The PHITS Monte Carlo Particle Transport Simulation Code

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Deterministic vs Monte Carlo (MC)

 In deterministic models, the output of the model is fully determined by the parameter values and the initial conditions.

$$\begin{array}{c} X1 \longrightarrow \\ X2 \longrightarrow \\ X3 \longrightarrow \end{array} \qquad \mathbf{f}(\mathbf{x}) = \mathbf{x}^2 \qquad \stackrel{\longrightarrow}{\longrightarrow} \begin{array}{c} Y1 \\ \longrightarrow \\ Y2 \\ \longrightarrow \\ Y3 \end{array}$$

- Monte Carlo methods are stochastic techniques to solve problems using probabilistic (statistical) methods that utilizes sequences of random numbers and probability distributions which define the range of outcomes.
- The Monte Carlo method provides approximate solutions to a variety of problems, which may have many variables.

$$\mathbf{E}_1 = \mathbf{E}_2 = \mathbf{E}_3 = \mathbf{E} \qquad \underbrace{\mathbf{E}_1}_{\mathbf{E}_2} \xrightarrow{\longrightarrow}_{\mathbf{E}_3} \mathbf{f}(\mathbf{x}) = \mathbf{?} \qquad \underbrace{\longrightarrow}_{\mathbf{N}_2}^{\mathbf{N}_1} \mathbf{N}_1 \neq \mathbf{N}_2 \neq \mathbf{N}_3$$

Deterministic Simulation Codes

Advantages

- Exact
- Fast
- Do not require powerful/fast computers.

Disadvantages

- Inaccurate in the case of complicated geometries.
- Do not reconstruct collisions & do not preserve all correlations.
 > It is not possible to model interdependent relationships between input variables.

Sensitivity Analysis.

With just a few cases, deterministic analysis makes it difficult to see which variables impact the outcome the most.

Scenario Analysis.

In deterministic models, it's very difficult to model different combinations of values for different inputs to see the effects of truly different scenarios.

Monte Carlo Simulation Codes

Advantages

- Accurate even in the case of complicated geometries.
- Reconstruct collisions & preserve all correlations.

> It is possible to model interdependent relationships between input variables.

Probabilistic Results.

> Results show not only what could happen, but how likely each outcome is.

Sensitivity Analysis.

It is easy to see which inputs had the largest effect on the results.

Scenario Analysis.

It can can see exactly which inputs had which values when certain outcomes occurred.

Disadvantages

- Slow
- Require often powerful/fast computers.

- Credit for inventing the Monte Carlo method is shared by Stanislaw Ulam, John von Neuman and Nicholas Metropolis, who invented the method to solve neutron diffusion problems for Manhattan Project (1939-46) at Los Alamos.
- The 1949 article "The Monte Carlo Method" in Journal of the American Statistical Association, 44 (247), 335-341 by Metropolis and Ulam is often considered as the birth of the Monte Carlo method.



Taylor & Francis

The Monte Carlo Method Author(s): Nicholas Metropolis and S. Ulam Source: *Journal of the American Statistical Association*, Sep., 1949, Vol. 44, No. 247 (Sep., 1949), pp. 335-341 Published by: Taylor & Francis, Ltd. on behalf of the American Statistical Association Stable URL: http://www.jstor.com/stable/2280232





John von Neumann (28.12.1903-8.02.1957)



Nicholas Constantine Metropolis (11.06.1915-17.10.1999)

Stanislaw Ulam Jol (13.04.1909-13.05.1984)

- Historic example: calculation of π
 - Numerically: look for an appropriate convergent series and evaluate this approximately.
 - By Monte Carlo: look for a stochastic model.
- Example: throw a needle on a sheet with equidistant parallel stripes.
 Distance between stripes: *d*.
 Length of needle: *I < d*.





Buffon's Needle Experiment – First stated in 1777



Georges Louis Leclerc Comte de Buffon (07.09.1707-16.04.1788)

- Buffon's original "experiment" was to drop a needle of length L on a lined sheet of paper and determine the probability of the needle crossing one of the lines on a paper with parallel lines with spacing D.
- Remarkable result: probability is directly related to the value of π.





