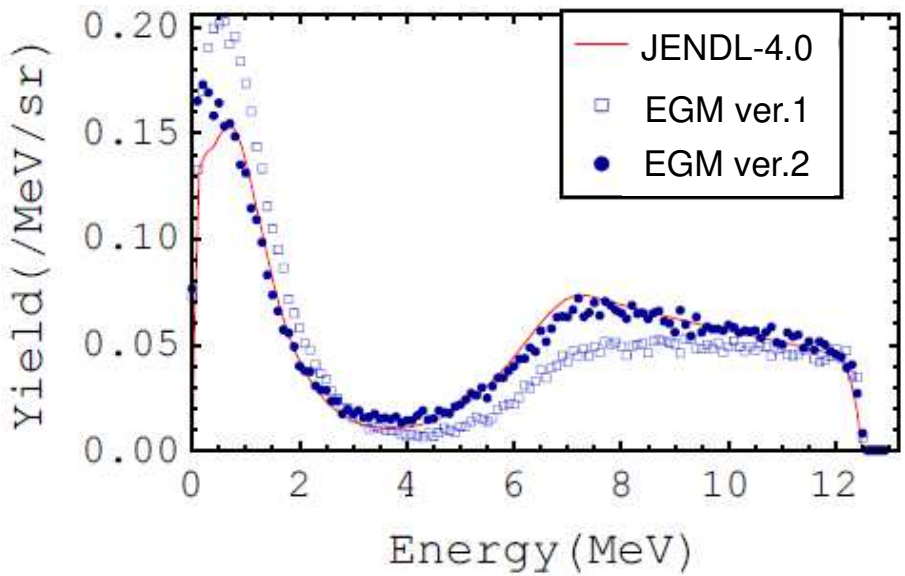
Difference between EGM and conventional method

EGM: Sample all secondary particles from 2D energy sampling space at once, considering energy & momentum conservation in an event

Conventional method: Sample particle by particle from 1D energy distribution



Energy sampling space



Secondary particle yields from ^{150}Nd(n,2n)

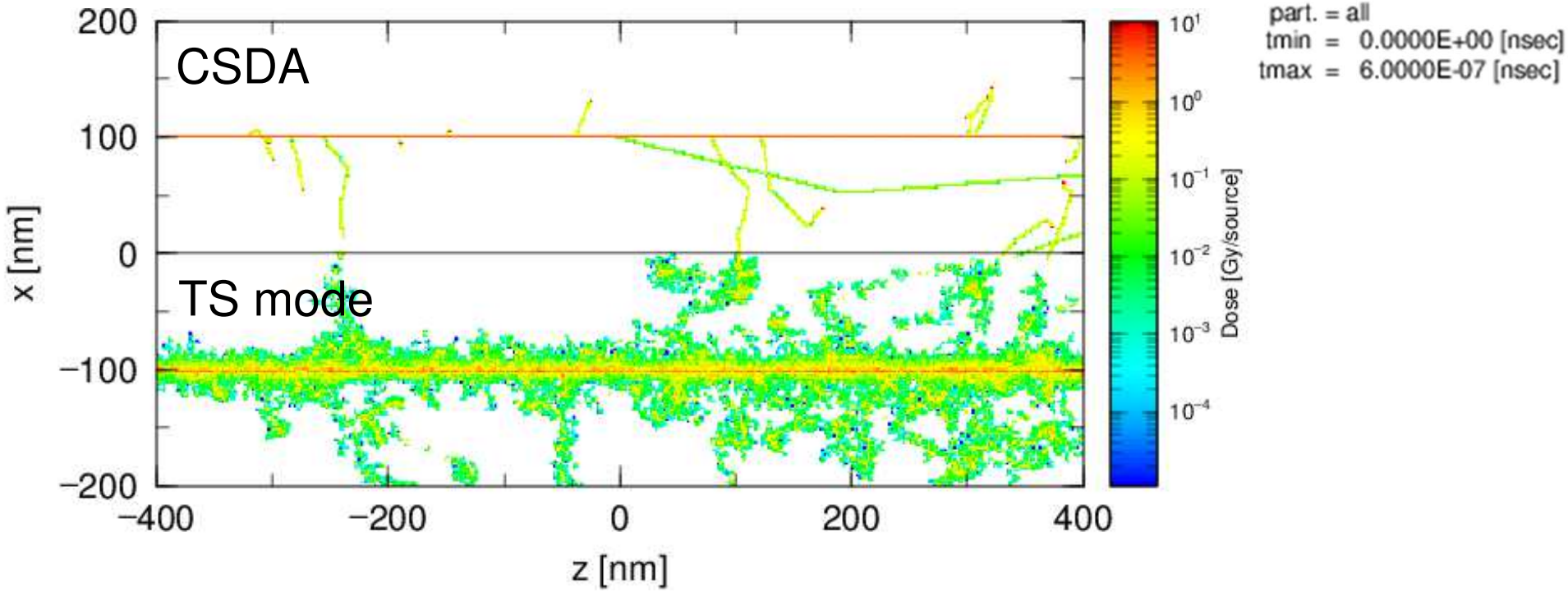
Indispensable in some cases such as detector response simulation

T.Ogawa *et al.*, *NIM A*, **763**, 575-590 (2014)

Track Structure (TS) Mode

Energy loss of charged particle in PHITS

- ✓ CSDA: combine a number of ionizations and excitations as an event
- ✓ TS mode: explicitly consider each ionization and excitation as an event



Trajectories of 5 MeV/n C ion simulated by CSDA and TS mode

Useful for applying PHITS to radiation biology such as DNA damage estimation

Y. Matsuya et al. Phys. Med. Biol. 66, 06NT02 (2021)

Benchmarks

Comprehensive benchmark results are published in an Open-Access paper*

JOURNAL OF NUCLEAR SCIENCE AND TECHNOLOGY, 2017
VOL. 54, NO. 5, 617–635
https://doi.org/10.1080/00223131.2017.1297742

Taylor & Francis
Taylor & Francis Group

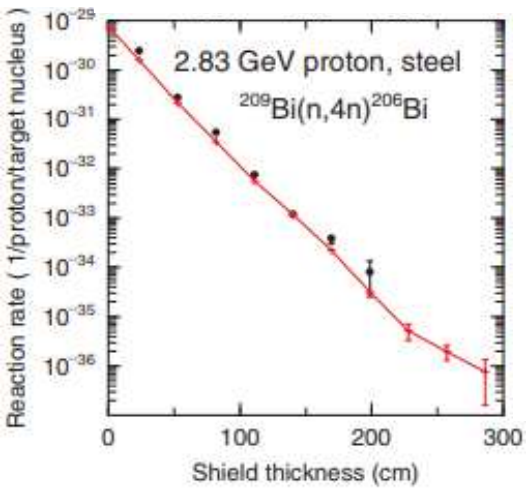
TECHNICAL MATERIAL

OPEN ACCESS Check for updates

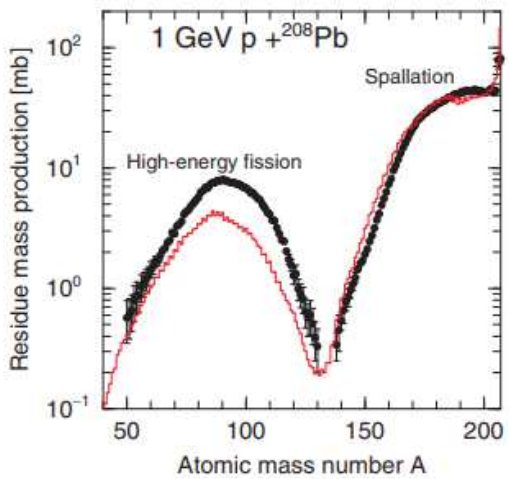
Benchmark study of the recent version of the PHITS code

Yosuke Iwamoto[a], Tatsuhiko Sato[a], Shintaro Hashimoto[a], Tatsuhiko Ogawa[a], Takuya Furuta[a], Shin-ichiro Abe[a], Takeshi Kai[a], Norihiro Matsuda[a], Ryuji Hosoyamada[b] and Koji Niita[b]

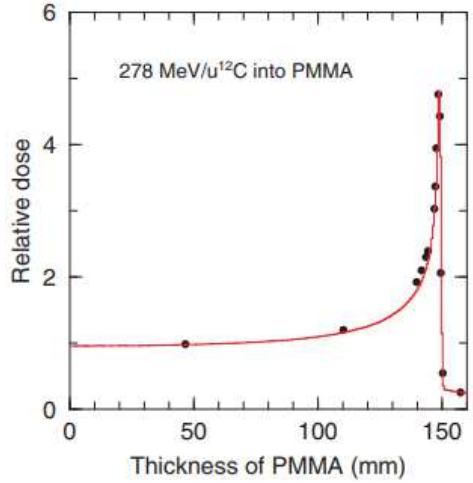
[a]Japan Atomic Energy Agency, Ibaraki, Japan; [b]Research Organization for Information Science and Technology, Ibaraki, Japan



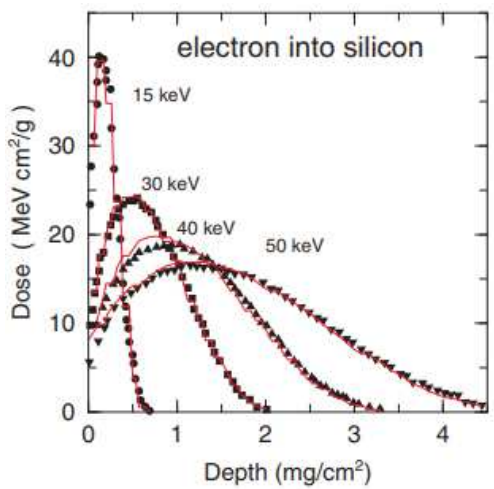
Shielding calculation



Fission yield



Particle therapy



Electron range

- ✓ All input files used for these benchmarks are included in /phits/sample/benchmark
- ✓ * https://www.tandfonline.com/doi/full/10.1080/00223131.2017.1297742

Table of Contents

Useful Functions for Facility Design

Variance reduction techniques

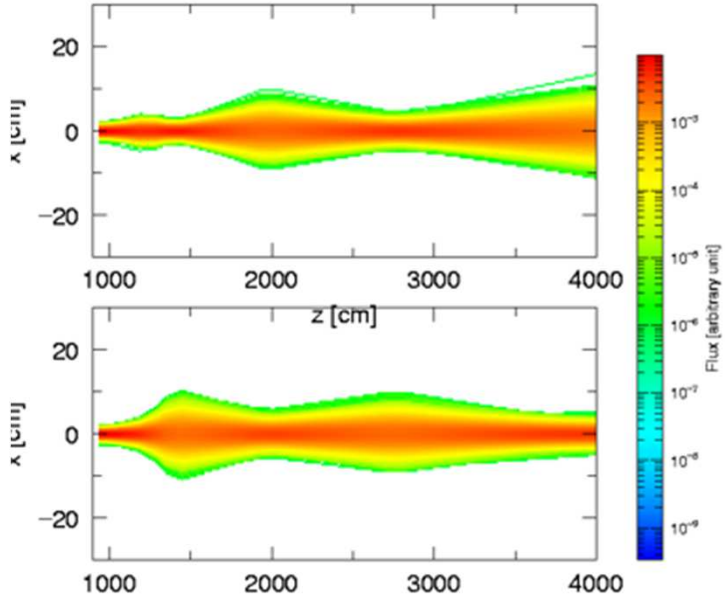
- ✓ Weight window generator
- ✓ Cell importance method

Electro-magnetic fields

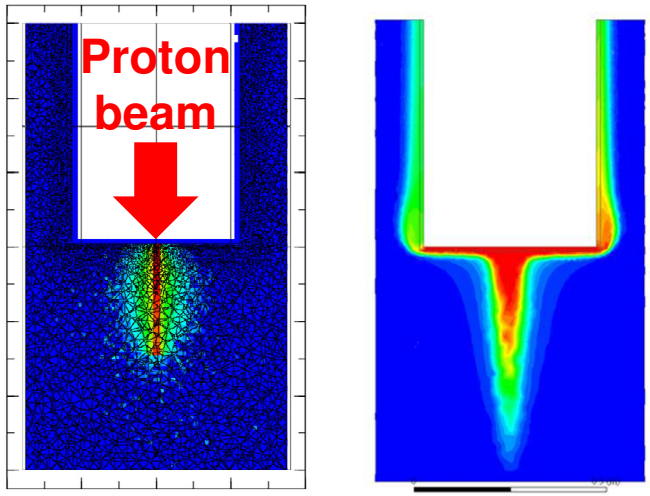
- ✓ Dipole & quadrupole magnet
- ✓ Wobbler magnet
- ✓ Parallel electric field
- ✓ Complex field map in xyz or r-z coordinate

Others

- ✓ Direct calculation of operational and protection quantities such as H*(10) & Effective dose
- ✓ Sensitivity analysis based on ANOVA
- ✓ Estimation of time evolution of induced activity considering decay chains of RI
- ✓ Phase space source based on RMS emittance
- ✓ Coupling with thermal analysis



