OpenMC(TD): Current status, future plans and experimental benchmarking in Monte Carlo simulations

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[2]Millennium Institute for Subatomic Physics at the High Energy Frontier (SAPHIR)
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UNAM, Ciudad de México - México
17th - 21th June - 2024

LASNPA XIV/2024

XIV Latin American Symposium on Nuclear Physics and Applications

Outline

1. Introduction

2. Current status of OpenMC(TD)

3. Code development plans

4. Benchmark experiments

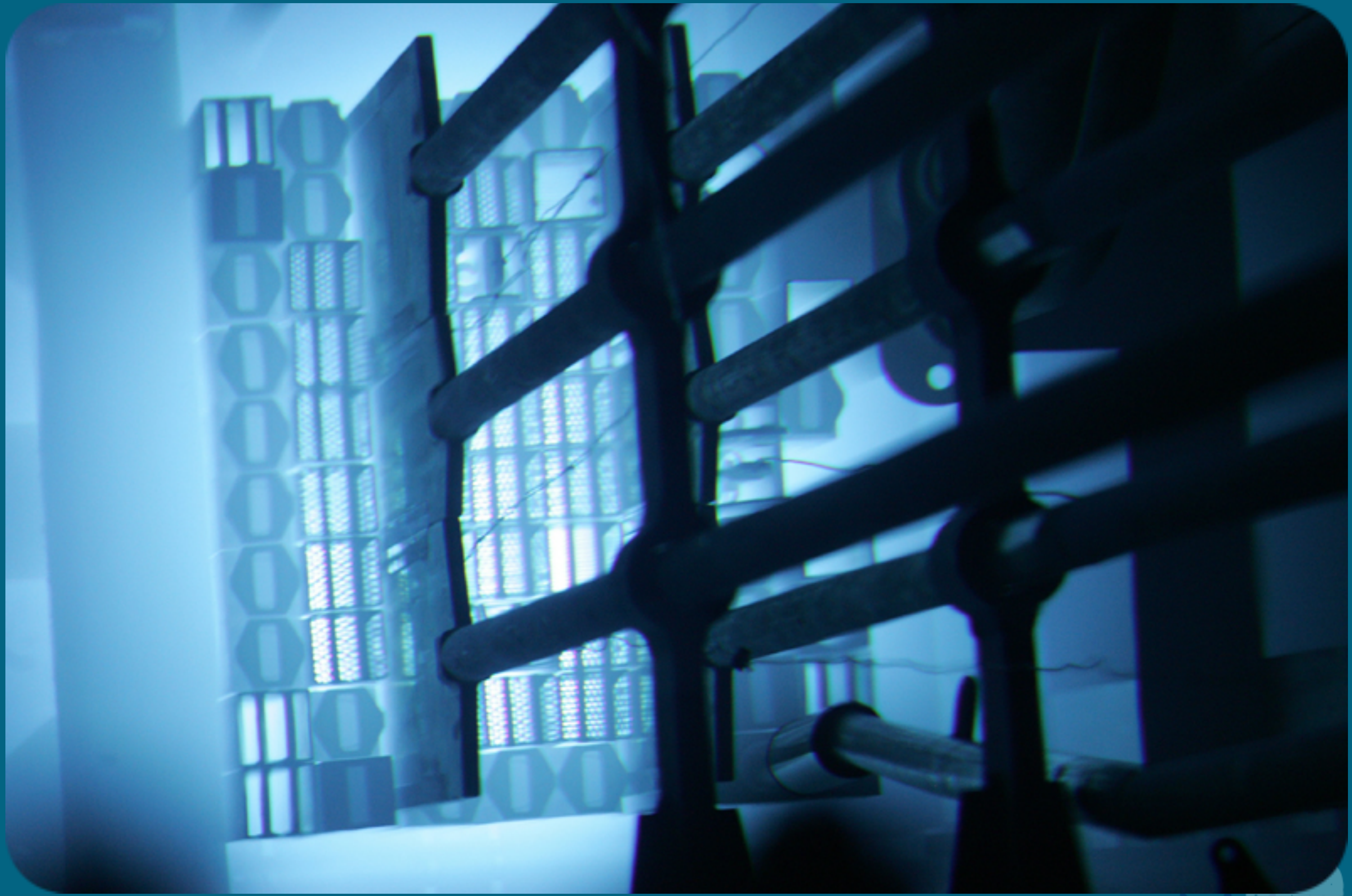
5. Conclusions

1. Introduction

Introduction

Motivation

How can we model the time evolution of neutron population in a fissile system such as a nuclear reactor?



Introduction

Neutron Transport Equation (NTE)

$$\left[\frac{1}{v}\frac{\partial}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla + \Sigma_{tot}(\mathbf{r}, E)\right] \psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \int_0^\infty dE' \int_0^{4\pi} d\hat{\mathbf{\Omega}}' \Sigma_S(E' \rightarrow E, \hat{\mathbf{\Omega}}' \rightarrow \hat{\mathbf{\Omega}}) \psi(\mathbf{r}, E', \hat{\mathbf{\Omega}}', t) + S(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$$