What is the probability P, that the needle crosses one of the lines?



$$P_{cut} = \int_0^{\pi} P_{cut}(\theta) \frac{d\theta}{\pi} = \int_0^{\pi} \frac{L\sin\theta}{D} \frac{d\theta}{\pi} = \frac{L}{\pi D} \int_0^{\pi} \sin\theta \, d\theta = \frac{2L}{\pi D}$$

• If we drop the needle *N* times and count *R* intersections, we obtain: $P_{cut} = \frac{R}{N} = \frac{2L}{\pi D} \implies \pi = \frac{2LN}{RD}$



NU	imber o	f Needle Dr	ops: O	
Nu	imber o	f Hits: 0	10	
	16 36 3	CDL D.D.		

History of Monte Carlo Method						
	Drop 1 Drop 100 Drop 1000 Start Over					
	Number of Needle Drops: 1					
	Estimate of PI: Infinity					



Number of Needle Drops: 11 Number of Hits: 8	Drop 1 Drop 10 Di	rop 100	Drop 1000	Start Over
Number of Needle Drops: 11 Number of Hits: 8	, 1 1	1		
Number of Needle Drops: 11 Number of Hits: 8	AIT	t		
Number of Needle Drops: 11 Number of Hits: 8	1TT			
Number of Needle Drops: 11 Number of Hits: 8	/ ¥		<u>17</u>	
Number of Hits: 8	Number of Needle Drops:	11		
Entimate of PI: 2.75	Number of Hits: 8			
Estimate of F1. 2.70	Estimate of PI: 2.75	J		









Laplace's method of calculating π (1886)



Pierre-Simon de Laplace (23.03.1749-05.03.1827)

"Hit or miss" approach



 $2\mathbf{r}$

Area of the square = $4r^2$

Area of the circle = πr^2

If we drop a small coin enough many times, *N*, randomly inside the square and count random hits inside circle N_c , we obtain P_{in} , the probability of random points inside the circle: $P_{in} = \frac{N_c}{N}$

 $P_{in} = \frac{N_C}{N} = \frac{\pi r^2}{4r^2} = \frac{\pi}{4} \longrightarrow \pi = \frac{4N_C}{N}$

What is PHITS?

Particle and Heavy Ion Transport code System

Capability

Transport and collision of nearly all particlesover wide energy rangeusing Monte Carlo methodneutron, proton, ions,
electron, photon etc10-4 eV to 1 TeV/u

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



Accelerator Design

Applications



Radiation Therapy & Protection



Space & Geoscience

Example of PHITS Calculation



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

Stochastically simulate the motion of each particle using cross sections \rightarrow Average behavior such as particle flux and mean deposition energy

User Interfaces of PHITS

- Source code: Fortran (Intel Fortran 11.1, Gfortran 4.71 or later)
- Input file: Free-format text

You do not have to write Fortran program nor compile PHITS

- Geometry >GG format
 - ► Graphic utility: ANGEL
 - Support software (ParaVIEW*, SuperMC**)
- Tally functions Geometry drawn by ANGEL
 Particle fluence, Heat, Particle yield etc.
- Output Data

Text data, histograms, contour maps

Platforms

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









ParaVIEW

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Comparison with other MC codes

Name	Develo per	Application	Language	Features
MCNP(X)	LANL	Nuc. Energy Radiology	FORTRAN	World standard of nuclear energy High reliability, Criticality
GEANT4	CERN etc.	High E Phys, Radiology, Astronomy	C++	Object-oriented, Platform to integrate models and tools developed all over the world
FLUKA	CERN, INFN	Accelerator, Radiology, Astronomy	FORTRAN	Applied to accelerator shielding design Particularly popular in EU
EGS	KEK, SLAC	Radiology	FORTRAN	EM cascade code Applied to mainly radiology
SuperMC	FDS	Fusion, Radiology	C++	Developed for ITER High CAD-affinity, Visualization
PHITS	JAEA, RIST, KEK	Accelerator, Radiology, Astronomy	FORTRAN	Easy start-up Applied to accelerator design, radiology, space science