Quadrupole magnet

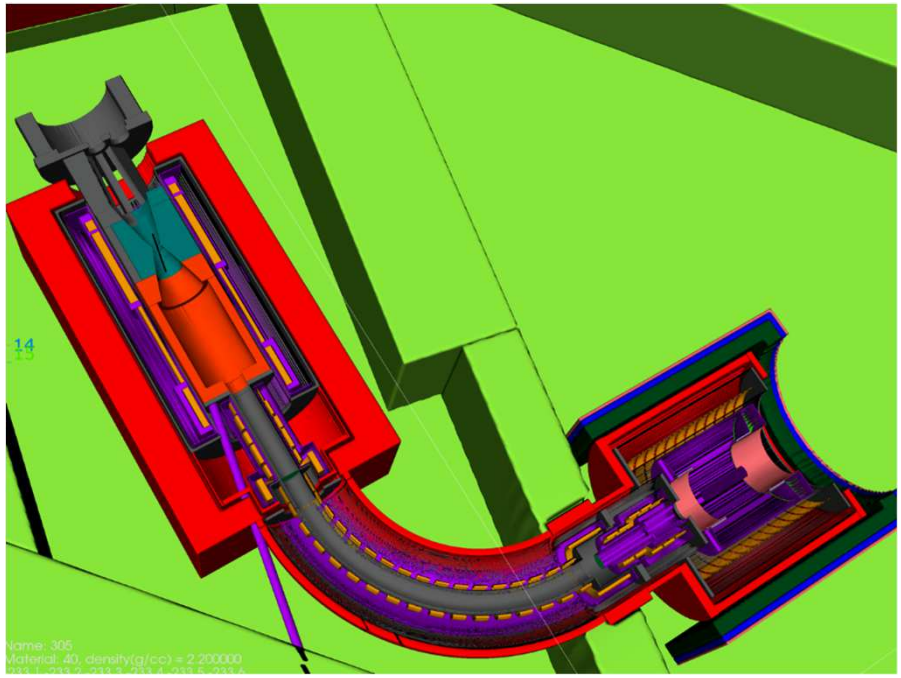


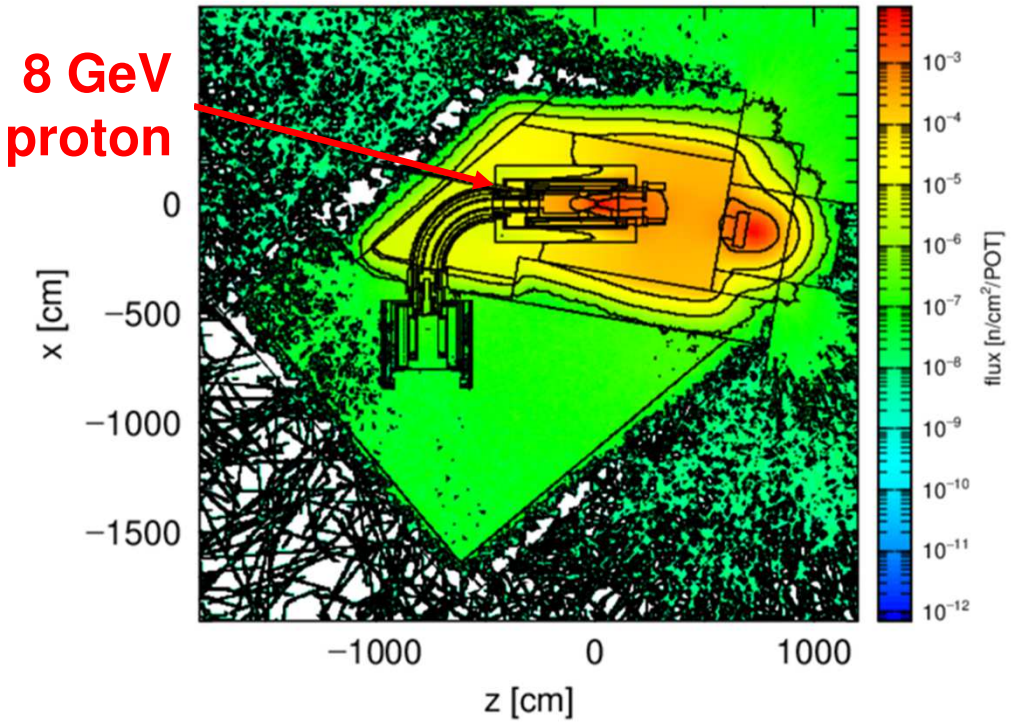
PHITS + Ansys Fluent

Design of J-PARC facilities

Japan Proton Accelerator Research Complex

- ✓ Constructed in Tokai-mura as the joint project between JAEA and KEK
- ✓ Consists of several proton accelerators with energies up to 30 GeV
- ✓ Used for various purposes such as particle physics and neutron generation





3D geometry view and flux distribution around COMET experimental facility

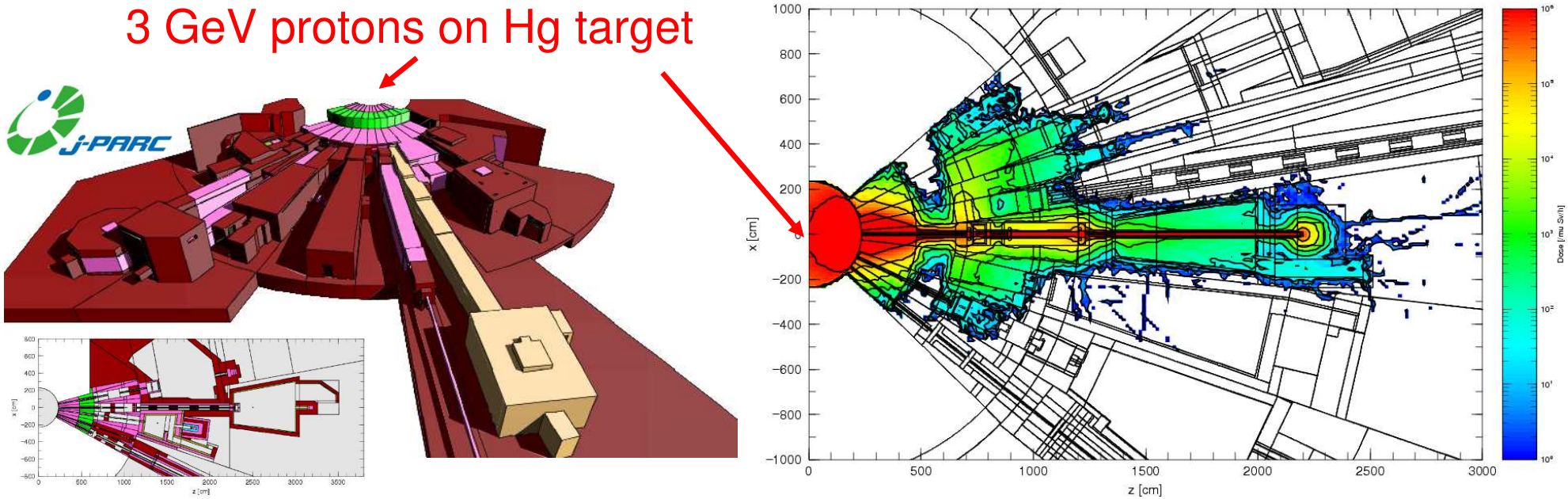
COMET searches for coherent neutrino-less conversion of a muon to an electron

Courtesy of COMET experiment team (https://comet.kek.jp/)

Design of Neutron Beam Line

Material and Life science experimental Facility (MLF) in J-PARC

3 GeV protons on Hg target



2D & 3D geometry views and dose distribution around a neutron beam line

Special functions for neutron beam line design

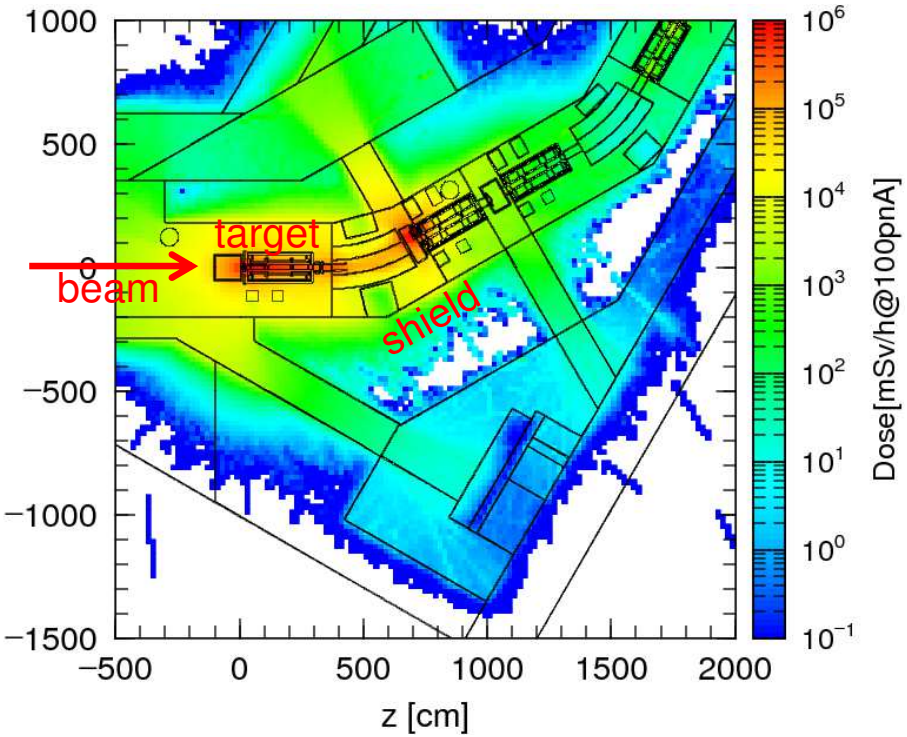
- Duct source option: Special variance reduction technique for long beam line
- Mechanical & optical devices: Multipole magnets, T0 chopper, Super mirror
- Gravity: Cold neutrons gradually go down to the ground direction

https://j-parc.jp/c/en/facilities/mlf/index.html

Design of RI Beam Factory

- ✓ Constructed by RIKEN for accelerating various unstable nuclides up to U
- ✓ Nihonium (Z=113) was discovered in this facility

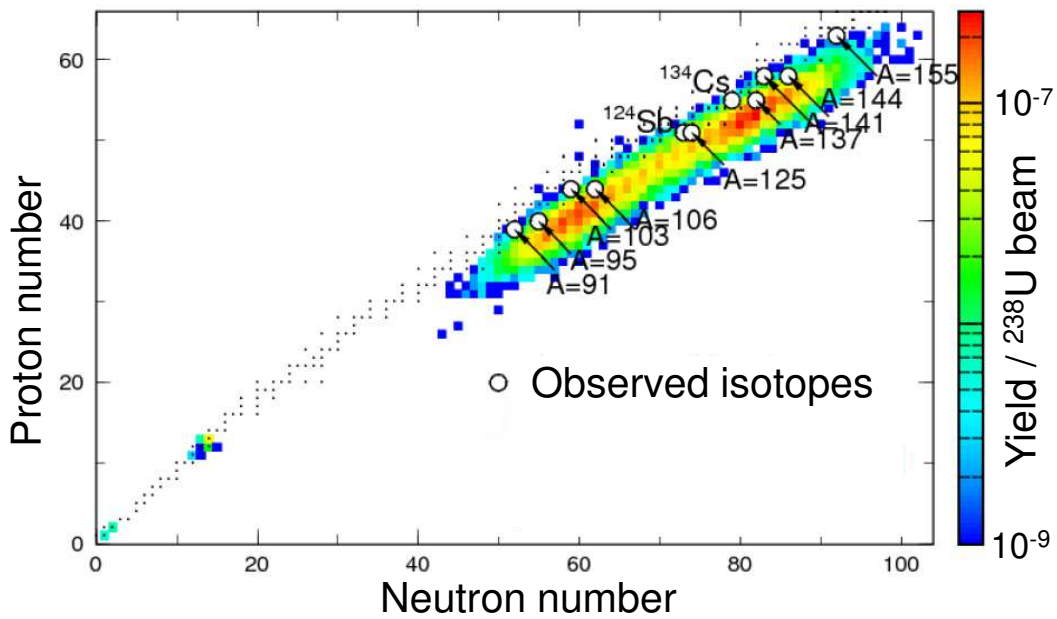
Shielding design



Dose distribution around BigRIPS*

*In-flight RI beam separator

Activation calculation



Yields of RI generated by ^{238}U beam

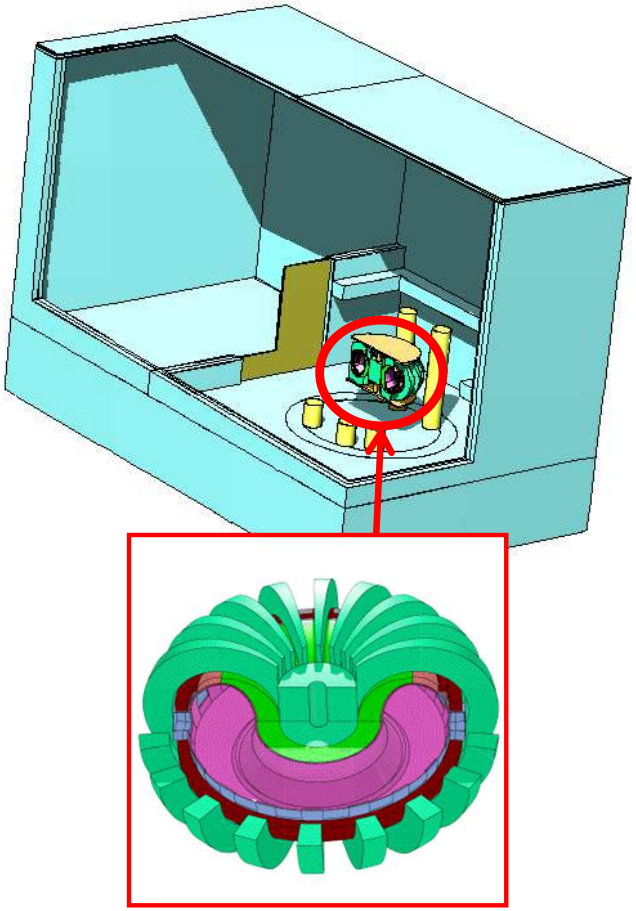
Function to plot the yield distribution on the nuclear chart