Neutron time change rate

Net number of neutrons

Neutrons collisioning in phase space

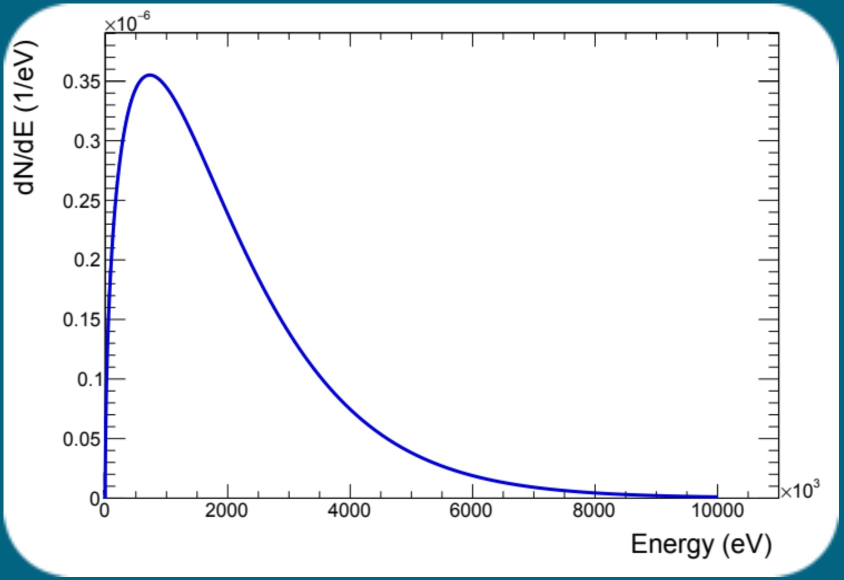
Neutrons scattering into phase space

Neutron source term

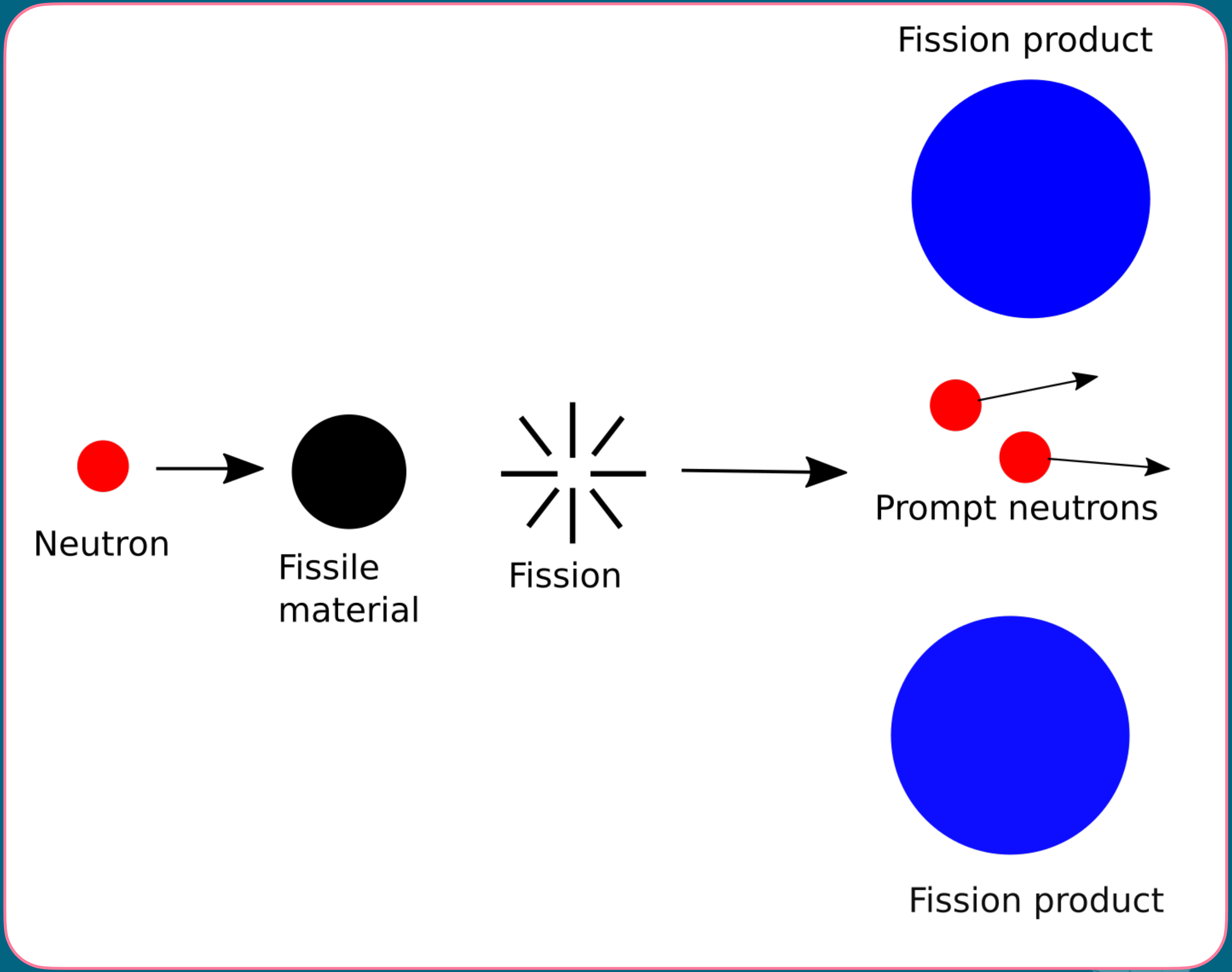
Introduction

Prompt neutrons

Mean energy of 2 MeV



^{235}U prompt fission neutron energy spectrum taken from ENDF-B/VIII.0

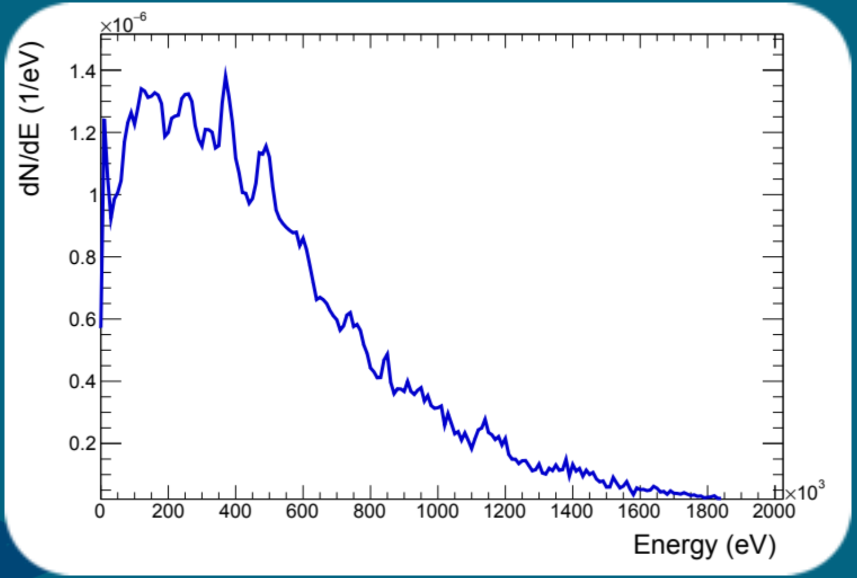


- Comprise ~99% released neutrons
- Emitted ~10^{-14} s after fission

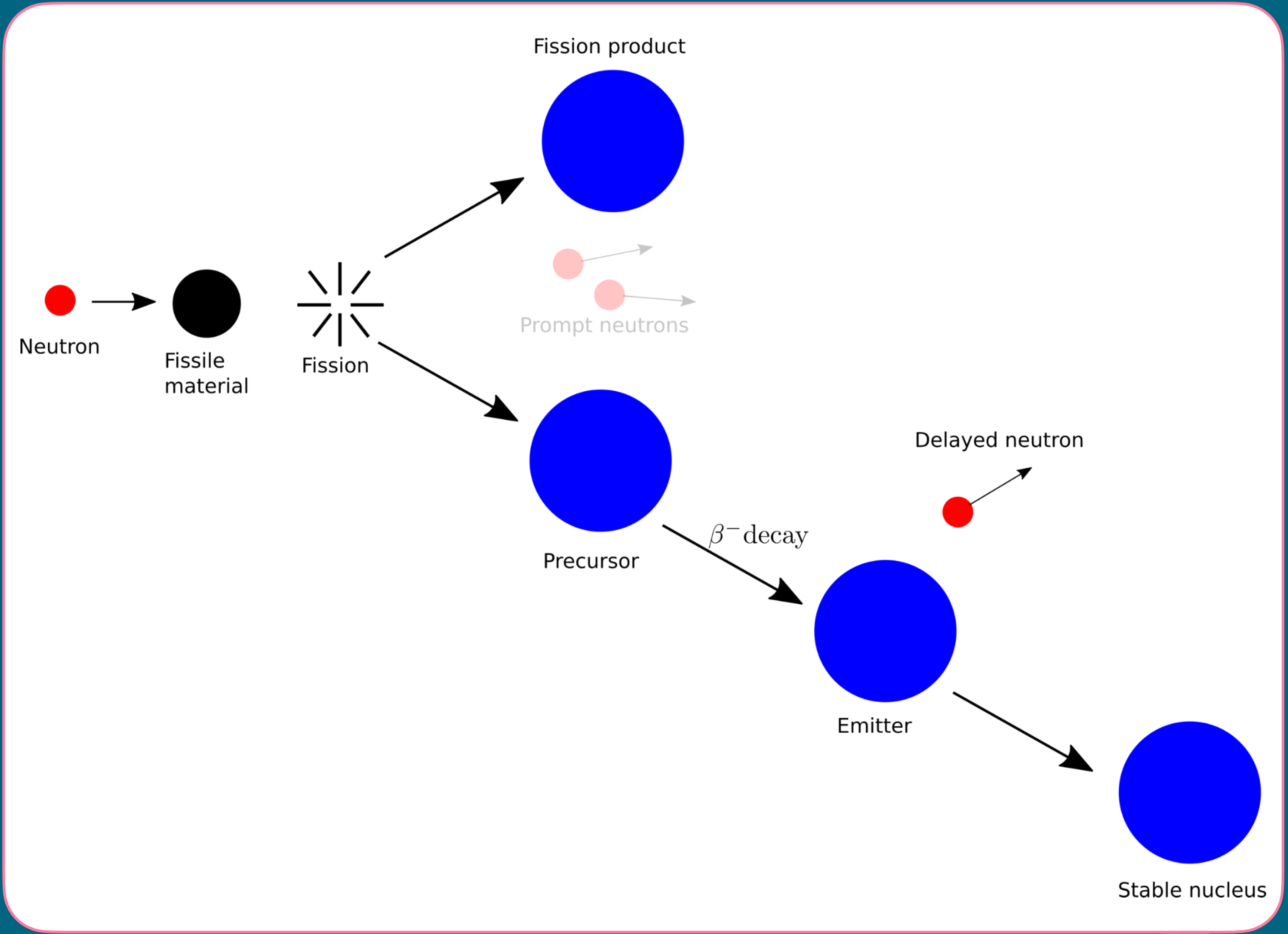
Introduction

Delayed neutrons

Mean energy of 484 keV



^{235}U delayed fission neutron energy spectrum taken from ENDF-B/VIII.0



- Comprise ~1% released neutrons
- Emitted between 10^{-3} s and 10^{2} s

Introduction

Neutron Transport Equation (NTE)

$$\left[\frac{1}{v}\frac{\partial}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla + \Sigma_{tot}(\mathbf{r}, E)\right]\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$$

$$= \int_0^\infty dE' \int_0^{4\pi} d\hat{\mathbf{\Omega}}' \Sigma_S(E' \rightarrow E, \hat{\mathbf{\Omega}}' \rightarrow \hat{\mathbf{\Omega}})\psi(\mathbf{r}, E', \hat{\mathbf{\Omega}}', t)$$

Prompt fission term

$$+\chi_p(E)(1 - \sum_i \beta^i) \int_0^\infty dE' \int_0^{4\pi} d\hat{\mathbf{\Omega}}' \nu(E')\Sigma_f(\mathbf{r}, E')\psi(\mathbf{r}, E', \hat{\mathbf{\Omega}}', t)$$

$$+ \sum_l \chi_l(E)\lambda_l C_l(\mathbf{r}, t)$$

Delayed fission term

And the NTE is coupled to the change in precursor concentration

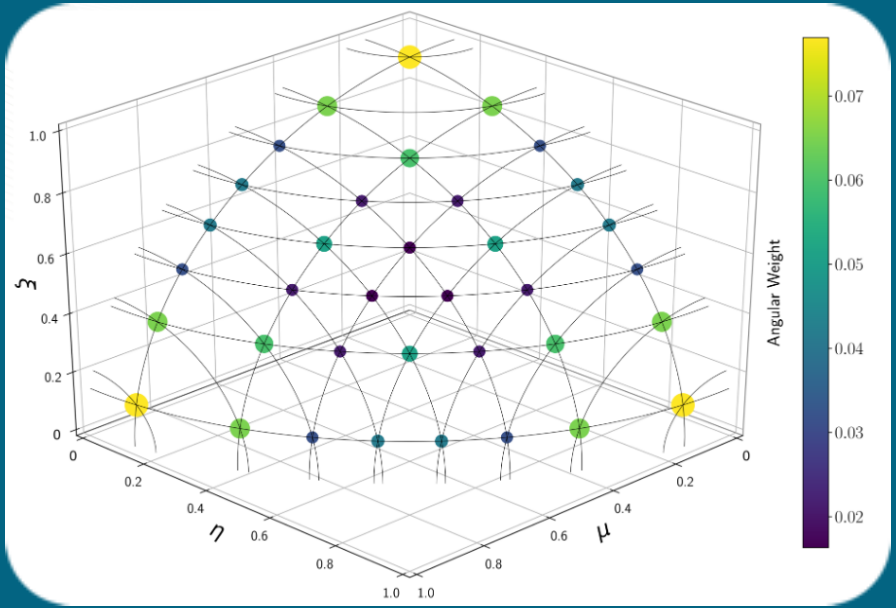
$$\frac{\partial}{\partial t} C_l(\mathbf{r}, t) = \sum_i \beta_l^i \int dE' \int d\hat{\mathbf{\Omega}}\, \nu(E')\Sigma_f(\mathbf{r}, E')\psi(\mathbf{r}, E', \hat{\mathbf{\Omega}}', t) - \lambda_l C_l(\mathbf{r}, t)$$

Introduction

Approaches to solve the NTE

Deterministic

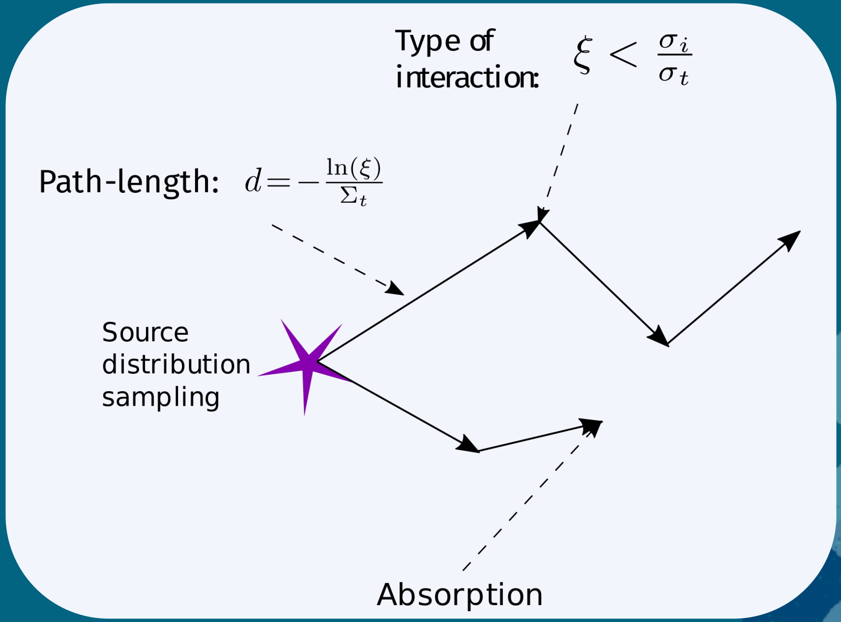
- Phase space is discretized
- Large memory requirements
- Constraints in memory may limit accuracy of results



Angular quadrature S16 to discretize angular variable. From Transport Methods Overview, Oak Ridge National Laboratory.

Stochastic

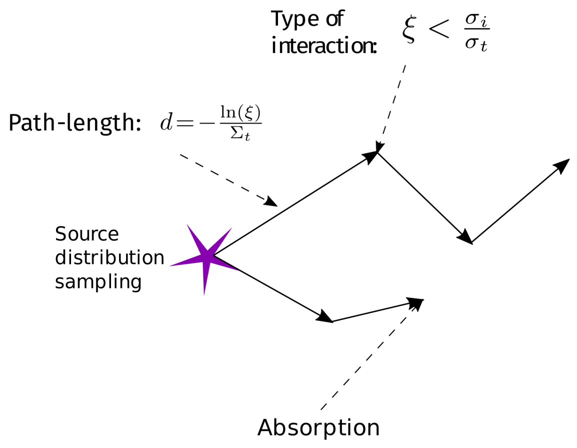
- Phase space is not discretized
- Transports particles
- Commonly used in stationary state



Introduction

Time in Monte Carlo simulations

Stationary state

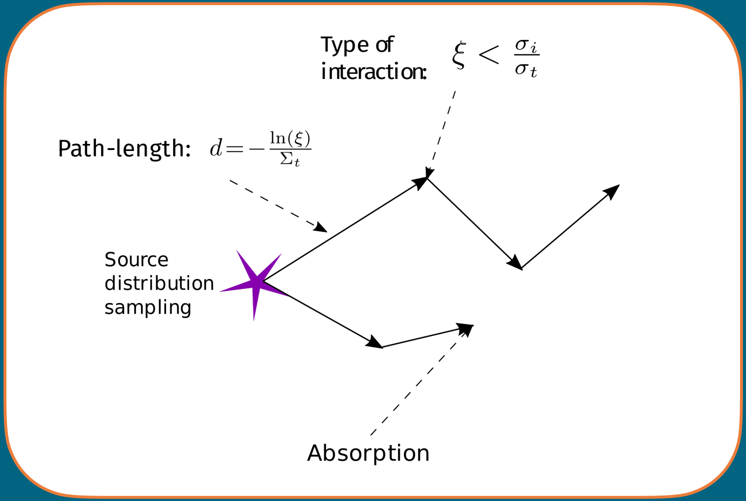


- Particles are emitted from a source.
- They either escape out of the system or travel in a straight line and collide
- Interaction probabilities are given by the cross sections.
- Time is not included in phase space.