Physical Processes included in PHITS

Collision Transport Collision

Transport	External Field and Optical devices	 Magnetic Field Gravity Super mirror (reflection) 			
between collisions	Ionization process for charge particle	 dE/dx : ATIMA code Continuous-slowing-down Approximation (CSDA) 			
		 δ-ray generation Microdosimetric function Track-structure simulation 			
Collision	Low-energy Neutrons Photons, Electrons	Nuclear Data (JENDL-4.0 etc.) + Event Generator Mode			
with nucleus	High-energy nucleons	Intra-Nuclear Cascade			
	Heavy lons	Quantum Molecular Dynamics			

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Basic idea of MC simulation





Transport: step length is controlled by 1) Interaction length of physics process 2) Geometrical boundary

Physics Interaction: sampling interaction probability

Transport of Nucleus in Matter



Calculation of Collision Distance d



Calculation of collision distance d



Calculation of d in Monte Carlo codes



Calculation of d in Monte Carlo Codes



depth in matter



Two-Step Model for high energy p+N and N+N Reactions*

Dynamical/Pre-equilibrium stage

- Intra-nuclear cascade or QMD models
- Fast process: interaction time (≈ 10⁻²² s)
- Pre-equilibrium nucleon emission

De-excitation stage

(mostly nucleon, cluster and γ evaporation and fission)

- Statistical equilibrium
 - 1. Excited remnants have forgotten the entrance channel
 - 2. De-excitation mechanisms:
 - Evaporation, Fission or Multifragmentation followed by Evaporation
- Slow process: de-excitation time (10⁻²⁰ 10⁻¹⁶ s)
- Energy and angular momentum release
- Final residue (A_{res}, Z_{res})

Nuclear Reaction Models - Dynamical Step

Intra-Nuclear Cascade (INC) Models



- Straight-line trajectories
- Mean-field potential
- Binary collisions with Pauli blocking
- Limitations
 - Mean free path > de Broglie wavelength

$$\Lambda = \frac{1}{\rho_0 \, \sigma_{NN} \, f_{\text{Pauli}}} \qquad \qquad \lambda = \frac{h}{\rho_{\text{la}}}$$

≻ E_{proj'lab} ≈ 20 MeV/nucleon – 3 GeV/nucleon

≻ A_{proj}: p, n, π^{+/-}, A < 4</p>

Quantum Molecular Dynamics (QMD) Models



- Nucleons as wave packets
- Curved trajectories
- Potential built from nucleon-nucleon interactions
- Two- or three-body forces
- Binary collisions with Pauli blocking
- Limitations
 - ≻ E_{proj/lab} ≈ 10 MeV/nucleon 3 GeV/nucleon
 - A_{proj}: any nucleus

De-excitation by Evaporation or Fission





Intra-Nuclear Cascade or QMD Model Excited Nucleus

Evaporation Model

or

Fission

De-excitation by SMM and Evaporation 0 **Evaporation** Excited Model Intra-Nuclear Cascade **Nucleus** or QMD Model

Map of Models Recommended to Use in PHITS

	Neutron	Proton, Pion (other hadrons)		Nucleus	Muon	e- / e+	Photon	
-	1 TeV	1 TeV 1 TeV/u					1 TeV	
	Intra-nuclea	ar cascade (JAM)			Virtual			
gh	+ Ev	aporation (GEM)			Photo-			
Ĩ	3.0 GeV				Nuclear			Photo-
1	Intra-nuclear c	ascade (INCL4.6)	d	Quantum Molecular	JAM/ JQMD		FPDI 97	Nuclear JAM/
λ		+	t	Dynamics	+	EGS5	or	JQMD
erç	Eva	aporation (GEM)	31.1	(JOMD)	GEM		EGS5	GEM
En	20 MeV		чпе	+ GEM	200 IVIEV			+
Ι	Nuclear		α	10 MeV/u	ATIMA			JENDL
≁	Data Library	1 MeV		Ionization	+			NRF
ΝC	(JENDL-4.0)	1 ko\/			Original	$\frac{1}{1}$	1 //	
Ľ	+			7 (1 11 11 / / /	Muonio		IKEV	
	EGM				atom +	structure	*Only in v	water
	0.01 meV				Capture	1 meV		

Physics models of PHITS and their switching energies

Switching energies can be changed in input file of PHITS

JAM (Jet AA Microscopic Transport) Model

- JAM is a Hadronic Cascade Model, which explicitly treats all established hadronic states including resonances with explicit spin and isospin as well as their anti-particles.
- We have parameterized all Hadron-Hadron Cross Sections, based on Resonance *Model* and *String Model* by fitting the available experimental data.