Tanaka et al. Progress in Nuclear Science and Technology 4, 201 (2014)

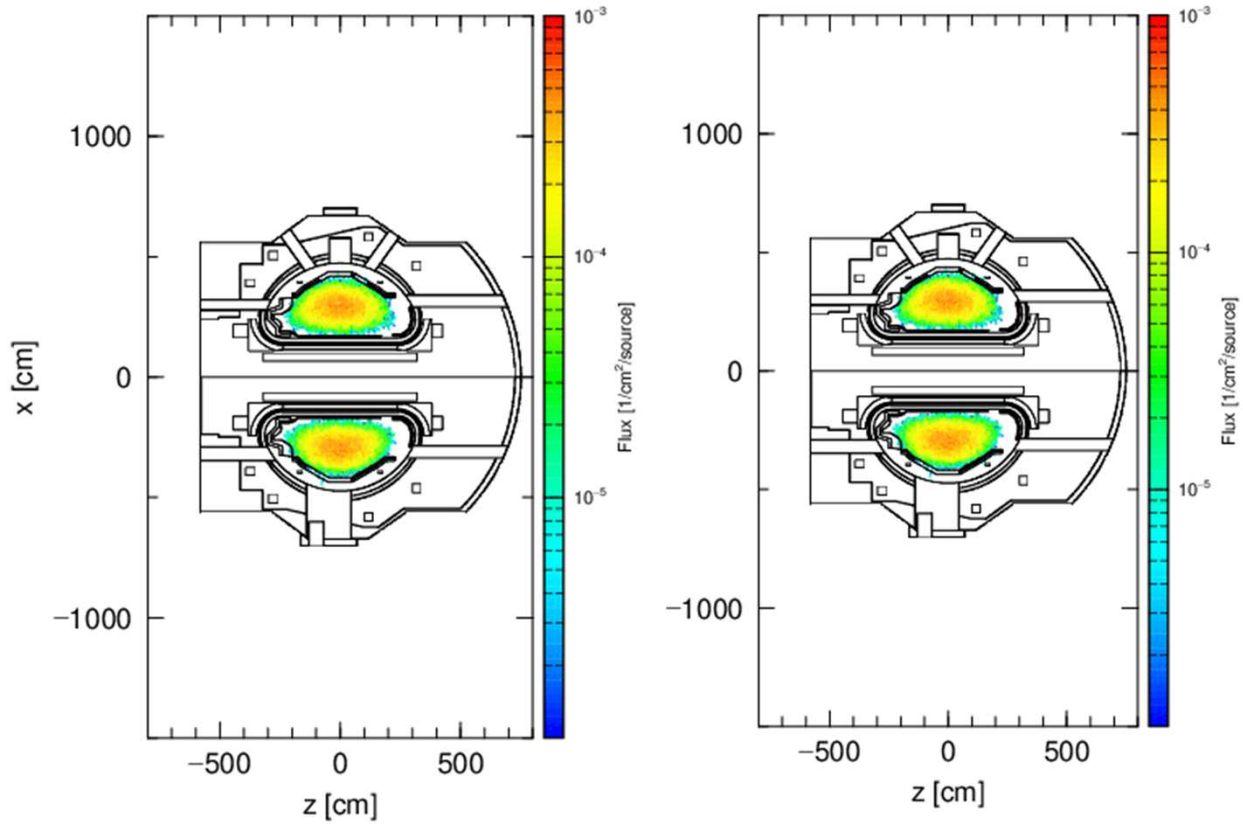
Akashio et al. EPJ Web of Conferences 153, 01022 (2017)

Design of Tokamak Fusion Device

Accurate prediction of heat, defect, and activation in complex Tokamak fusion device geometry is indispensable for its design



3D view of JT-60

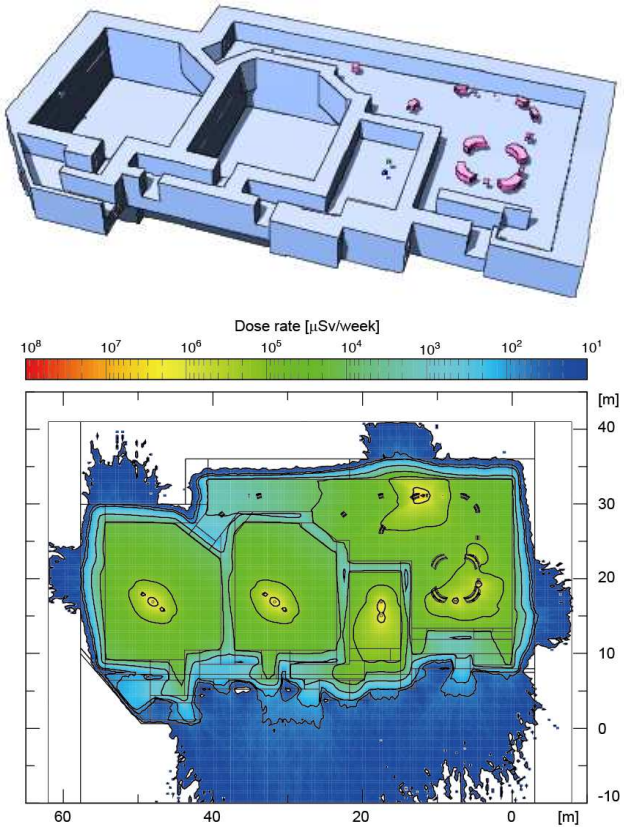


Neutron flux distributions in the vicinity of device with / without considering shielding effect

A. Sukegawa et al. Prog. Nucl. Sci. Technol. 1, 36-39 (2011)

Design of Other Facilities

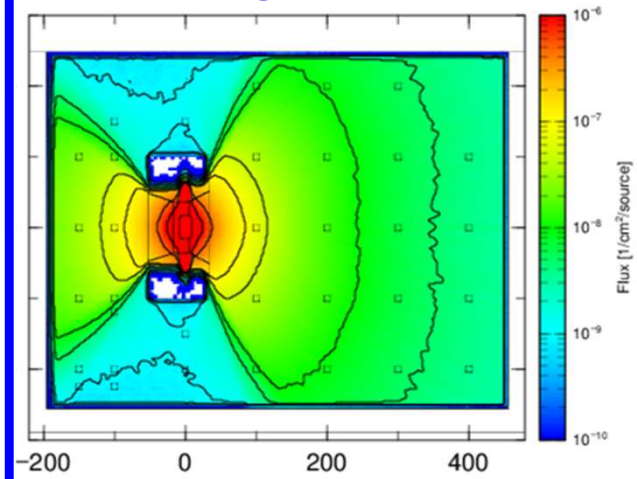
Particle therapy

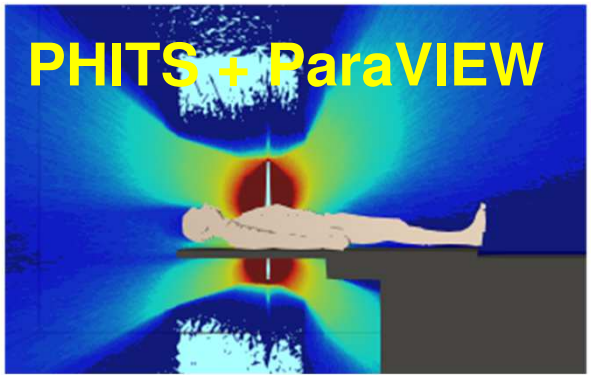


Fukui Prefectural Hospital Proton Therapy Center

Satoh et al. J. Nucl. Sci. Technol. 49, 1097 (2012)

Diagnostics

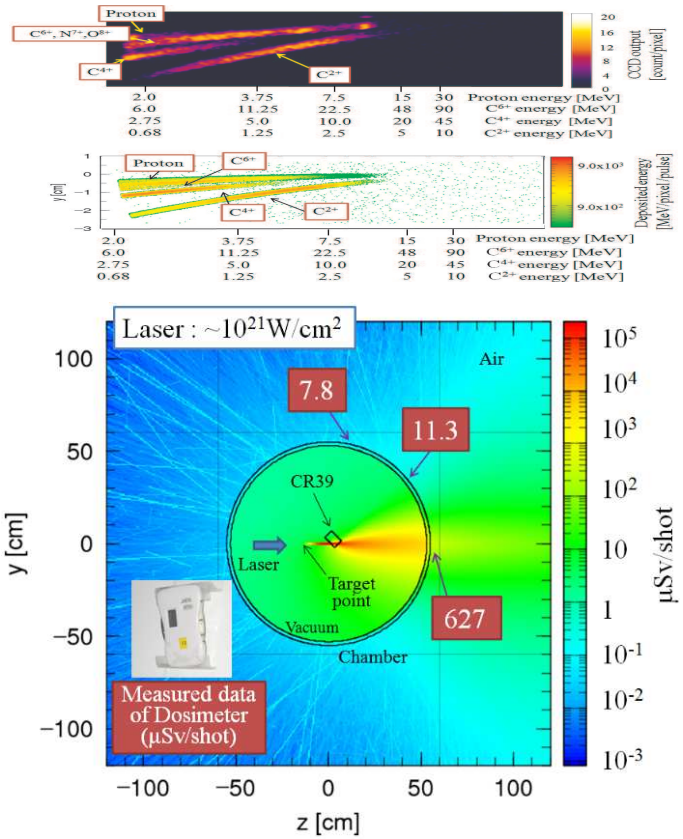




CT room in Kyushu University

Fujibuchi et al. Japanese J. Radio Tech 75, 1297 (2019)

Laser accelerator



J-KAREN laser system in QST Kansai

Sakaki et al. Rev. Sci Instr. 85, 02A705 (2014)

Used for getting the permission from Nuclear Regulation Authority in Japan

Table of Contents

Useful Functions for Medical Application

RI source generation function

Reproduce the decay of any RI with or without considering the contributions from its daughter nuclides, based on ICRP 107

Voxel & mesh phantoms

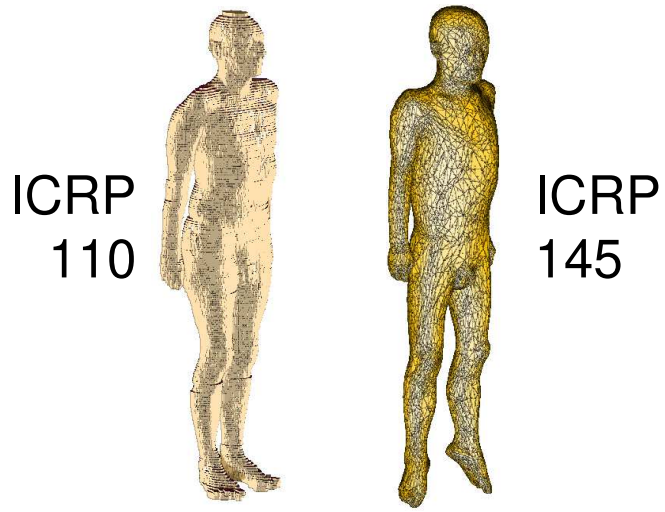
- ✓ Represent fine structures of human body by volume pixels (voxel) or tetrahedral meshes
- ✓ Special algorithm to reduce the computational time of particle transport in tetrahedral mesh*

Microdosimetric function

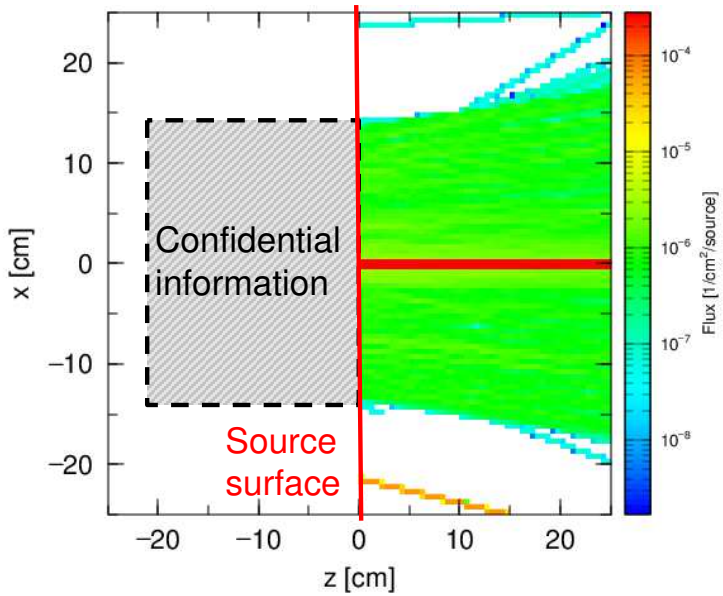
Special tally named [t-sed] for calculating microdosimetric quantities (*y* & *z*) without performing track structure simulation**

Phase-space file converter (PSFC)

Automatically convert PS source information compiled by IAEA to PHITS source format for simulating medical accelerator beams



Voxel & mesh phantoms



Simulation using PSFC

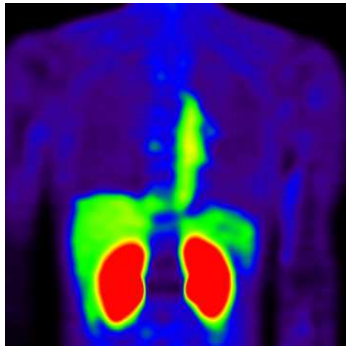
*Furuta et al. Phys. Med. Biol. 62, 4798 (2017) **Sato et al. Radiat. Prot. Dosim. 122, 41 (2006)

RT-PHITS (RadioTherapy package based on PHITS)

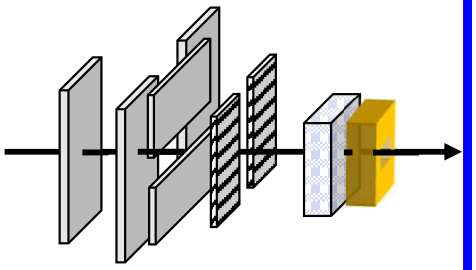
- ✓ Convert DICOM image (CT, PET, SPECT) and plan data to PHITS input
- ✓ Convert dose distribution calculated by PHITS to DICOM RT-Dose data

DICOM image & plan data

CT

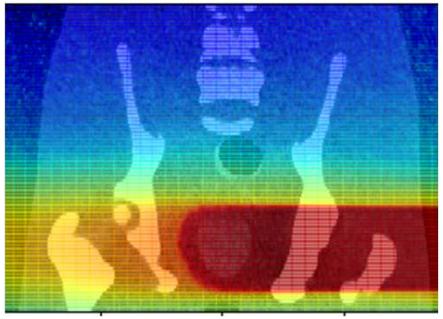


PET/SPECT



RT-plan

DICOM Software



RT-dose

- ✓ROI
- ✓DVH

RT-PHITS (CT2PHITS, PET2PHITS, Plan2PHITS, PHITS2DICOM etc.)