Introduction

Time in Monte Carlo simulations

Stationary state



- Particles are emitted from a source.
- They either escape out of the system or travel in a straight line and collide
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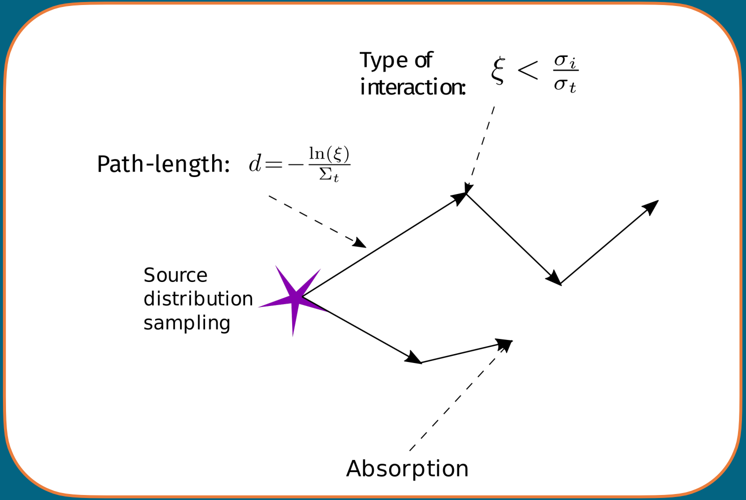
Time-dependence

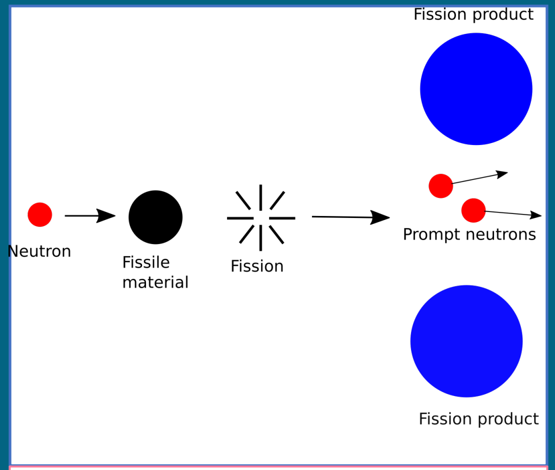


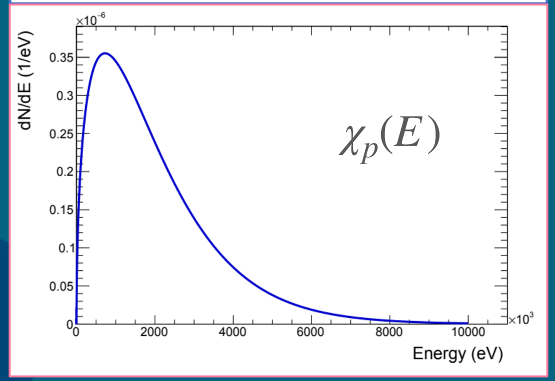
+

- Time evolution of neutrons
- Capability to score time dependent quantities (e.g. flux as a function of time)
- Division of simulation time in discrete time

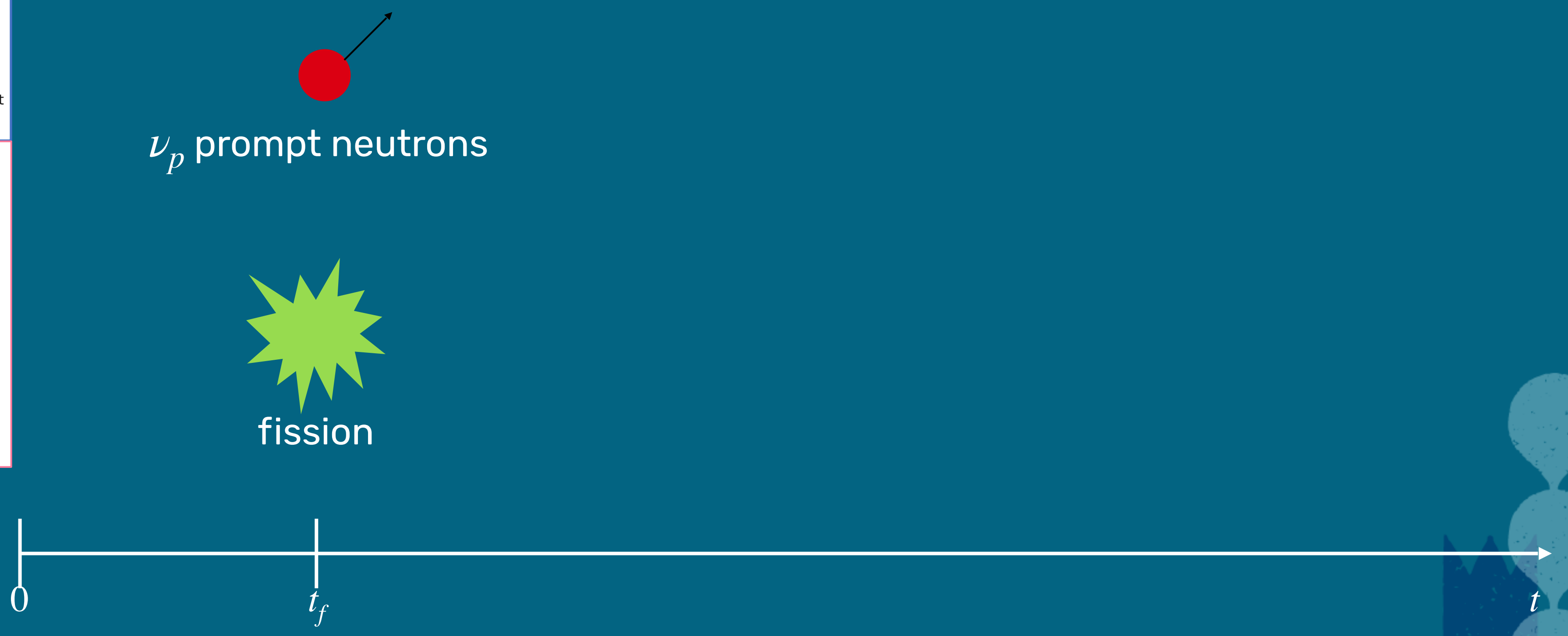
Introduction

β-delayed emission in analog Monte Carlo simulations



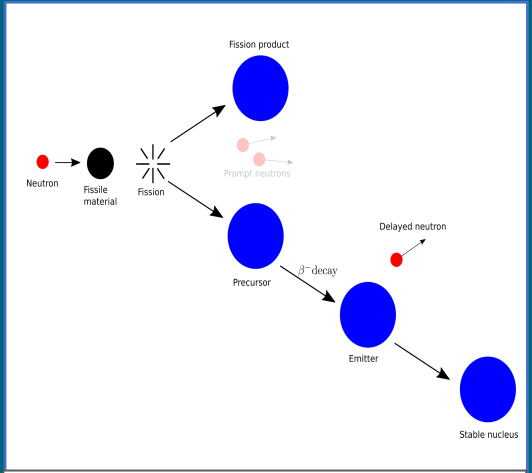


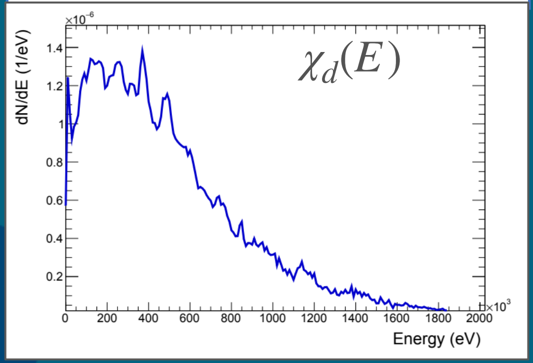
- prompt neutron energy sampled from $\chi_p(E)$
- neutron time t_f



Introduction

β-delayed emission in analog Monte Carlo simulations





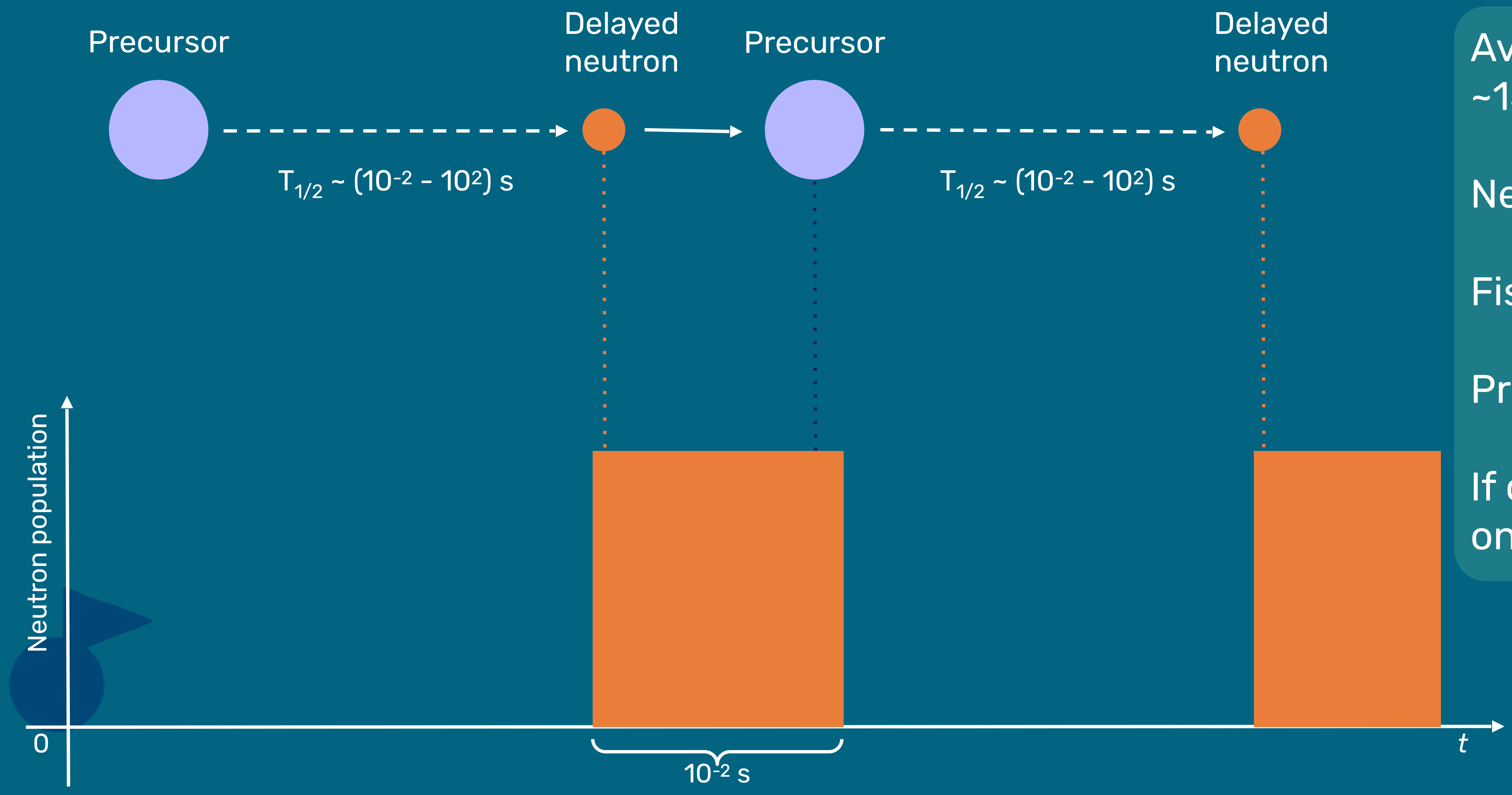
- delayed neutron energy sampled from $\chi_d(E)$
- neutron time $t_f + t_d$ obtained from precursor decay probability:

$$p_i(t) = \lambda_i e^{-\lambda_i (t - t_0)} \theta(t - t_0)$$

ν_d delayed neutrons

Introduction

β-delayed emission in analog Monte Carlo simulations



Average fission chain length ~150 neutrons

Neutron lifetime ~ 10^{-4} s

Fission chain lifetime ~ 10^{-2} s

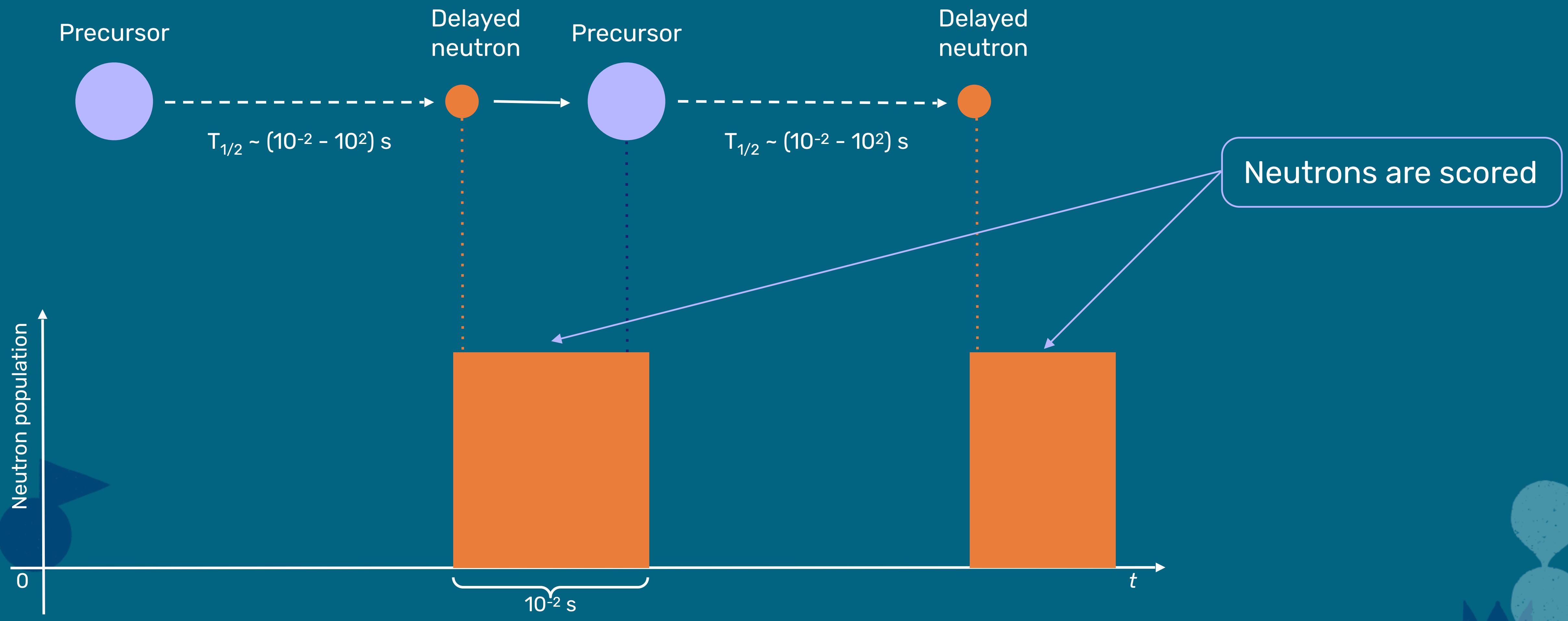
Precursor half life ~ (10^{-2} - 10^{2}) s

If critical, each prompt chain will on average create 1 precursor

Sjenitzer et al., Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations, Nucl. Sci. Eng.,175:1, 94-107, (2013)

Introduction

β-delayed emission in analog Monte Carlo simulations



Sjenitzer et al., Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations, Nucl. Sci. Eng.,175:1, 94-107, (2013)

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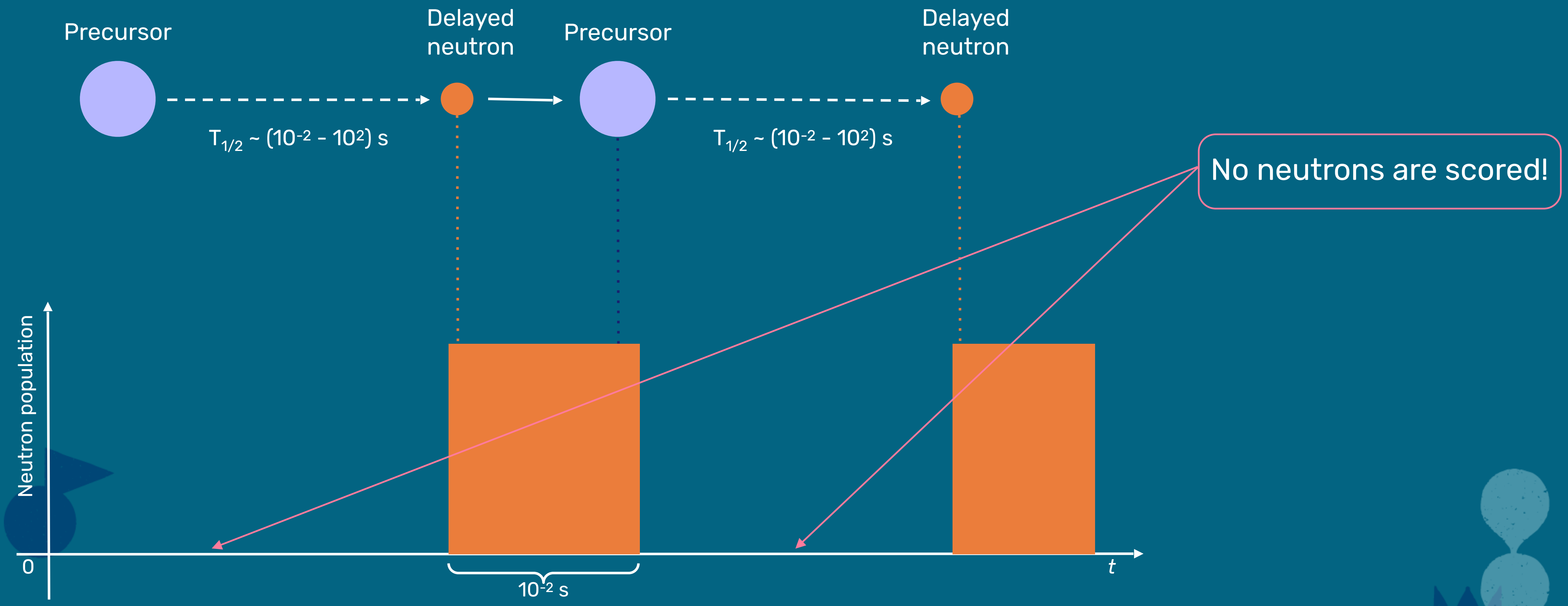
β-delayed emission in analog Monte Carlo simulations



Sjenitzer et al., Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations, Nucl. Sci. Eng.,175:1, 94-107, (2013)

Introduction

β-delayed emission in analog Monte Carlo simulations

The different timescales associated to prompt and delayed events would lead to large variances.

This means that β-**delayed emission** must be simulated another way.

ed!

Neutron population

0

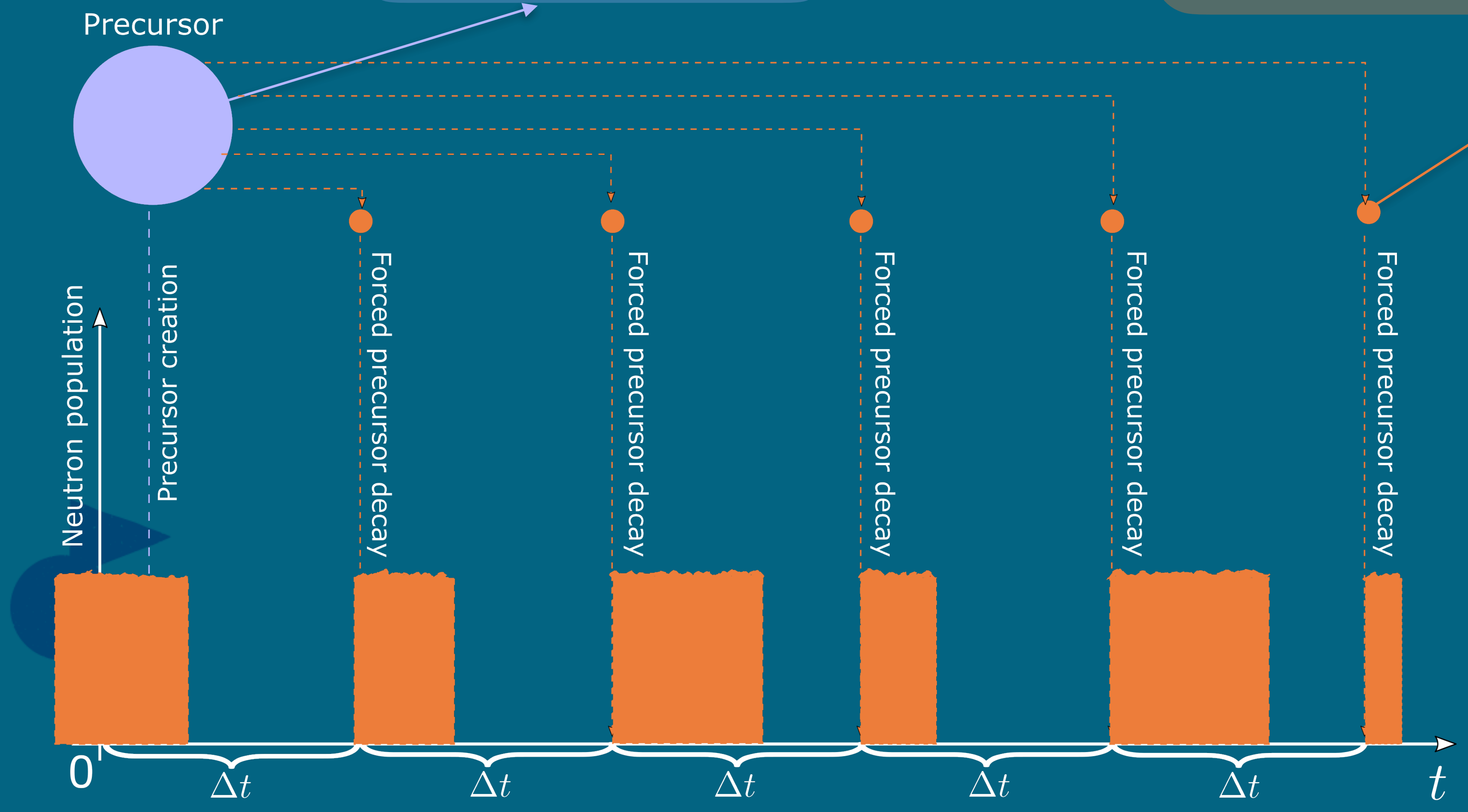
Sjenitzer et al., Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations, Nucl. Sci. Eng.,175:1, 94-107, (2013)

Introduction

β-delayed emission in a <u>non-analog</u> Monte Carlo simulations

$$w_p(t) = w_c \sum_i \Gamma_i e^{-\lambda_i (t - t_0)}$$

$$w_d(t) = \frac{p(t)}{\bar{p}(t)} = w_c \Delta t \sum_i \Gamma \lambda_i e^{-\lambda_i (t - t_0)} \quad \text{with} \quad t_j < t < t_{j+1}$$



$$\bar{p}(t) = \frac{1}{t_{j+1} - t_j} = \frac{1}{\Delta t}$$

Monte Carlo fair game is preserved by changing the delayed neutron weight and population control is enforced at the end of each time interval.