JQMD (JAERI Quantum Molecular Dynamics) Model

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



K. Niita et al, Phys. Rev. C52 (1995) 2620,

T. Ogawa et al., Phys. Rev. C92 (2015) 024614

Limitations with QMD

- QMD calculates the interaction of every single particle and can be used to calculate particle multiplicities and fragment yields.
- However, in QMD models, nuclei are often falsely disintegrated or excited during time evolution, mainly owing to a nonrelativistic equation of motion due to a nonrelativistic description of the Hamiltonian.
 - > The spurious excitation or decay can suppressed by:
 - ✓ introducing Pauli force and freezing the nucleons until impact;
 - disregard peripheral collisions and spurious reactions by limiting the impact parameter.
 - Coalescence models are often used to simulate cluster formation; however, they cannot be applied to the formation of heavy residues.
 - These treatments result in non-conservation of energy, an incorrect specific heat of the nucleus, or inaccurate simulation of peripheral collisions

Hence, QMD has problems to calculate the residual nucleus production!



- JAMQMD is a combination of the JAM and JQMD models and is composed of binary reactions of elastic, resonant and non-resonant channels, a relativistic equation of motion, interaction by mean field, and "clusterization" in the final state.
- Artificial corrections are not necessary because nuclei are formed and sustained by the interaction between nucleons.
- The calculations are fast and can reasonably well simulate particle production and fragment yield in high-energy nucleus-nucleus reactions of up to 1 TeV/u of incident energy.

$$m_T^2 = m^2 + p_x^2 + p_y^2 = E^2 - p_z^2$$



Proton transverse mass distribution in central Pb-Pb collisions at 20, 40, 80, and 158 GeV/u. Symbols are experimental data taken

Nuclear Data Library

Cross sections for low energy neutrons strongly depends on nuclear structure

Physics models are inadequate

Isotopic cross section data library is necessary



http://wwwndc.jaea.go.jp/jendl/j40/J40_J.html

Event Generator Mode

What is event generator mode (EGM)?

Sample all secondary particles from DDX contained in nuclear data library, considering energy & momentum conservation in an event

Indispensable for detector response and soft-error rate calculation

How does it work?

Conventional method: Sample particle by particle from energy distribution
 EGM: Sample all particles at once from energy sampling space



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



Japan Proton Accelerator Research Complex



Constructed under joint project of JAEA and KEK in Tokai-mura

Shielding Design around Spallation Target



M. Harada et al. J. Nucl. Material 343, 197 (2005)

Shielding Design around Neutron Beam Line



23 neutron beam lines in material and life science facility

Duct source option

- Source generation program specialized for shielding design of long beam lines
- "Weight" of each source particle is automatically adjusted
- obtain good statistics within reasonable computational time in whole area

Functions for Beam Transport

Charged particles

- Angular and energy straggling
- Dipole and Quadrupole Magnetic field
- Magnetic field map in xyz or r-z coordinate

Low energy neutrons

- Dipole, Quadrupole and Sextupole
- Magnetic field map in xyz or r-z coordinate
- Pulse (Time dependent) Magnetic field
- Optical devices; Super mirror
- Mechanical devices; T0 chopper,
- Gravity

PHITS can simulate not only trajectories, but also collisions and ionization at the same time.





CT Dosimetry System: WAZA-ARI

What is WAZA-ARI?

- Web-based system for calculating patient doses from CT examination
- Organ dose data calculated by PHITS coupled with Japanese voxel phantoms for male & female





F. Takahashi et al. Health Phys., 109, 104-112 (2015), https://waza-ari.nirs.qst.go.jp/

Application to Particle Therapy



Application to BNCT



Treatment planning system: JCDS

H. Kumada et al. *J. Phys.: Conf. Ser.* **74**, 021010 (2007)



Application to Nuclear Medicine

PHITS-based Application for Radionuclide Dosimetry In Meshes



- 1. Select human or mouse tetra-mesh phantom
- 2. Input retention time of Radioiodine (RI) in each organ visualization
- 3. Automatically generate PHITS input for the condition and execute
- 4. Visualize the calculated dose distributions in TPS or ParaVIEW

Developed by MSKCC and Opened to Public for free!