PHITS input file

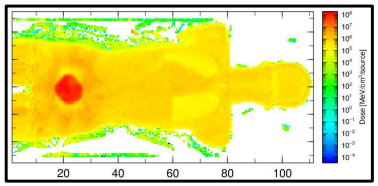
Voxel phantom

- ✓ RI-source with xyz
- ✓ Phase space file

[source] section

PHITS

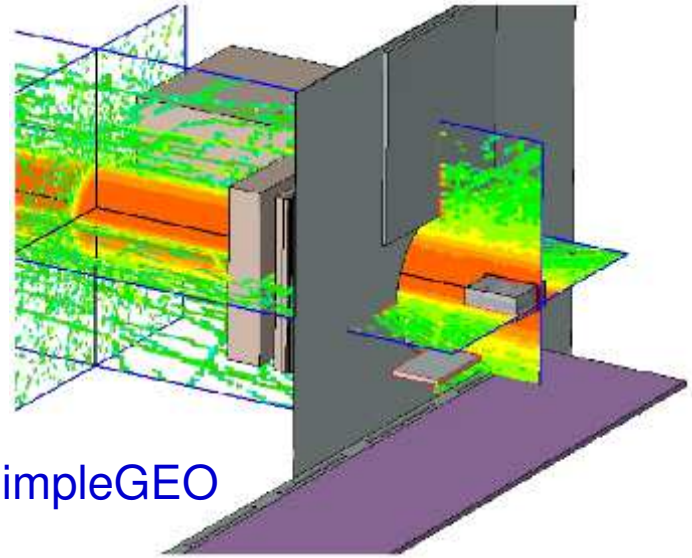
PHITS output file



Dose distribution

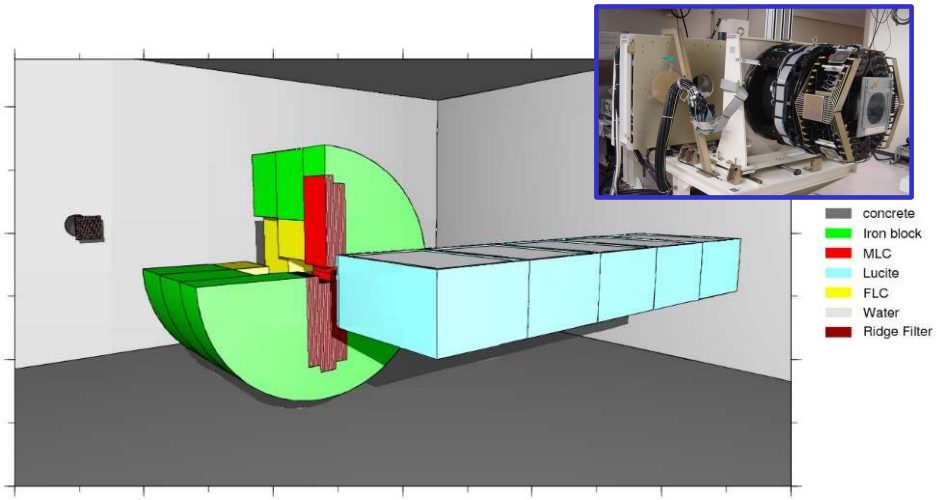
phits/utility/RT-phits

Applications to Particle Therapy



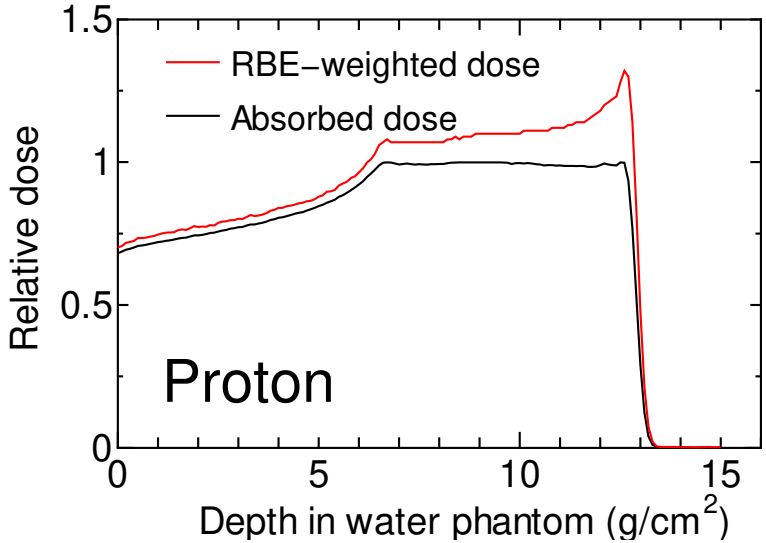
drawn by
PHITS+SimpleGEO

O. Ploc et al. IEEE Aerospace Conf. (2017)

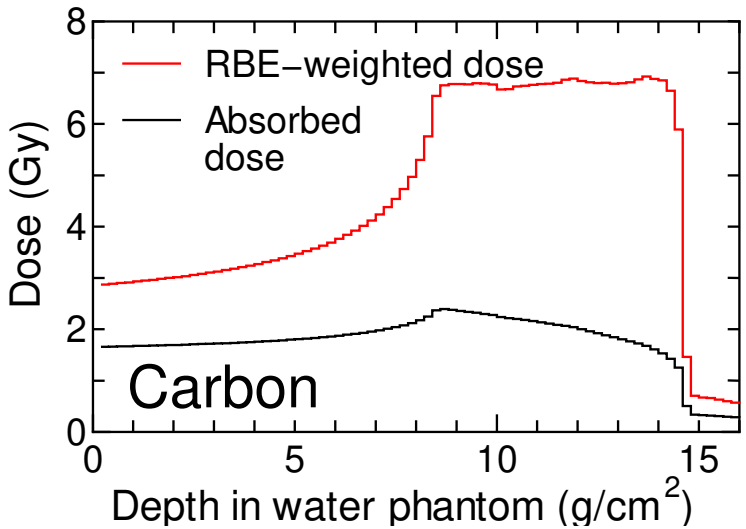


S. Yonai et al. Med Phys. 39, 5028-39 (2012)

Secondary dose estimation



K. Takada et al. JRR 59, 91-99 (2018)

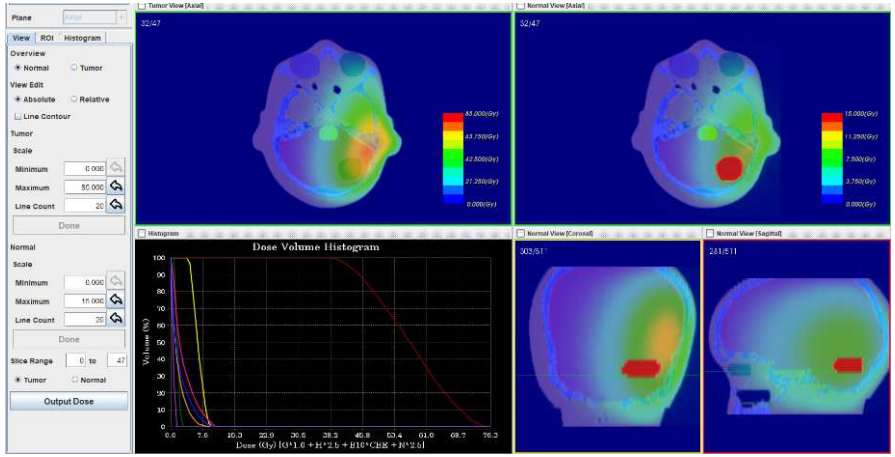


T. Sato et al. Radiat. Res. 171, 107-117 (2009)

RBE-weighted dose estimation

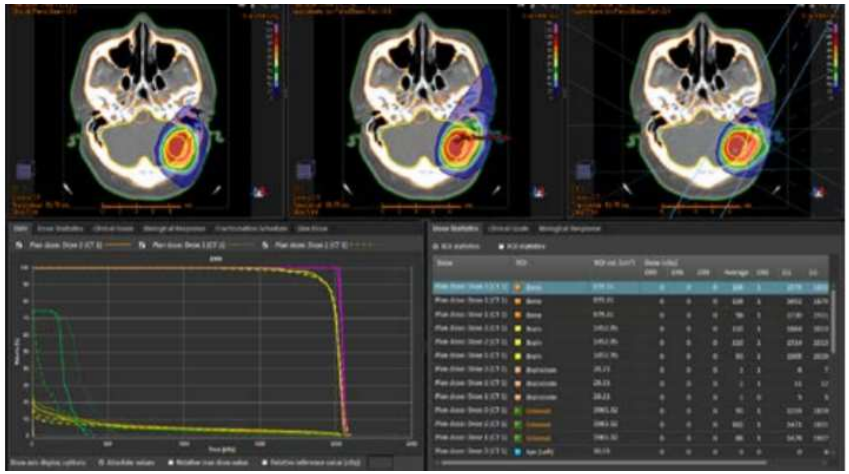
Applications to BNCT

Treatment Planning System



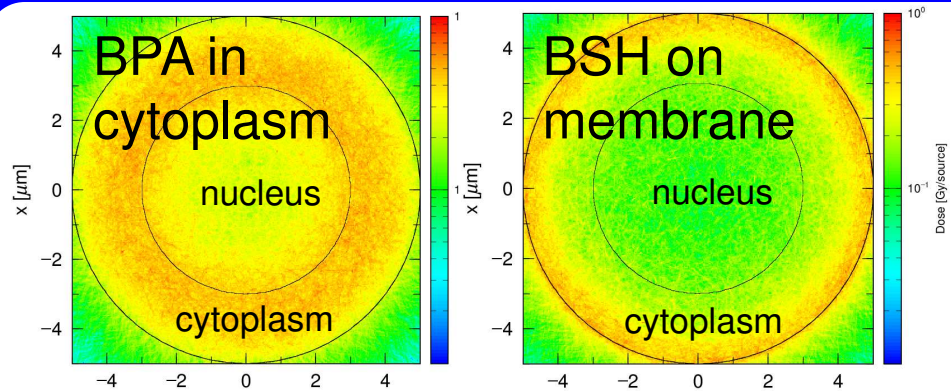
Tsukuba Plan

Kumada et al. Appl. Radiat. Iso. 166, 109222 (2020)

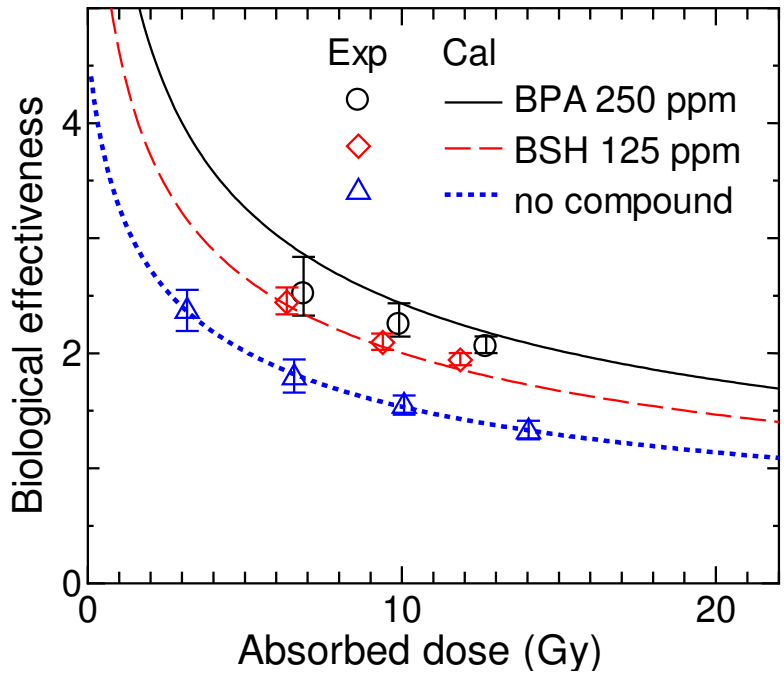


NeuCure™ by S.H.I.