Sjenitzer et al., Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations, Nucl. Sci. Eng.,175:1, 94-107, (2013)

Introduction

Grouped β-delayed emitter precursors

J. Nuclear Energy, 1957, Vol. 6, pp. 1 to 21. Pergamon Press Ltd., London

DELAYED NEUTRONS FROM FISSIONABLE ISOTOPES OF URANIUM, PLUTONIUM AND THORIUM*

G. R. KEEPIN, T. F. WIMETT and R. K. ZEIGLER
University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico

Abstract—The periods, relative abundances, and absolute yields of delayed neutrons from "fast" fission of six nuclides (^{235}U, ^{233}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{232}Th) and thermal fission of three nuclides (^{235}U, ^{233}U, and ^{239}Pu) have been measured. "Godiva," the bare ^{235}U metal assembly at Los Alamos, was the neutron source. Six exponential periods were found necessary and sufficient for optimum least-squares fit to the data. Despite evident perturbations, general agreement among delayed neutron periods was obtained for all nuclides. Measured absolute total yields in delayed neutrons per fission (for the pure isotopes) are:

^{235}U: 0·0165 ± 0·0005 ^{239}Pu: 0·0063 ± 0·0003
^{233}U: 0·0070 ± 0·0004 ^{240}Pu: 0·0088 ± 0·0006
^{239}U: 0·0412 ± 0·0017 ^{232}Th: 0·0496 ± 0·0020

Representative of general delayed neutron periods (half-lives) and abundances are the ^{235}U fast-fission data:

Half-life (sec)	Relative abundance
54·51 ± 0·94	0·038 ± 0·003
21·84 ± 0·54	0·213 ± 0·005
6·00 ± 0·17	0·188 ± 0·016
2·23 ± 0·06	0·407 ± 0·007
0·496 ± 0·029	0·128 ± 0·008
0·179 ± 0·017	0·026 ± 0·003

	Possible precursor nuclei	Mean energy (MeV)	Average half-life of the group [s]			Delayed neutron fraction [%]		
i			235U	239Pu	233U	235U	239Pu	233U
1	87Br, 142Cs	0.25	55.72	54.28	55.0	0.021	0.0072	0.0226
2	137I, 88Br	0.56	22.72	23.4	20.57	0.140	0.0626	0.0786
3	138I, 89Br, (93,94)Rb	0.43	6.22	5.60	5.00	0.126	0.0444	0.0658
4	139I, (93,94)Kr 143Xe, (90,92)Br	0.62	2.3	2.13	2.13	0.252	0.0685	0.0730
5	140I, 145Cs	0.42	0.61	0.618	0.615	0.074	0.018	0.0135
6	(Br, Rb, As etc.)	-	0.23	0.257	0.277	0.027	0.0093	0.0087
		Total				0.64	0.21	0.26

Assumption (6 groups):

$$A(i) = \sum_{j=1}^{6} a_j \exp(-\lambda_j t)$$

Although there are more than 269 precursors in ^{235}U fission, they are grouped in 6 families.

Introduction

New data on precursors of β-delayed neutron emitters

International Atomic Energy Agency
Nuclear Data Services
قسم البيانات النووية مقدمة من

Search

CRP Meetings
- RCM-3 2017
- RCM-2 2015
- RCM-1 2013
- CM 2011

IAEA Docs
- INDC(NDS)-0735
- INDC(NDS)-0683
- INDC(NDS)-0643
- INDC(NDS)-0599
- INDC(NDS)-0107/G

CRPs/DDPs
- Reference Database for Beta-Delayed Neutron Emission (2013-2018)
- Total Absorption Gamma-

Reference Database for Beta-Delayed Neutron Emission

The overall objective of the Coordinated Research Project (2013-2018) was to create a Reference Database for Beta-Delayed Neutron Emission that contains an orga experimental, evaluated and theoretical data on beta-delayed neutron emission, and is readily available.

Microscopic Database	Macroscopic Database
The database includes a compilation of all existing measured beta-decay half-lives and delayed-neutron emission probabilities of individual precursors, and the recommended values based on evaluations performed by the CRP evaluators. Where a delayed-neutron spectrum has been measured there is a link to the corresponding spectrum file. The database also provides access to theoretical models and systematic parameterizations.	The macroscopic database includes all published experimental and evaluate (nubars), delayed neutron decay paramaters (a_i,T_i), and composite delayed fissioning systems. New recommendations for 6- and 8-group parameters a

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Nuclear Data Sheets
Nuclear Data Sheets 173 (2021) 144–238
www.elsevier.com/locate/nds

Development of a Reference Database for Beta-Delayed Neutron Emission

P. Dimitriou,[1,*] I. Dillmann,[2,3] B. Singh,[4] V. Piksaikin,[5] K.P. Rykaczewski,[6] J.L. Tain,[7] A. Algora,[7] K. Banerjee,[8] I.N. Borzov,[9,10] D. Cano-Ott,[11] S. Chiba,[12] M. Fallot,[13] D. Foligno,[14] R. Grzywacz,[15,6] X. Huang,[16] T. Marketin,[17] F. Minato,[18] G. Mukherjee,[8] B.C. Rasco,[19,6,15,20] A. Sonzogni,[21] M. Verpelli,[1] A. Egorov,[5] M. Estienne,[13] L. Giot,[13] D. Gremyachkin,[5] M. Madurga,[15] E.A. McCutchan,[21] E. Mendoza,[11] K.V. Mitrofanov,[5] M. Narbonne,[13] P. Romojaro,[11] A. Sanchez-Caballero,[11] and N.D. Scielzo[22]

These efforts brings the opportunity to explore how this new individual precursor data impacts on simulations of fissile systems.

Introduction

Inclusion of individual precursors

Libraries:
-JEFF-3.1.1
-ENDF-B/VIII.0

→

269 **individual precursors**
products of ^{235}U fission

→

β-delayed neutron emission

i-th precursor
cumulative yield

i-th precursor
relative importance

$$I_i = \frac{CY_i P_{n,i}}{\nu_d}$$

i-th precursor
delayed neutron
emission probability

Delayed neutron
yield

Introduction

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About OpenMC

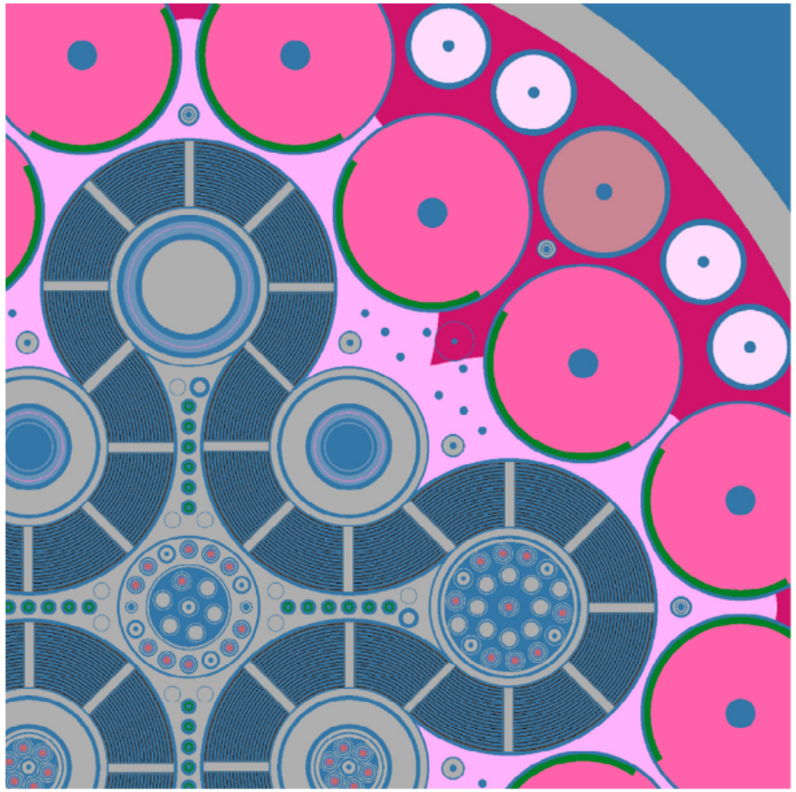

Fig. 1. Cross-sectional view of a section of an OpenMC model of the Advanced Test Reactor (ATR).

- Monte Carlo code for particle transport
- K-eigenvalue, fixed source and subcritical multiplication problems
- Continuous energy nuclear cross section data follows HDF5 format
- Active community that contributes to its development

Code license allows to "...including without limitation the rights to use, copy, modify, merge, publish, distribute..."

Modified code in this work was called Time-Dependent OpenMC or OpenMC(TD)

Romano et al., "OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development," Ann. Nucl. Energy, 82, 90–97 (2015).

2. Current status of OpenMC(TD)

OpenMC(TD) current status

LASNPA XIV/2024

Some results so far: Publications

Nuclear Engineering and Technology 54 (2022) 811–816

Contents lists available at ScienceDirect

Nuclear Engineering and Technology

journal homepage: www.elsevier.com/locate/net

Original article

Calculation of kinetic parameters β_{eff} and Λ with modified open source Monte Carlo code OpenMC(TD)

Check for updates

J. Romero-Barrientos [a, b, *], J.I. Márquez Damián [c], F. Molina [a, e], M. Zambra [a, f], P. Aguilera [a, d], F. López-Usquiano [a, b], B. Parra [g], A. Ruiz [a, d]

[a] Comisión Chilena de Energía Nuclear, Nueva Bilbao, 12501, Las C...des, Santiago, Chile
[b] Departamento de Física, Facultad de Ciencias Físicas y M... Universidad de Chile, Blanco Encalada, 2008, Santiago, Chile
[c] Spallation Physics Group, European Spallation S... 76, 22100, Lund, Sweden
[d] Facultad de Ciencias, Departamento de Físic... s Palmeras, 425, Ñuñoa, Santiago, Chile
[e] Departamento de Ciencias Físicas, Universida... 837-0136, Santiago, Chile
[f] Universidad Diego Portales, Manuel Rodríguez ... Chile
[g] Instituto de Física Corpuscular, Parque Científic... catrático José Beltrán, 2, E-46980, Paterna, Spain

2022

Nuclear Engineering and Design 423 (2024) 113189

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Nuclear Engineering and Design

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Transient Monte Carlo simulations with OpenMC(TD): A catalyst towards advancing research in next-generation reactors and to improve fission nuclear data

J. Romero-Barrientos [a,*], F. Molina [a,b,c], M. Zambra [a,d], F. López-Usquiano [a,c]

[a] Centro de Investigación en Física Nuclear y Espectroscopía de Neutrones CEFNEN, Comisión Chilena de Energía Nuclear, Nueva Bilbao, Las Condes, 12501, Santiago, Chile
[b] Millennium Institute for Subatomic physics at high energy frontier - SAPHIR, Fernández Concha 700, Las Condes, Santiago, Chile
[c] Departamento de Ciencias Físicas, Universidad Andres Bello, Sazié 2212, 837-0136, Santiago, Chile
[d] Universidad Diego Portales, Manuel Rodríguez Sur 415, Santiago, Chile

2024

Nuclear Engineering and Technology 55 (2023) 1593–1603

Contents lists available at ScienceDirect

Nuclear Engineering and Technology

journal homepage: www.elsevier.com/locate/net

Original Article

Development of transient Monte Carlo in a fissile system with β-delayed emission from individual precursors using modified open source code OpenMC(TD)

Check for updates

http://crossmark.crossref.or... doi=10.1016/j.net.2023.02.0...