Carter et al. J. Nucl. Med (2019) (https://www.paradim-dose.org/)

d 0a-01

0.05

ParaVIEW

Calculation of Dose Conversion Coefficients

supervision of ICRP C2 Task groups

PHITS Simulation Conditions

Incident particle: neutron, proton, pion, muon, heavy ions (~Ni)
Incident energy: 1 MeV/n* up to 100 GeV/n

- •Irradiation geometry: ISO, AP, PA, LLAT, RLAT, ROT
- Calculated quantity: dose, Q(L),Q(y)&Q_{NASA}-based dose equivalent



*from 1 meV for neutron

T. Sato et al. Phys. Med. Biol. 54, 1997, (2009), T. Sato et al. Phys. Med. Biol. 55, 2235, (2010)₄₉

Applications to Radiation Biology



Linear Energy Transfer (LET)



LET is the amount of energy deposited per unit length of a material as a charged particle traverses the material

LET_w has the unit MeV/cm (or more common keV/µm)

Light vs. Heavy lons at the same LET (140 keV/µm)



10 mm





10 10

Microscopic Track Structure Simulation



Microdosimetric Function ~ Comparison with Track Structure Simulation ~



PHITS can almost perfectly reproduce the track structure simulation data
 Computational time: PHITS << Track structure simulation (~10⁻⁶)

MATROSHKA Experiment



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

Aircrew Dose Estimation



Impact of Solar Flares on Earth

WArning System for AVIation Exposure to Solar Energetic Particle

WASAVIES

- Nowcast radiation doses during large solar particle events based on the satellite observation and ground-level neutron monitors
- $\checkmark\,$ PHITS was used for analyzing the motion of solar particles in the atmosphere



R. Kataoka et al. Space Weather (2018); T. Sato et al. Space Weather (2018)

Calculation of Radiation Damage: DPA

What is DPA?

Average number of displaced atoms per atom of a material
PHITS-DPA considers not only Coulomb scattering of charged particles but also nuclear interactions.



Y. Iwamoto et al., Nucl. Instr. and Meth. B, 274 (2012) 57. Y. Iwamoto et al., J. Nucl. Sci. Technol. 51 (2014) 98.

Semiconductor soft error rate evaluation

Semiconductor soft error ?

- The information stored in semiconductor memory is flipped by incident radiations through the energy deposition process
- At ground level, errors are induced by reactions of cosmic ray neutrons

Simulation of secondary particle production by neutrons is necessary



SER analyses with device simulator or multiple sensitive volume model

S. Abe et al. J. Nucl. Sci. Technol. 53, 451-458 (2015)

Semiconductor soft error rate evaluation



- SEU occurs when deposition energy exceeds a certain threshold
- SEU probability = 0 from non-event generator simulation

→ Critical mistake!

• SEU probability = 10⁻⁶/source from event generator simulation

Decontamination effect estimation system

- Software to evaluate decontamination effect based on ambient dose
- PHITS was used to calculate ambient dose in contaminated environment



http://nsed.jaea.go.jp/josen/ (~Provided as freeware)

Typical Features of PHITS

- Capability of transporting nearly all particles Over a wide energy range in any materials
- Simple user interface and graphical output tools
- Sophisticated nuclear reaction models and libraries
 INCL4.6, INC-ELF, JQMD, JAM, JAMQMD, JENDL-4, EGS5 etc.
- Special functions for various purposes
 - Event generator mode
 - Microdosimetric function
 - Beam transport functions

PHITS has been used by more than 4,000 users in many countries

Future Plans

Improve nuclear reaction models and data library

- Full set of JENDL-4.0/HE
- Fission & intra-nuclear cascade models

Implement new functions

- Improvement of track-structure model
- Estimation of uncertainties using the high-energy particle induced radioactivity calculation code DCHAIN-SP
- Estimation of systematic uncertainties
- Improve user support functions
 - Special editor for making PHITS input file
 - Completion of error & warning ID lists

Subscribe to PHITS mailing list for update information

see http://phits.jaea.go.jp/howtoget.html and Email to phits-office@jaea.go.jp

Thank you very much for your kind attention!!