Approved by PMDA : 30200BZX00083000



Dose analysis in cellular scale



Estimation of therapeutic effect

T. Sato et al. Sci. Rep. 8, 988 (2018)

Applications to Nuclear Medicine

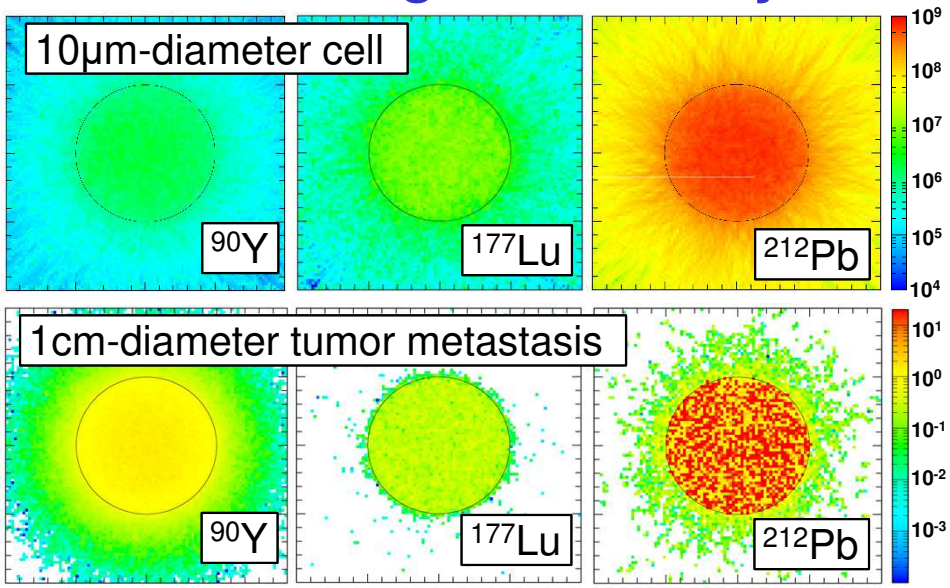
PHITS-based Application for Radionuclide Dosimetry In Meshes

- ✓ Developed by MSKCC and opened to public for free
- ✓ Automatically generate PHITS input file based on mesh phantoms by supplying the concentration of RI in each organ

https://www.paradim-dose.org/

Carter et al. J. Nucl. Med 60, 1802 (2019)

Small target dosimetry



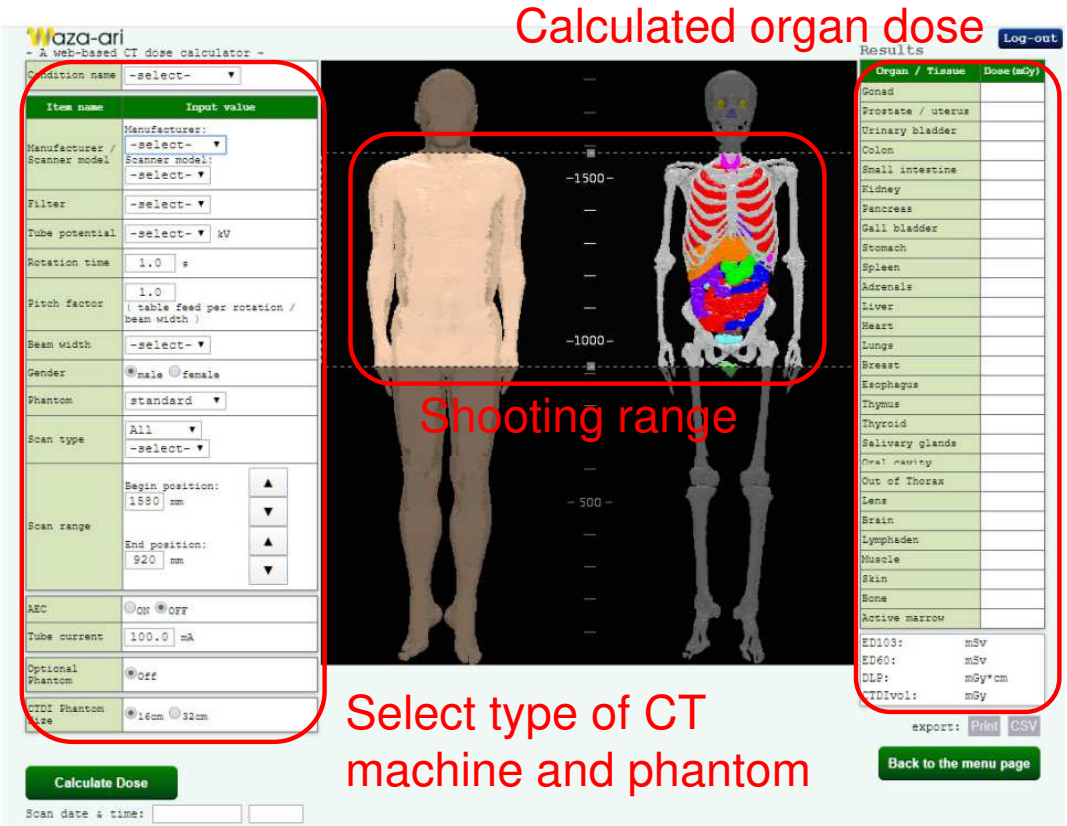
Dose distributions around 10-μm cell and 1-cm tumor metastasis

- ✓ Doses are highly heterogeneous in microscopic scales in the case of α or low-energy β emitters
- ✓ PHITS was used in calculating S-values for cellular and tumor-metastasis scale targets

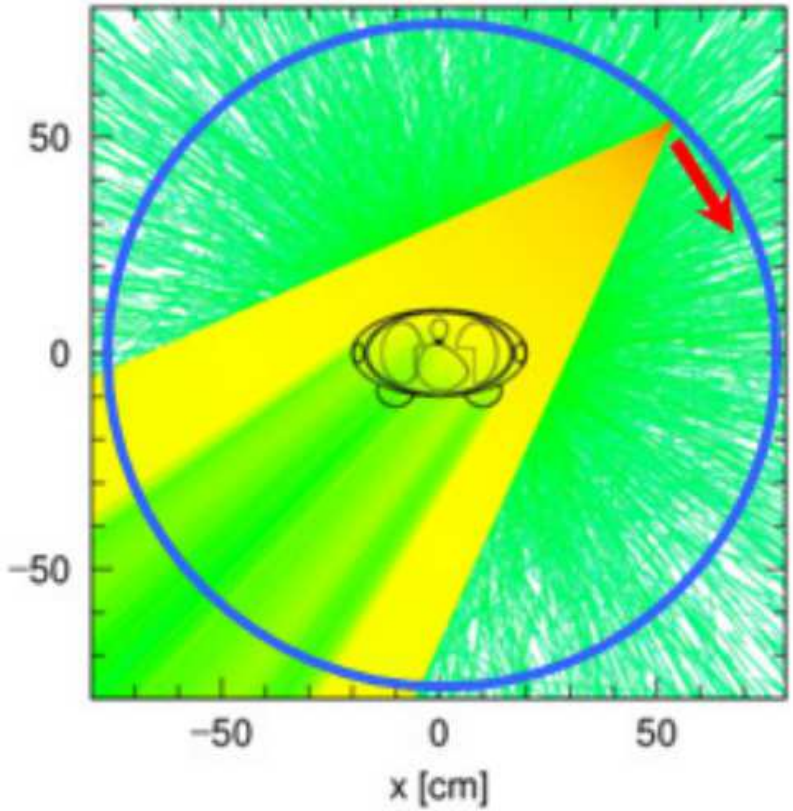
Lee et al. Radiat. Res. 190, 236 (2018)

Applications to Diagnostics

A Web-based CT dose calculator: WAZA-ARI



Interface of WAZA-ARI



Example of PHITS simulation

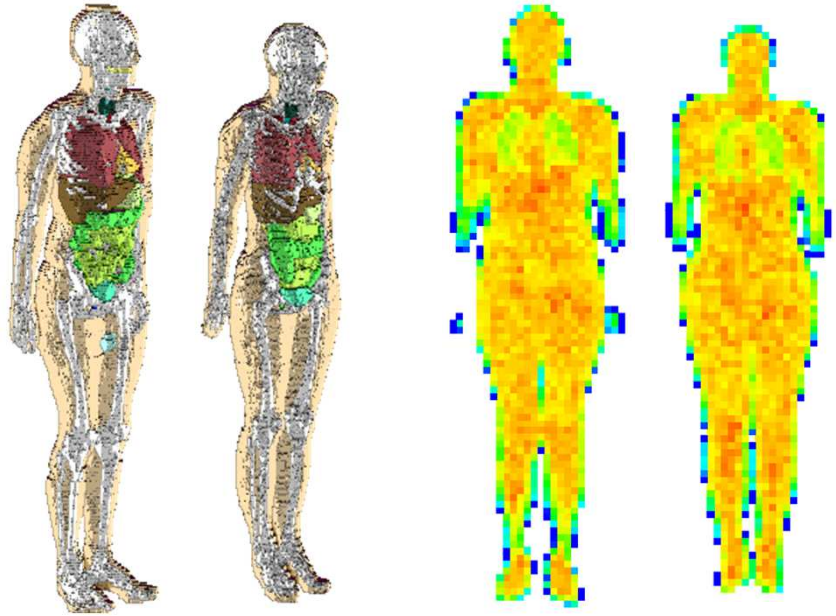
X-ray spectra of various CT machines are precisely reproduced and irradiated to Japanese voxel phantoms with different anatomies in PHITS

Approximately 2,000 facilities have been used for calculating CT-patient doses

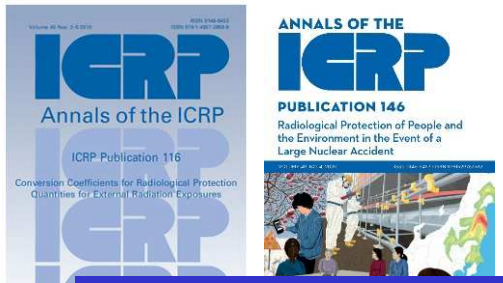
F. Takahashi et al. Health Phys. 109, 104 (2015), https://waza-ari.nirs.qst.go.jp/