J. Romero-Barrientos [a, *], F. Molina [a, b, c], J.I. Márquez Damián [d], M. Zambra [a, e], P. Aguiler... F. López-Usquiano [a, c, f], S. Parra [a]

[a] Centro de Investigación en Física Nuclear y Espectroscopía de Neutrones CEFNEN, Comisión Chilena de Energía Nuclear, Nueva Bilba... Santiago, Chile
[b] Millennium Institute for Subatomic Physics at High Energy Frontier - SAPHIR, Fernández Concha 700, Las Condes, Santiago, Chile
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[e] Universidad Diego Portales, Manuel Rodríguez Sur 415, Santiago, Chile
[f] Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Blanco Encalada, 2008, Santiago, Chile

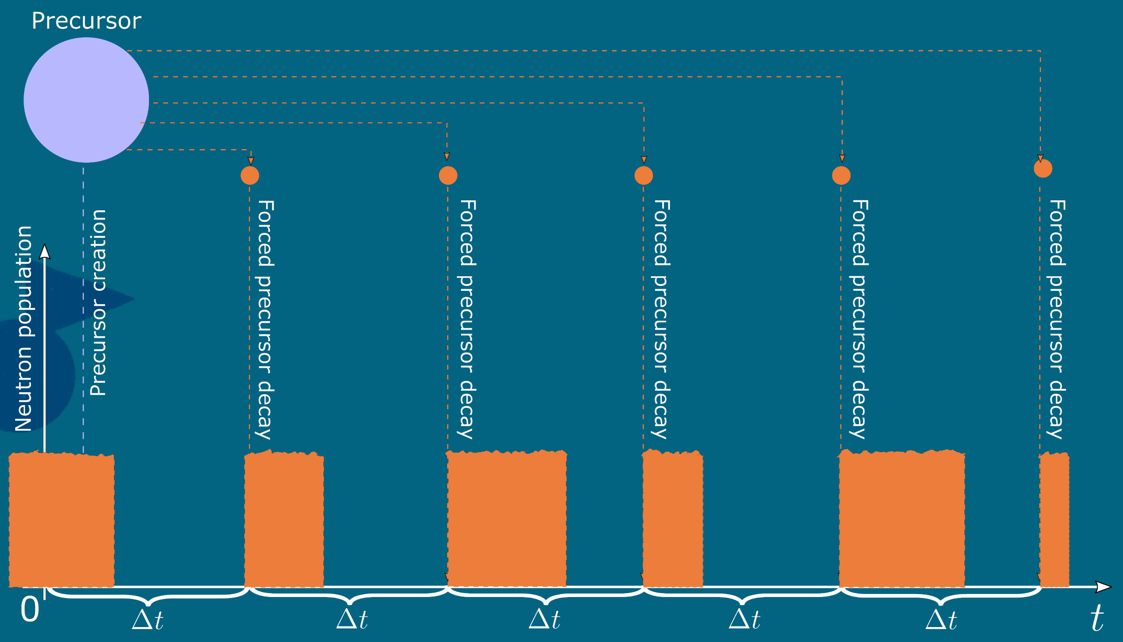
2023

OpenMC(TD) current status

Current OpenMC(TD) capabilities

Time-dependence related to β-delayed neutron emission

Forced decay and population control



Individual precursors instead of 6-group precursor structure

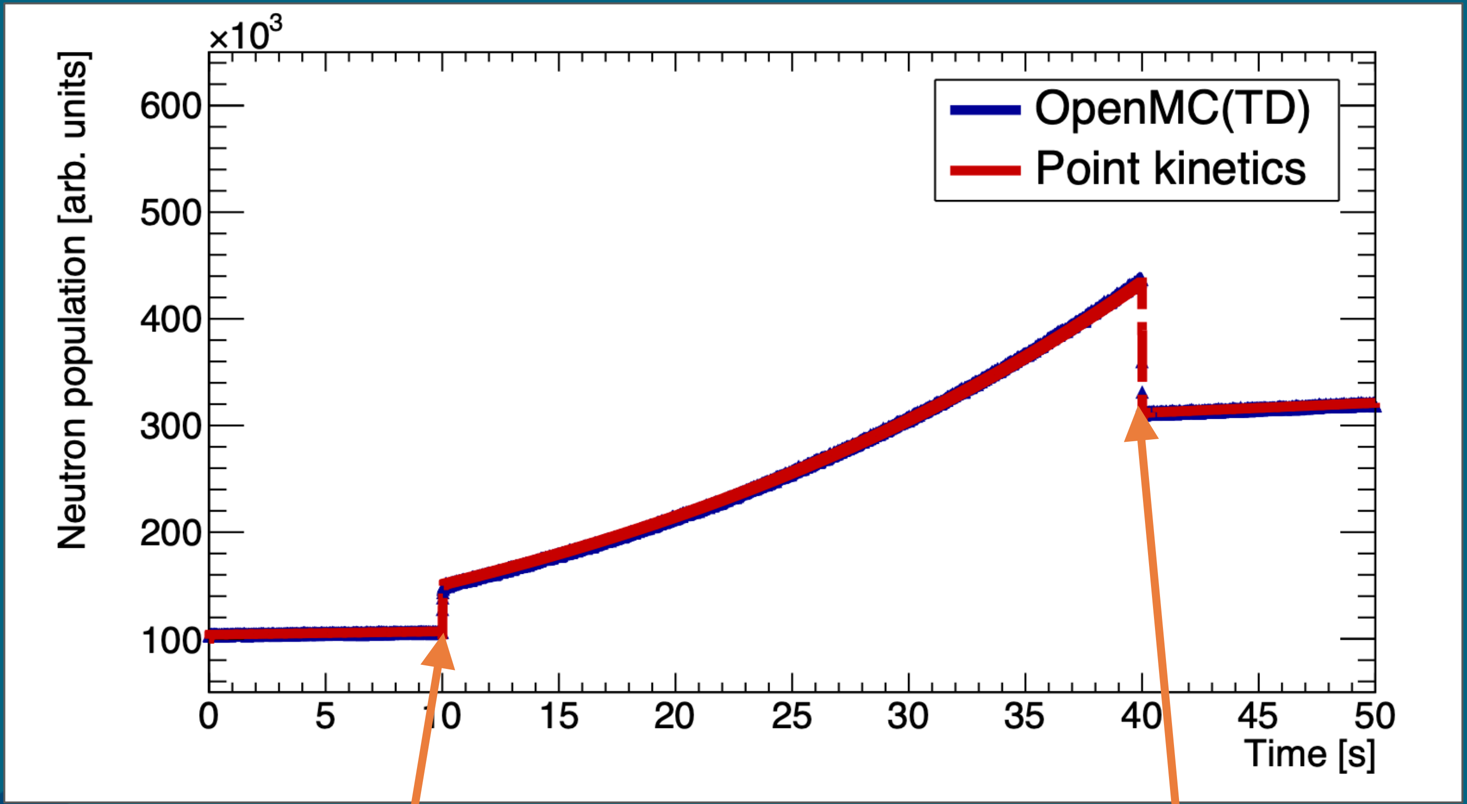
Individual precursor implementation

$$I_i = \frac{CY_i P_{n,i}}{\nu_d}$$

Romero-Barrientos et al., Nuclear Engineering and Technology , 55, 1593–1603 (2023).

OpenMC(TD) current status

Some results so far: 1 group point kinetics vs simulation



- Monoenergetic fissile system
- Rectangular box of (10x12x20) cm^3
- Constant cross-sections
- 1-group precursor structure.

+211 pcm
[Σ_a = 0.5870 cm^{-1}]

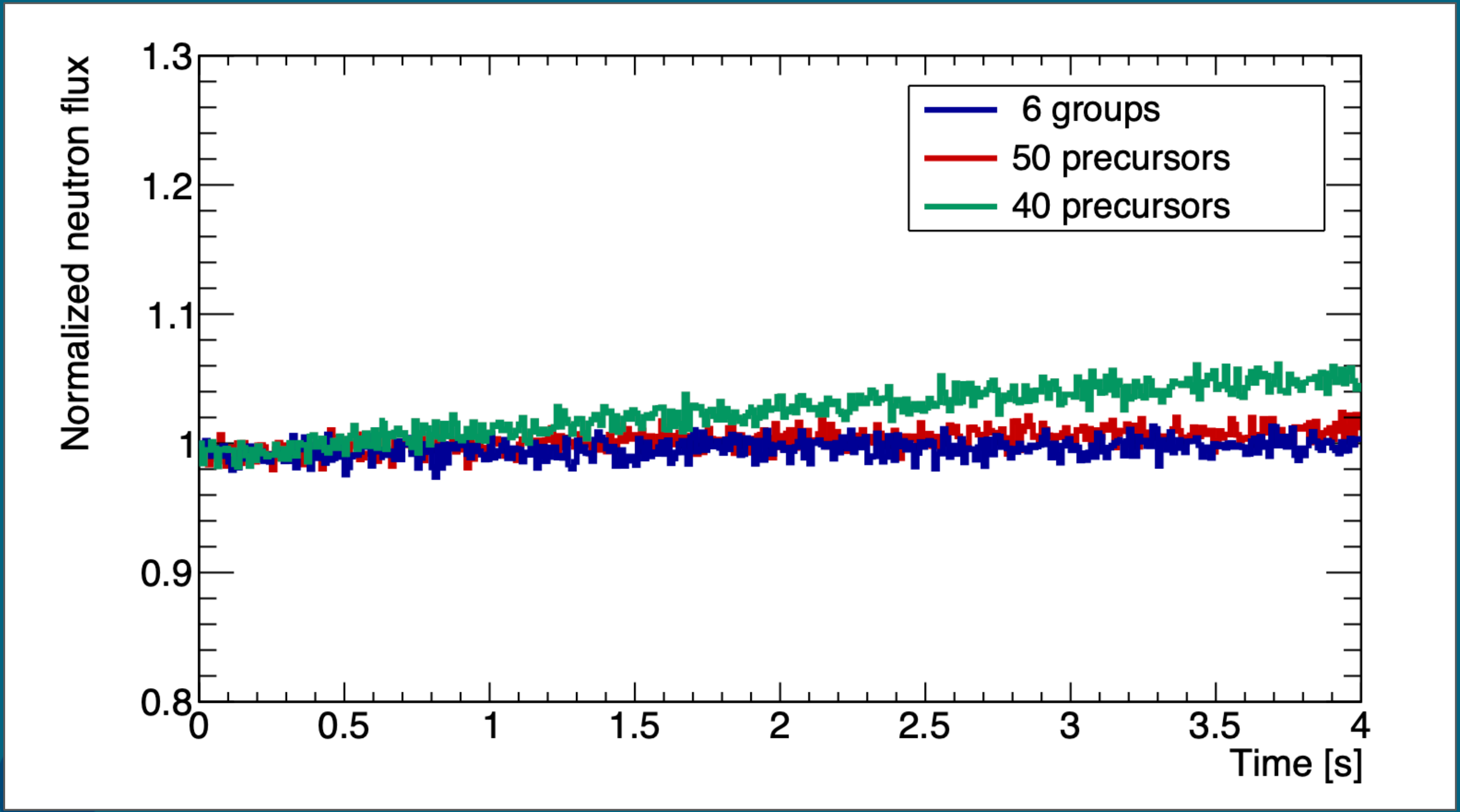
Back to slightly supercritical
[Σ_a = 0.5882 cm^{-1}]

Batches	25
Simulation time (s)	25
No. time intervals	50000
Time interval length (ms)	10

Romero-Barrientos et al., Nuclear Engineering and Technology , 55, 1593–1603 (2023).

OpenMC(TD) current status

Some results so far: Different number of precursors



- Energy-dependent fissile system
- Box surrounded by a 4.29 cm thickness light-water moderator.
- ^{235}U cross sections
- 50 individual precursors
- Slightly supercritical system k_{eff}=1.00025(3)
- Wall-clock time ~ 400 h

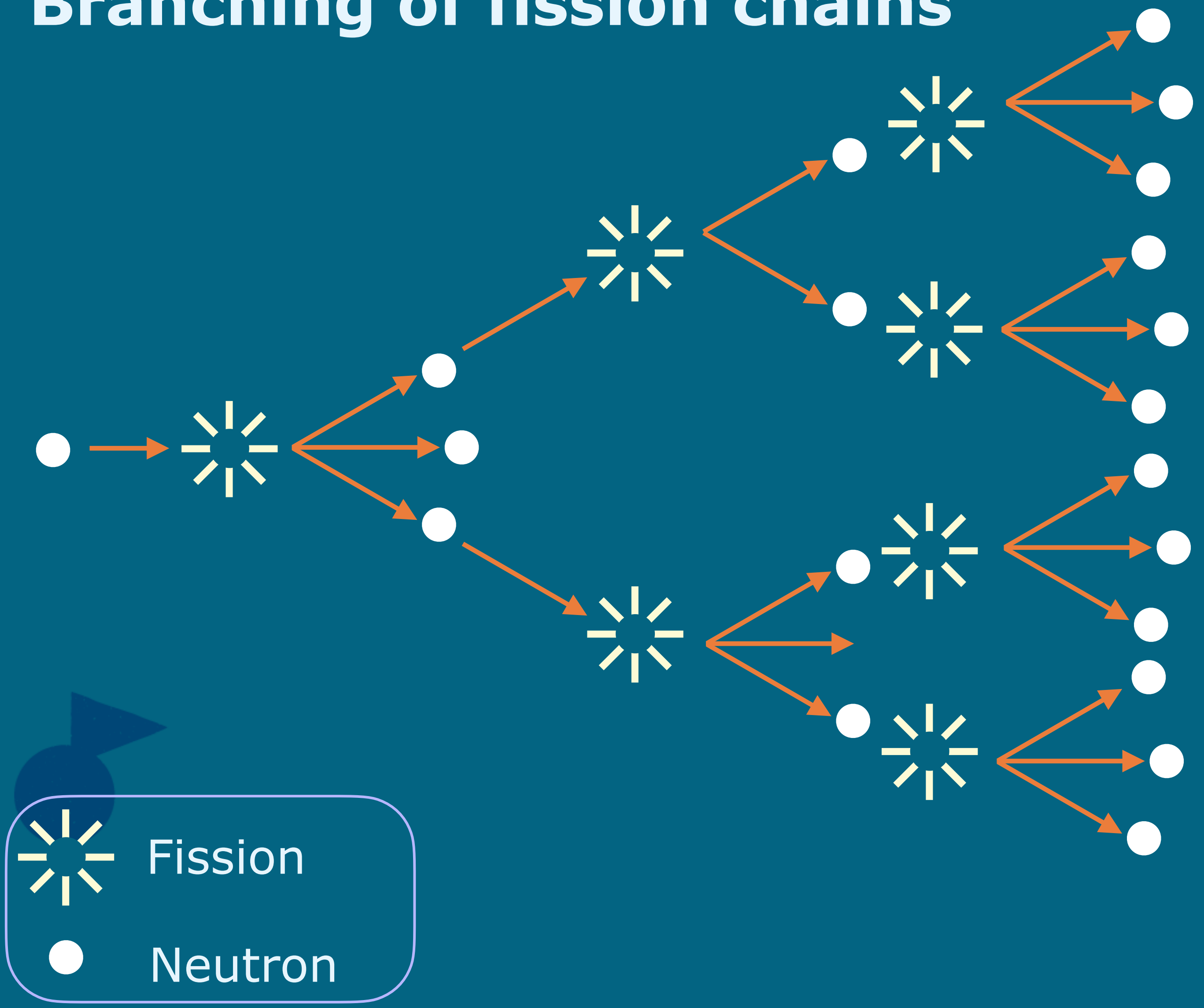
Simulation is stable and results are in agreement with the reduction in the number of precursors, but with high calculation times.

Romero-Barrientos et al., Nuclear Engineering and Technology , 55, 1593–1603 (2023).

3. Code development plans

OpenMC(TD) development plans

Branching of fission chains



Longer calculation times in critical and supercritical systems

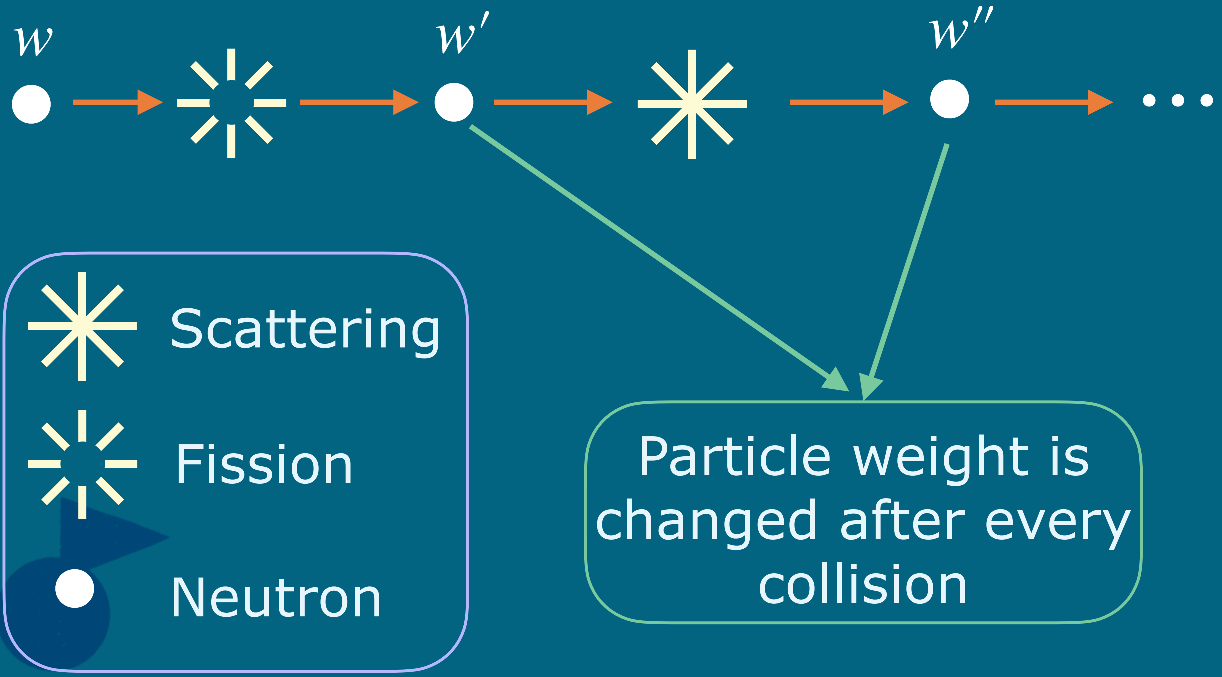
Solution: branchless collisions

Sjentizer et al., Annals of Nuclear Energy 38 (2011) 2195–2203

OpenMC(TD) development plans

Branchless collision method

To prevent branching, exactly one particle is emitted after a collision



Scattering event probability

$$P_s = \frac{\sigma_s(E)}{\nu_f(E)\sigma_f(E) + \sigma_s(E)}$$

Fission event probability

$$P_f = \frac{\nu_f(E)\sigma_f(E)}{\nu_f(E)\sigma_f(E) + \sigma_s(E)}$$

Statistical weight after collision

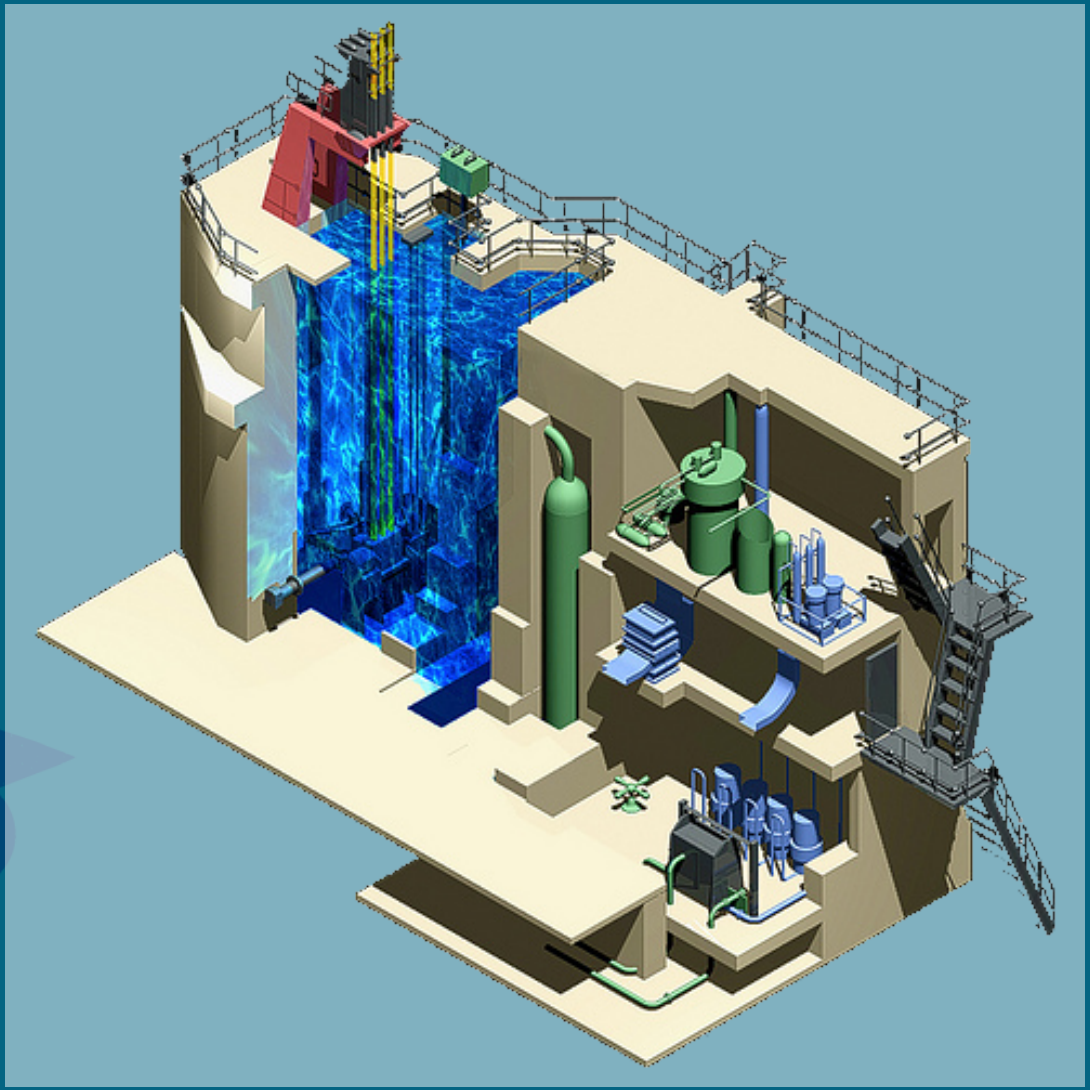
$$w' = w\frac{\nu_f(E)\sigma_f(E) + \sigma_s(E)}{\sigma_t(E)}$$

Simulations then will be performed using Guacolda-Leftraru supercomputer @ National Laboratory for High Performance Computing Chile

Belanger et al., “The Effect of Branchless Collisions on Neutron Clustering”, M&C 2023, (2023).