Applications to Radiological Protection

Dose conversion coefficient



ICRP reference phantoms

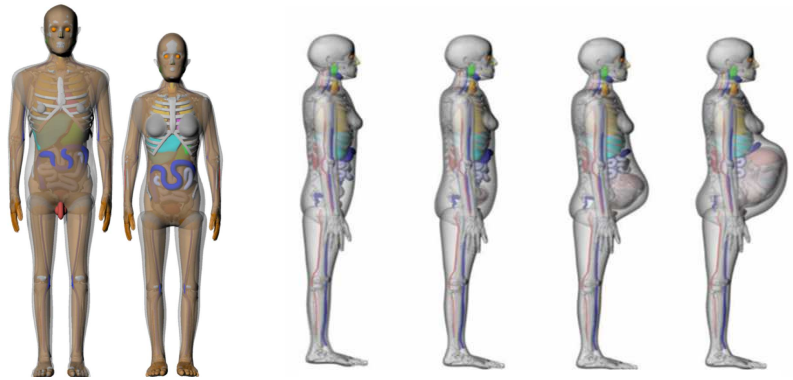


ICRP Publication 116, 123, 146

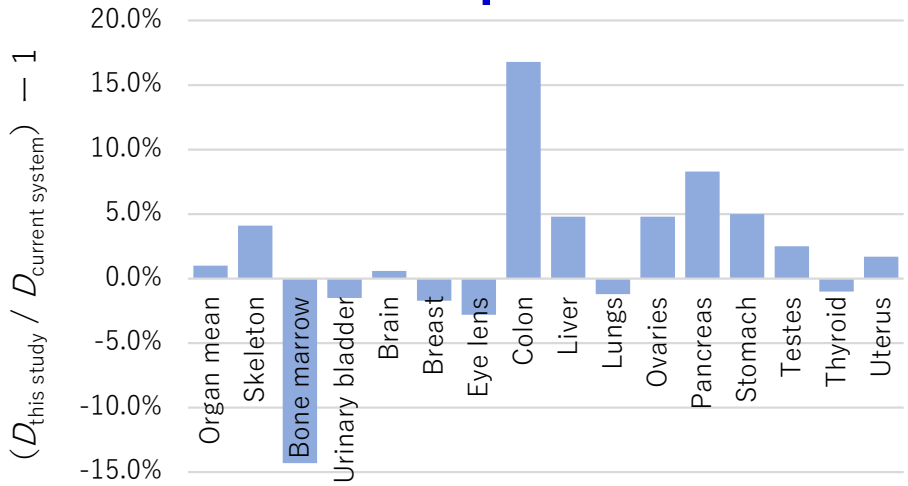
Used in evaluation by ICRP

T. Sato et al. *Phys. Med. Biol.* 54, 1997 (2009)
D. Satoh et al. JNST 53, 69-81 (2015)

Atomic-bomb survivor dose



J45 series phantom

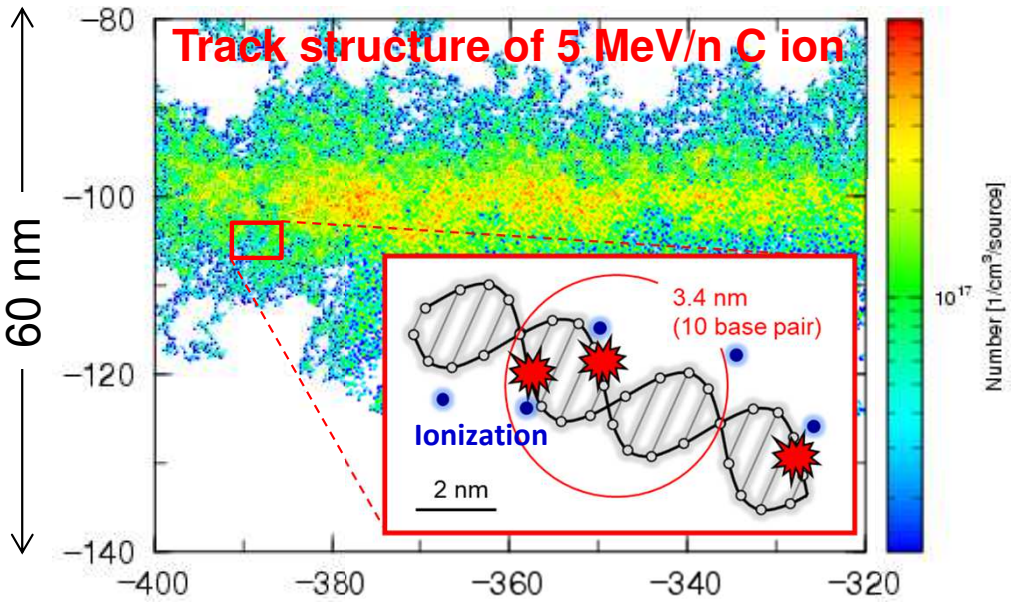


Differences between new & old systems

To be used in epidemiological study

C. Paulbeck et al. *Radiat. Res.* 192, 538 (2019)
T. Sato et al. *Radiat. Res.* 194, 390 (2020)

Applications to DNA-damage Estimation



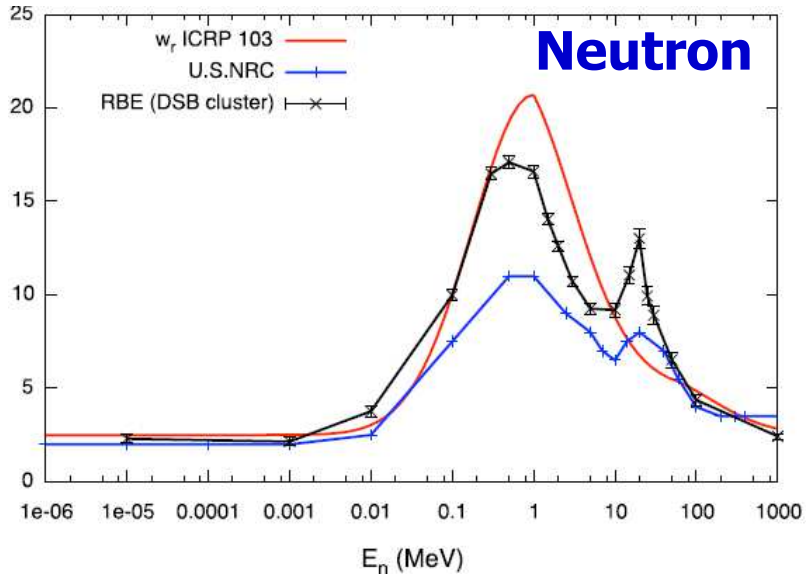
Spatial pattern of ionization & excitation

Special user-defined tally

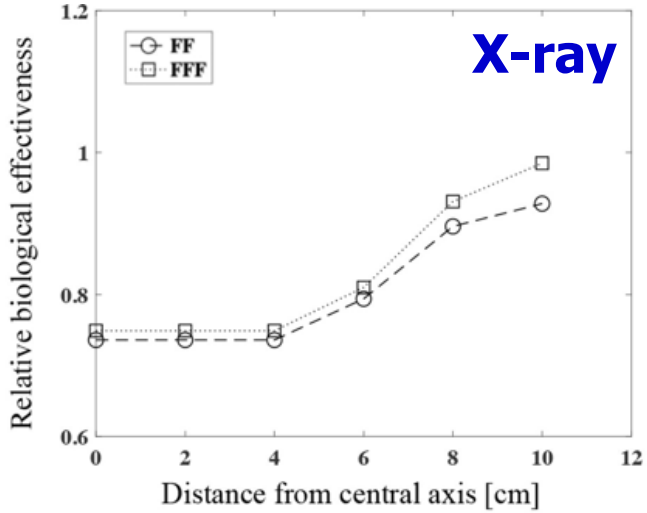
- ✓ Cluster of the events within 10 base pair of DNA to identify DSB and cluster damage
- ✓ Output the data in Standard DNA Damage (SSD) format

Matsuya J. App. Phys. 126, 124701 (2019)

RBE estimation of DSB yields



Baiocco et al., Sci Rep 6, 34033 (2016)



Nakano et al., BJR Open, 3, 1 (2021)

Table of Contents

Useful Functions for Space Research

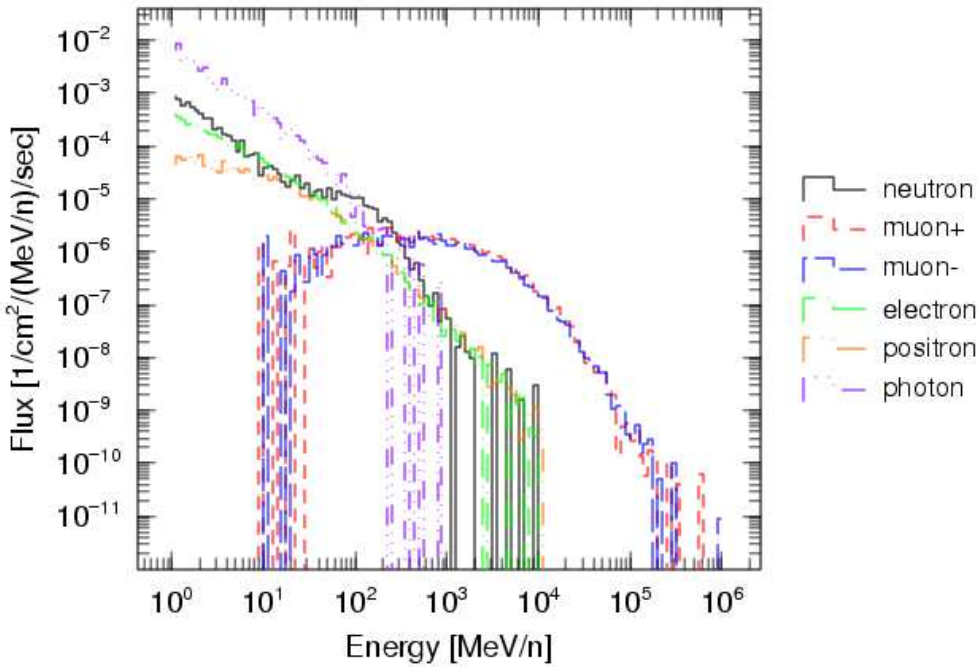
Comic-ray source mode

Applicable particle types

- ✓ Galactic cosmic ray (GCR) in space
- ✓ GCR in the atmosphere including secondary particles
- ✓ Solar energetic particle (SEP) in space for 5 historically large events

Input parameters

- ✓ Time (Year/Month/Day)
- ✓ location (latitude, longitude, altitude)
- ✓ Energy and angular ranges

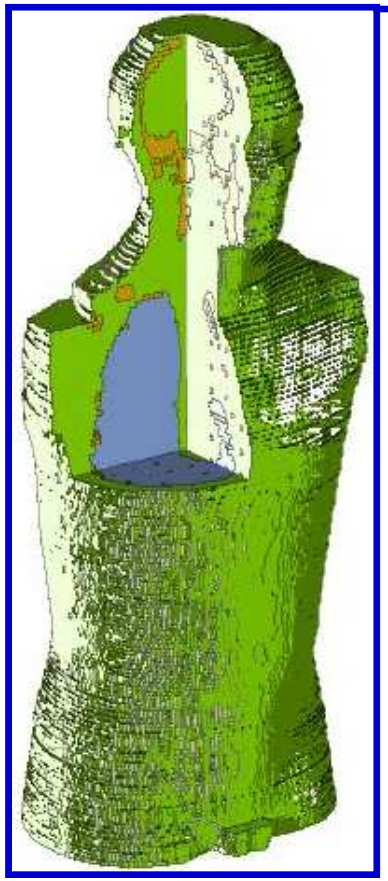


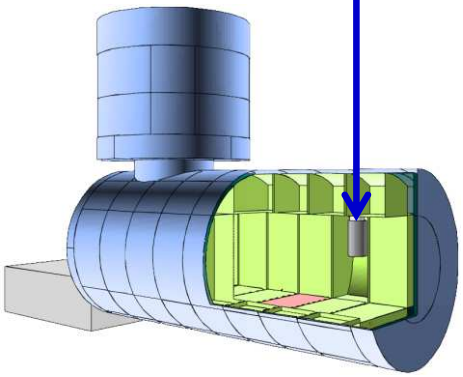
Cosmic-ray fluxes at ground level in New York

Dose equivalent estimator

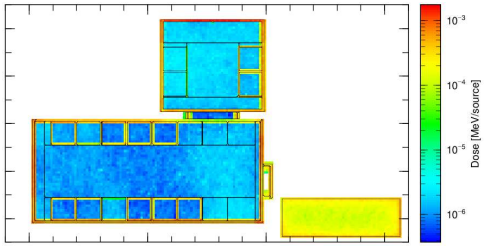
- ✓ Conversion coefficients for dose equivalent for adult male & female is implemented
- ✓ Direct calculation of dose equivalent by weighting $Q(L)$ on dose is feasible

Astronaut Dose Estimation



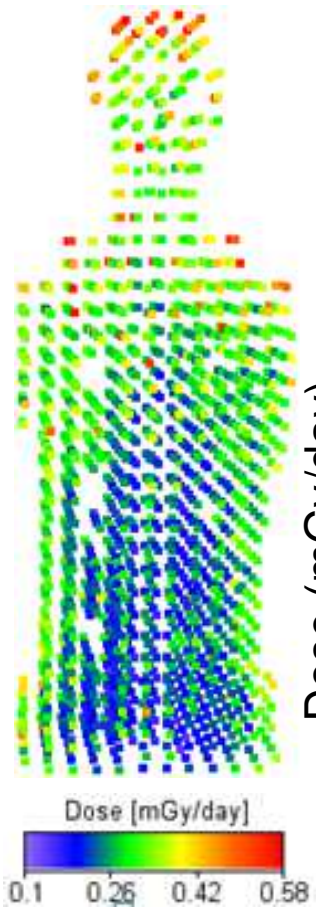


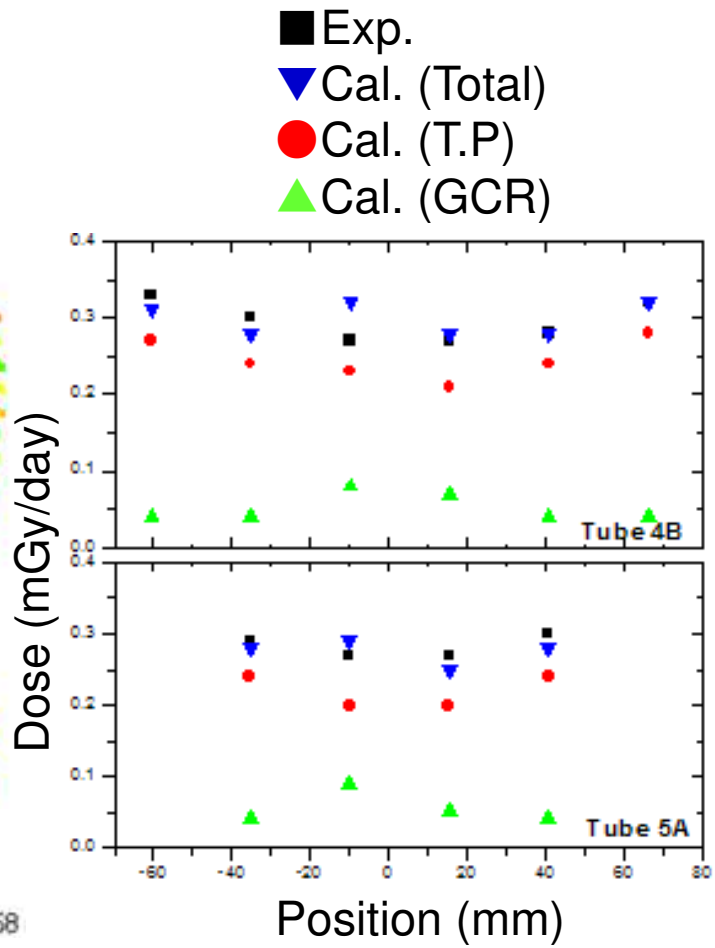
Virtual Kibo Module



MATROSHKA Project

Measure doses inside a human phantom mounted on ISS



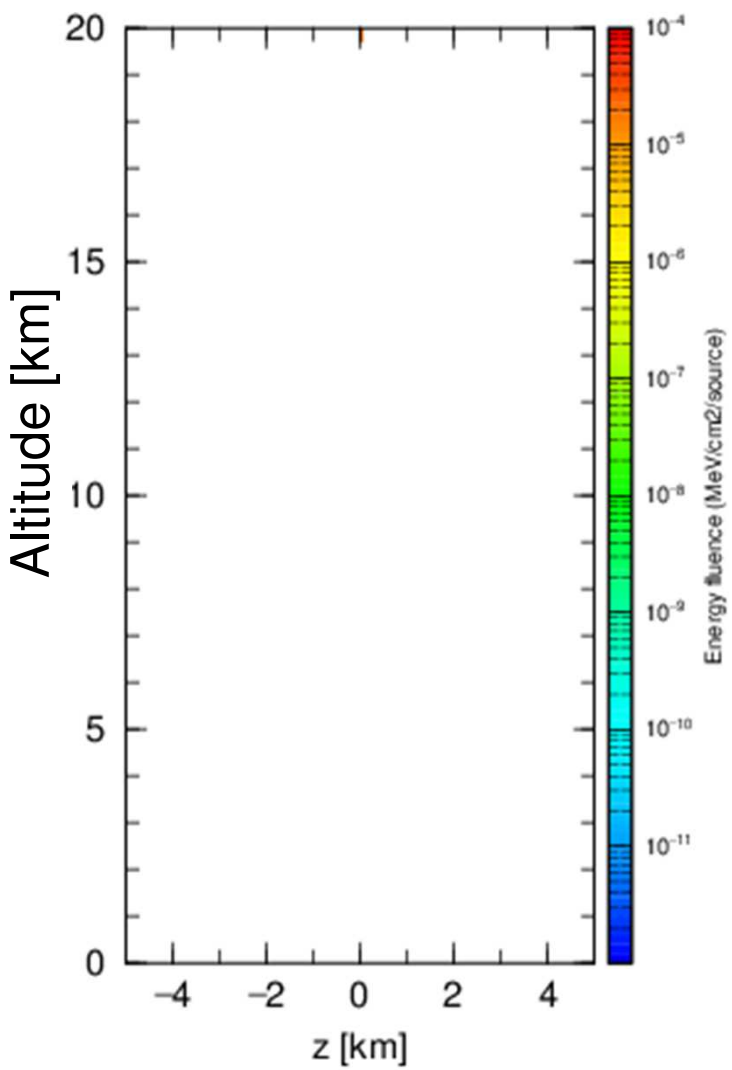


PHITS simulation results

Used in the verification of experimental results

L.Sihver et al. Radiat. Environ. Biophys. 49, 351 (2010); M.Puchalska et al., Adv. Space Res. (2012)

Cosmic-ray fluxes in the Atmosphere



Airshower simulation

Purposes

- ✓ Estimate of the effects of cosmic-ray exposure on human, devices, and the Earth
- ✓ Design of cosmogenic nuclide dating and muon radiography

PHITS Simulation and Modelling

- ✓ Airshower simulation for various conditions
- ✓ The results were modeled to instantaneously predict the cosmic-ray fluxes anytime and anywhere in the atmosphere

Outcomes

- ✓ PARMA: Implemented in PHITS as the generator of cosmic-ray source mode
- ✓ EXPACS: EXCEL version of PARMA https://phits.jaea.go.jp/expacs

Used in various research fields including geosciences (e.g. cosmoclimatology)

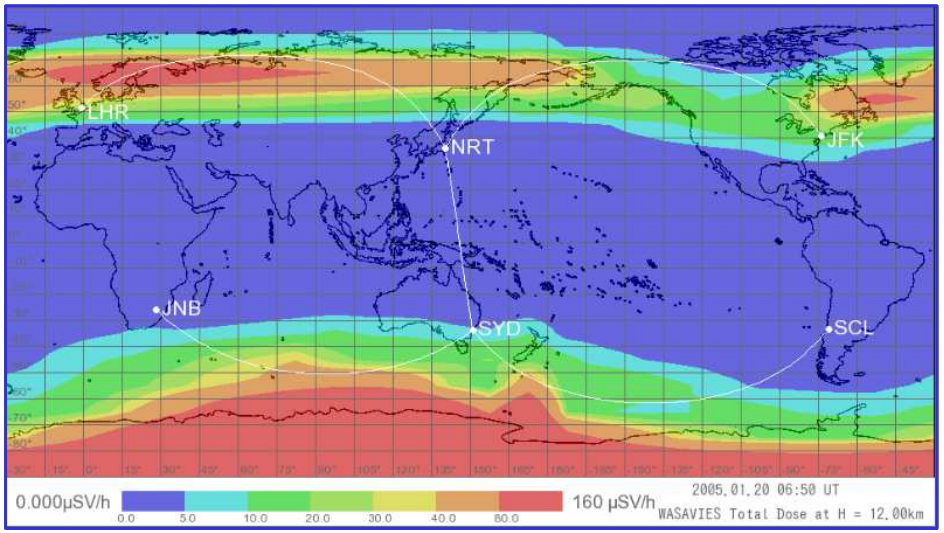
T.Sato, PLOS ONE 10, e0144679 (2015); T.Sato, PLOS ONE 11, e0160390 (2016)

Estimate of Solar Flare Impact

Development of WASAVIES

WArning System for AVIation Exposure to Solar energetic particles

- ✓ Determine cosmic-ray dose rates at flight altitudes during large solar flare
- ✓ PHITS was used for analyzing the airshower induced by solar particles

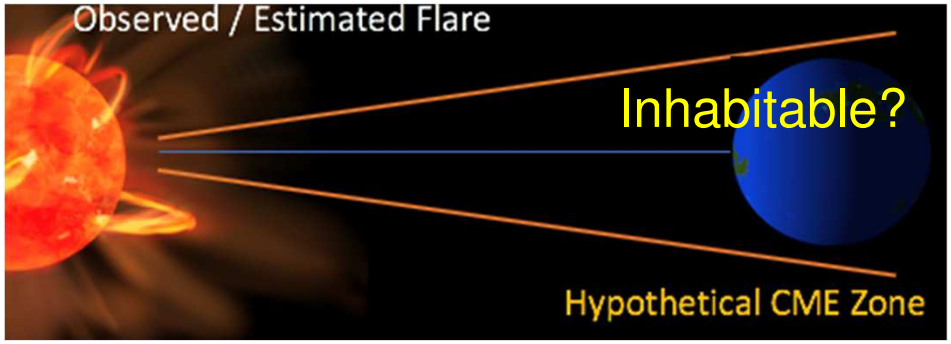


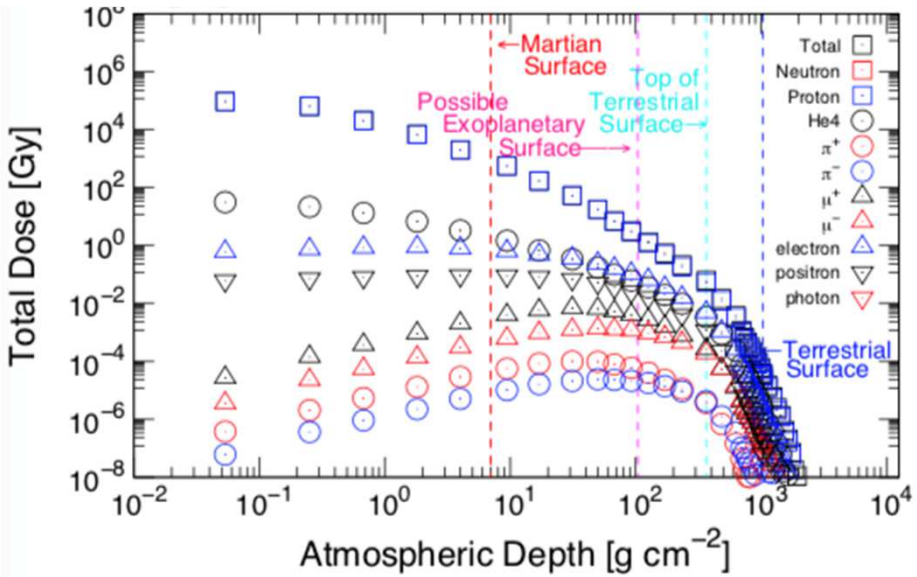
Radiation dose rate map at flight altitude during solar flare on Jan. 2005

T. Sato et al. Space Weather 16, 924 (2018)

https://wasavies.nict.go.jp/index_e.html

Impact of solar flare on planetary habiltability





Maximum radiation doses in the exoplanetary atmosphere

YA Yamashiki et al. ApJ 881, 114 (2019)

Table of Contents

Useful Functions for Detector Design

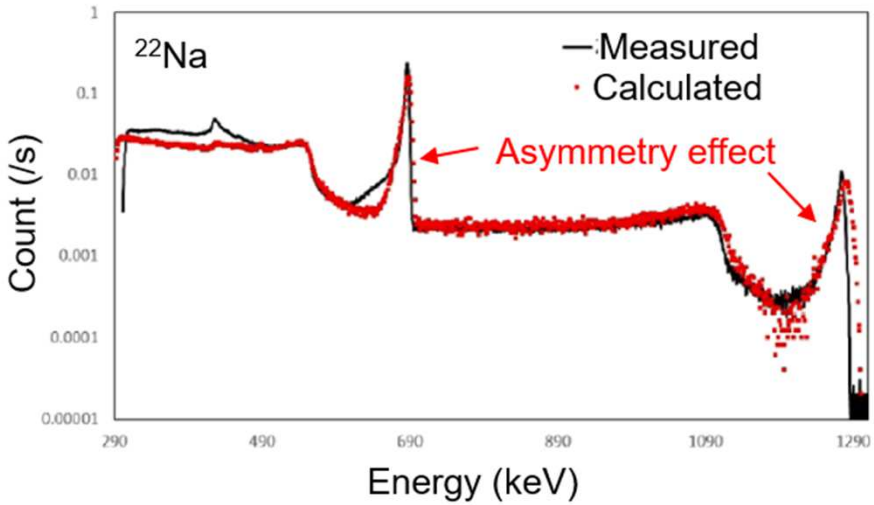
Detector resolution

- ✓ Gaussian distribution with Fano factor

$$f(E_L) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(E_L - E)^2}{2\sigma^2}\right]$$

with $\sigma = \sqrt{\sigma_r^2 + FE}$

- ✓ User original function

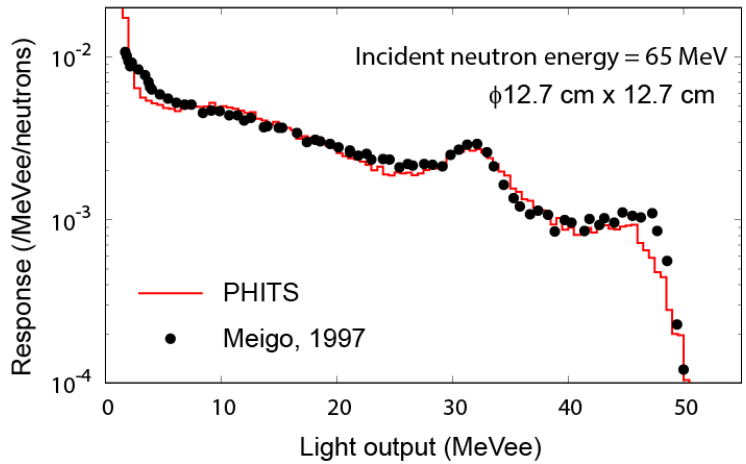


Response of CdZnTe calculated with consideration of the asymmetry effect

SCINFUL-QMD* mode

- ✓ Widely-used response calculation code for organic scintillators
- ✓ High precision *n*(C,*x*) database
- ✓ Conversion table from deposition energy to light output

Response function for complicated geometry and source definitions



Response of a liquid organic scintillator irradiated with 65 MeV neutron

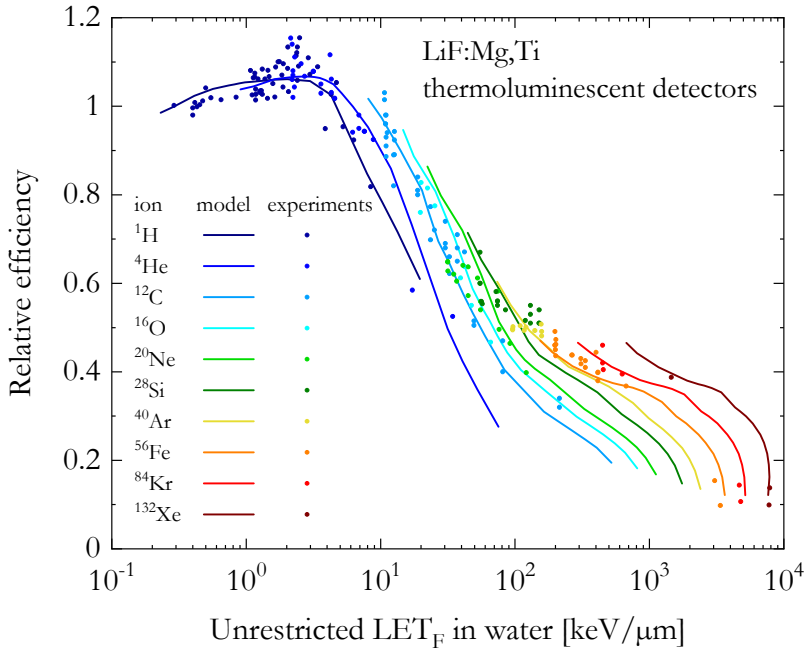
Meleshenkovskii et al. NIM B467, 108 (2020)

*Satoh et al. JAEA-Data/Code (2006)

Applications to Detector Design

Microdosimetric *d*(*z*) Model

- ✓ Universally determine detector responses for different radiation qualities based on *z* instead of LET
- ✓ Microdosimetric function in PHITS plays an indispensable role

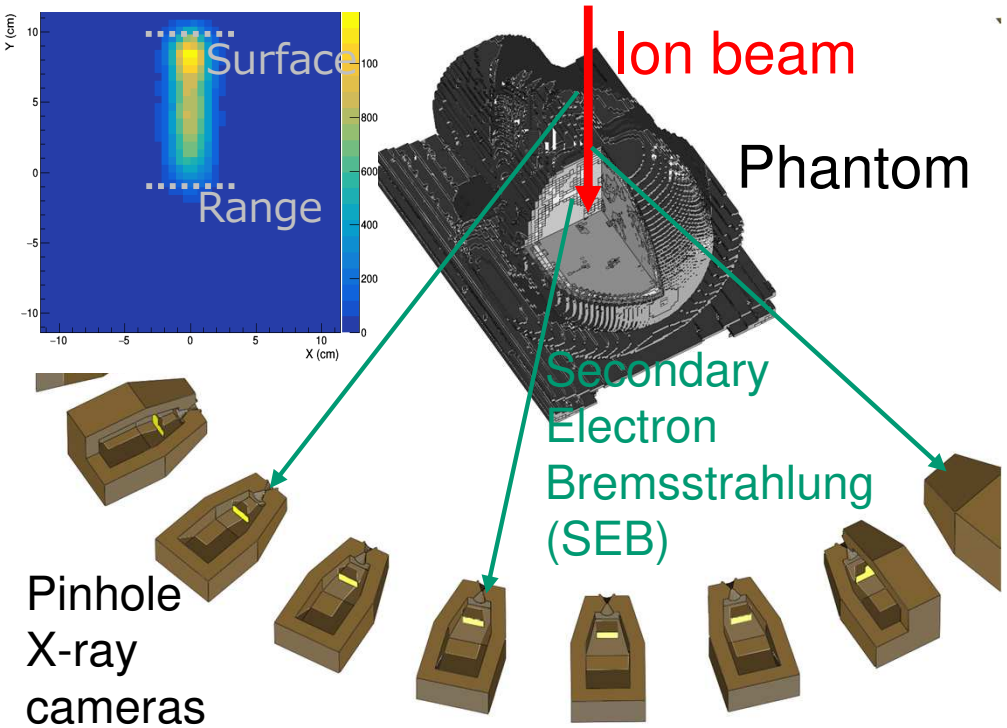


Response of TLD (LiF:Mg,Ti) for various ions as a function of LET

Parisi et al. Radiat. Meas. 123, 1 (2018)

Ion beam imaging system

- ✓ Precise estimation of SEB spectra is the key issue
- ✓ δ-ray production and activation calculation functions in PHITS play important roles



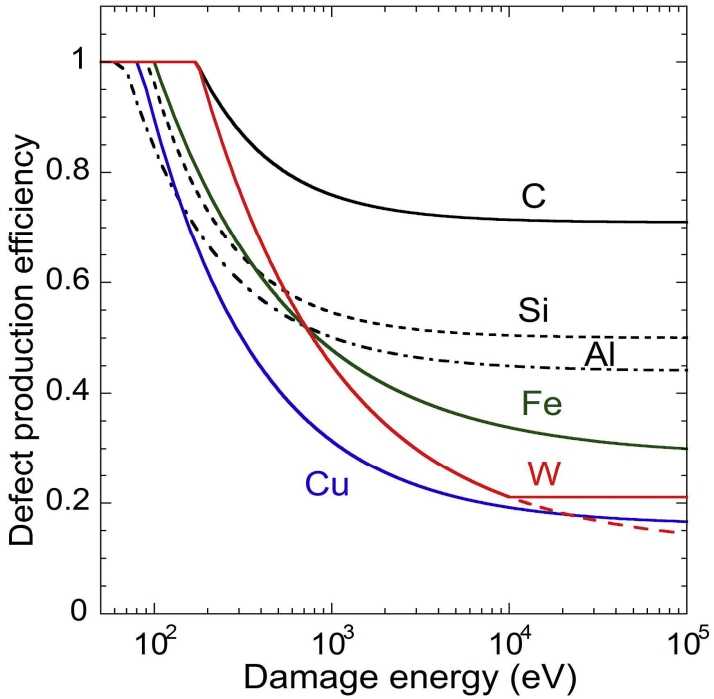
Schematic view of the imaging system

Yamaguchi et al. PMB 63, 045016 (2018)

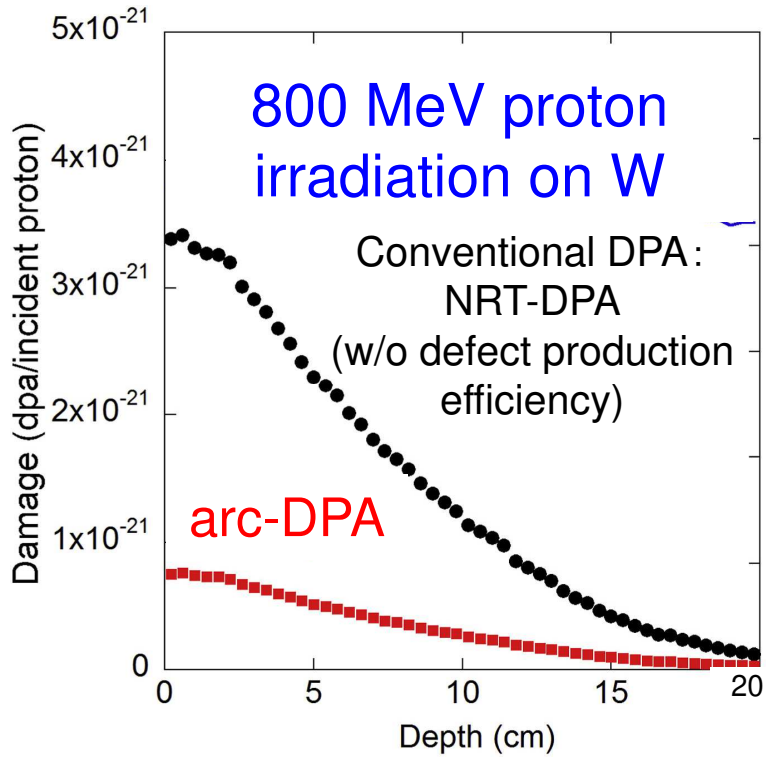
Application to Material Science

Tally for scoring DPA

- ✓ DPA: Average number of Displaced atoms Per Atom of a material
  → Index of radiation damage
- ✓ DPA tally in PHITS can score not only conventional index (NRT-DPA) but also newly proposed index (arc-DPA), considering defect production efficiency



Examples of defect production efficiencies



DPA depth distribution in tungsten

Y. Iwamoto et al., Journal of Nuclear Materials, 538, 152261 (2020)

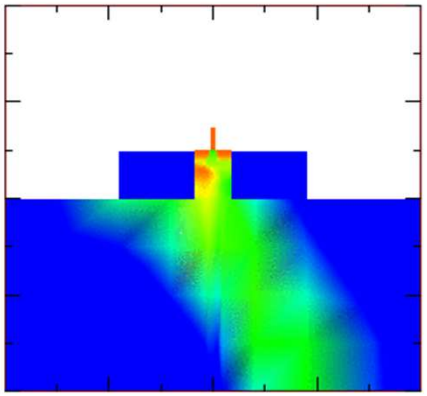
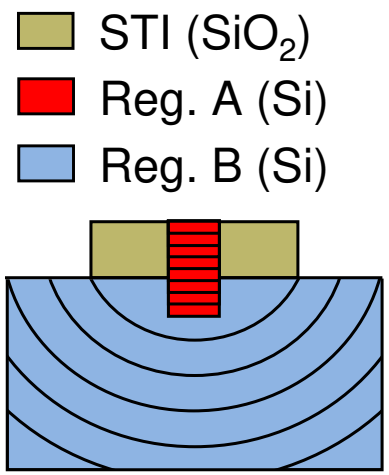
Application to Device Engineering

Estimate of soft error rate (SER) of semiconductor

- ✓ The information stored in semiconductor memory is flipped by incident radiations through the energy deposition process
- ✓ Cosmic ray neutron is the dominant contributor to SER at ground level

Event generator and cosmic-ray source modes are indispensable

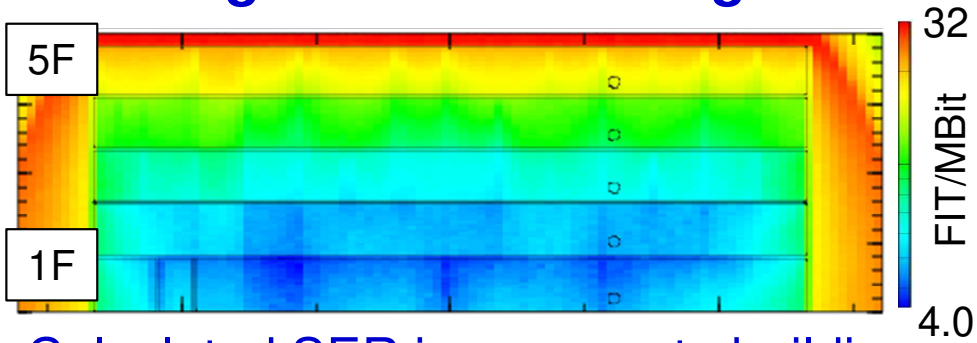
PHITS-based SER estimators

Device simulator	MSV model
	

Accurate! Fast!

Abe et al. J. Nucl. Sci. Technol. 53, 451 (2015)

Investigation of shielding effect



Calculated SER in a concrete building

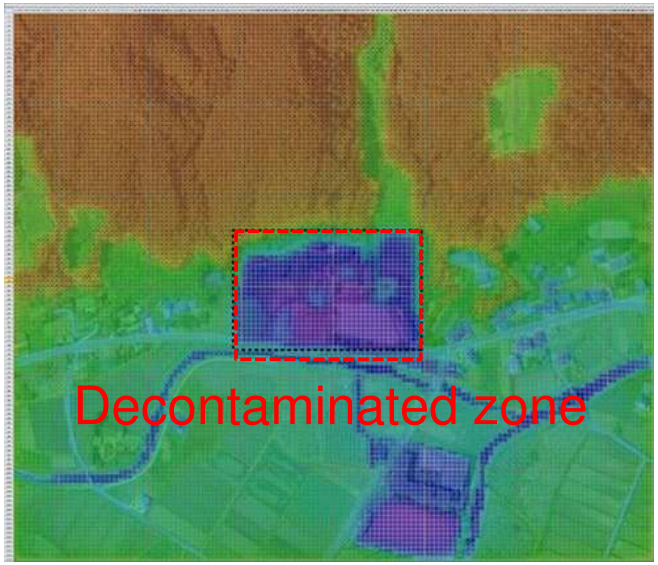
- ✓ Neutron-induced SER is dramatically reduced by concrete shielding
- ✓ Muon contribution to total SER is not negligible (up to 10% at 1st floor)

Abe et al. RADECS (2016)

Applications to Severe Nuclear Accident

Decontamination

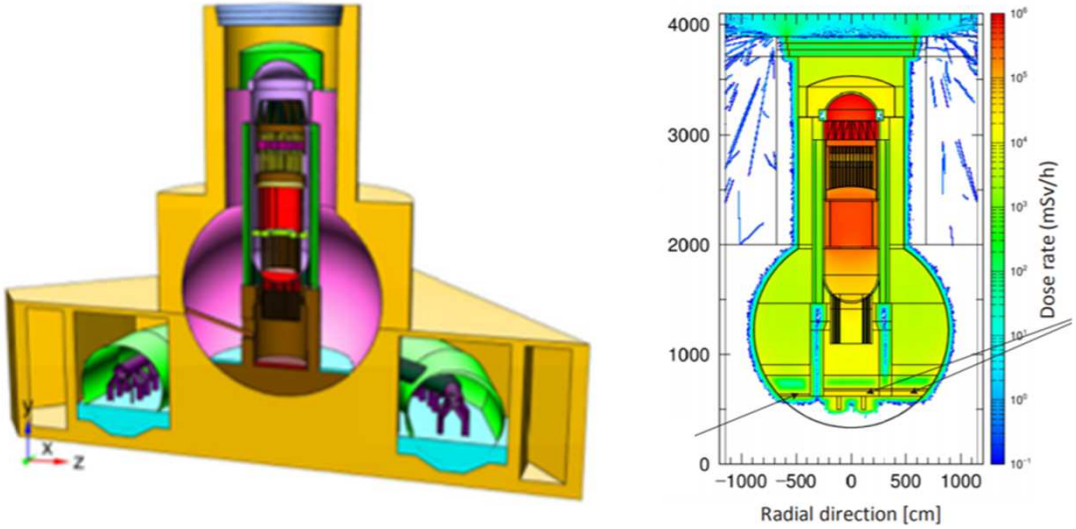
- ✓ JAEA developed software to evaluate decontamination effect (CDE)
- ✓ PHITS was used to make database of ambient doses in contaminated environment



Ambient dose estimated by CDE

Decommissioning of NPP

- ✓ Estimation of radiation dose distribution inside NPP is indispensable.
- ✓ PHITS was used to predict most probable dose rates by fully reproducing its geometry estimated based on the internal investigation results



Predicted dose rates inside Fukushima Daiichi NPP at the end of 2021

http://nsed.jaea.go.jp/josen/

Okumura et al. JAEA-Conf 2018-001

Table of Contents

Important Features of PHITS

- ✓ **Capability of transporting nearly all particles**

  Over a wide energy range in any materials

- ✓ **User-friendly interface and graphical output tools**

  ANGEL, PHIG-3D etc.

- ✓ **Sophisticated reaction models and libraries**

  JQMD, JENDL with event generator mode, track structure mode etc.

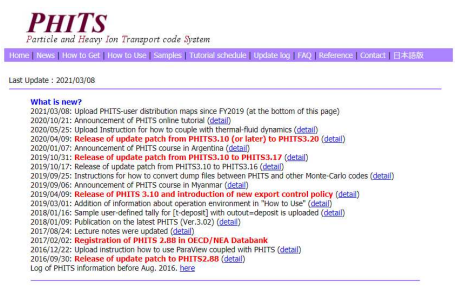
- ✓ **Useful functions and tools for various purposes**

  RI & cosmic-ray sources, RT-PHITS, microdosimetric function etc.

- ✓ **PHITS has been used in more than 50 countries**
- ✓ **Number of registered users increases ~ 1,000 per year**

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

More Information



Official Website

- ✓ Major update & tutorial announcements
- ✓ Confidential questions and bug reports to PHITS office

http://phits.jaea.go.jp/

Facebook

Press "like"

More frequently updated. Announcement of bug & tips

https://www.facebook.com/phitscommunity

User Forum

Recommended!

User communication site. Question & answer

https://meteor.nucl.kyushu-u.ac.jp/phitsforum/

Youtube

Promotional video. Tutorial contents (in future)

https://www.youtube.com/watch?v=G6-XTIctRgA