Nuclear reactor simulation

RECH-1 research reactor overview



Type	Pool type reactor
Power	5 MW thermal
Moderation and cooling	Light-water cooled and moderated
Control	6 Cd control rods
Irradiation sites	6 in-core irradiation sites
Experimental beams	5 beam tubes

Molina et al., Applied Radiation and Isotopes 129 (2017) 28–34

4. Benchmark experiments

Reactor benchmark experiments

Transient experiments

To compare transient simulation results with experimental results

→ Transient experimental experiments

- Insertion and withdrawal of control plates
- Insertion and withdrawal of a small absorber

Estimated prompt generation time of research nuclear reactor is ~60 μs → Temporal resolution needed is ~ 1 μs

Two detection systems proposed: in-core SPND and ex-core ^{3}He neutron detector

Burn-up state of the core will be considered if needed (fresh fuel)

5. Conclusions

Conclusions and outlook

LASNPA XIV/2024

- Time dependence related to the β-delayed neutron emission from individual precursors was included in a Monte Carlo code.
- This code was named OpenMC(TD) has shown promising results in transient Monte Carlo simulations of fissile systems, using individual precursors instead of the traditional 6-groups or families.
- OpenMC(TD) development plan includes the implementation of the branchless collision technique to reduce calculation times.
- Associated experimental measurements are planned to validate simulation results.
- It is expected to propose transient benchmark experiments to evaluate existing and future transient Monte Carlo codes.
- OpenMC(TD) could be a valuable tool to explore the impact of precursor individual data on results obtained for complex fissile systems, like a nuclear reactor.

Acknowledgments

- Jaime Romero-Barrientos acknowledges support from ANID Fondecyt Iniciación Project 11240321 and from ANID - Millennium Science Initiative Program - ICN2019_044.

- Francisco Molina acknowledges support from ANID Fondecyt Regular Project 1221364 and from ANID - Millennium Science Initiative Program - ICN2019_044.

Thank you for your attention

BACKUP SLIDES

Transient Monte Carlo simulations

β-delayed emission from individual precursors

Group structure (current codes)

Delayed fission takes place

↓

Delayed neutron sampled

↓

j-th precursor **group** is chosen from the group relative abundances a_j

↓

Associated delayed time sampled from group decay probability $p_j(t)$ and λ_j

↓

Delayed neutron energy is chosen from the j-th delayed neutron energy group spectra

Individual precursors (this work)

Delayed fission takes place

↓

Precursor is created[†]

↓

i-th **individual** precursor is chosen to decay from *relative importance* I_i

↓

Associated delayed time is sampled from $p_i(t)$ and λ_i

↓

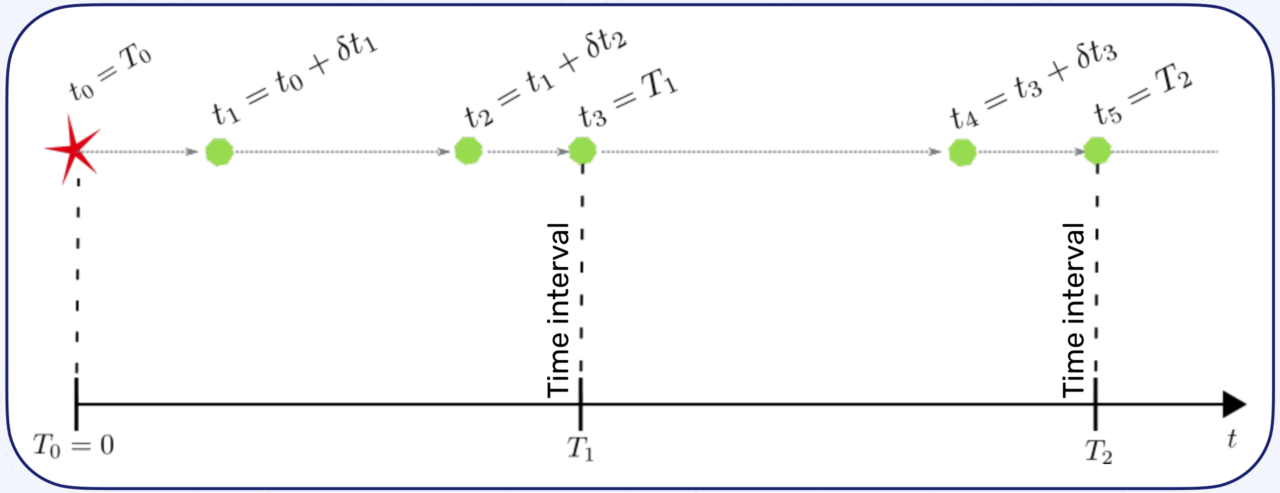
Delayed neutron energy is chosen as the mean energy from i-th precursor delayed neutron energy spectrum

[†] Sjenitzer et al., "Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations", Nucl Sci Eng, 175:1, 94–107 (2012).

Simulaciones Monte Carlo transientes

Inclusion of time-dependence in a MC simulation

1. Time evolution of neutrons†
2. Time filter†
3. Simulation time divided in time intervals

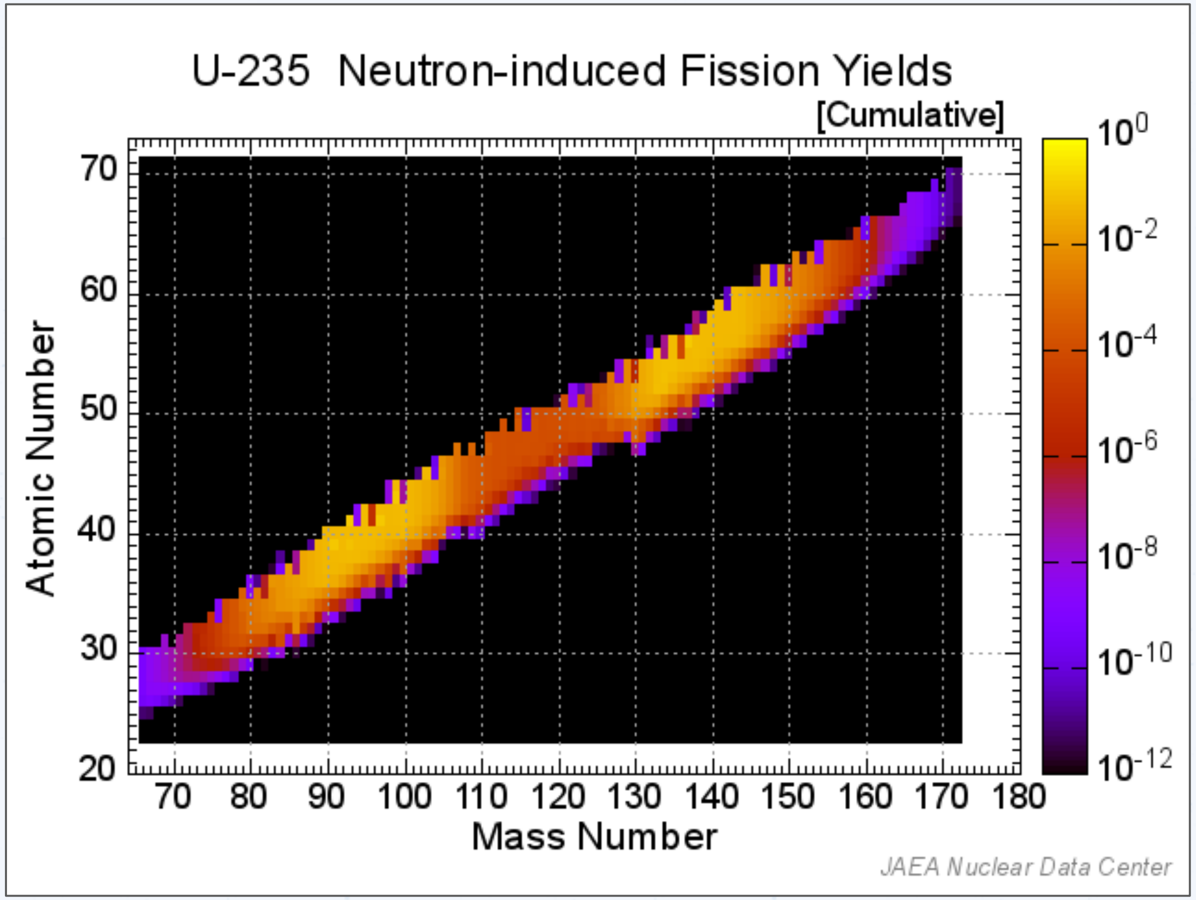


Sjenitzer et al., Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations, Nucl. Sci. Eng.,175:1, 94-107, (2013)

Transient Monte Carlo simulations

Producción (*yield*) cumulativo

$$I_i \equiv \frac{CY_i \, P_{n,i}}{\nu_d}$$



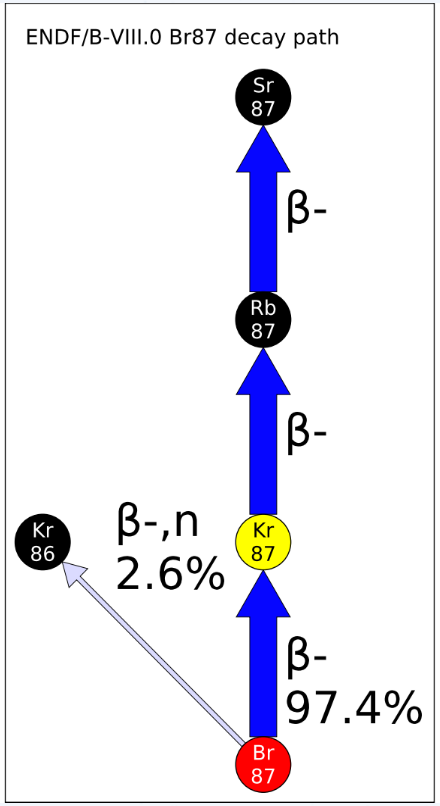
Cumulative fission yield (CY): number of atoms of a specific nuclei produced directly from fission and via decay of precursors.

CY for ^{87}Br is 2.03% which means that 203 atoms of ^{87}Br are created per 10,000 fissions.

Transient Monte Carlo simulations

Probabilidad de emisión de precursor de neutrones retardados

$$I_i \equiv \frac{CY_i \, P_{n,i}}{\nu_d}$$



Precursor delayed neutron emission probability ($P_{n,i}$): represents the probability of a neutron emission.

^{87}Br has a 2.6% probability of decaying to ^{86}Kr, emitting a delayed neutron in the process.

So, if 203 atoms of ^{87}Br are created per 10,000 fissions, and they have a 2.6% probability of decaying to ^{86}Kr, then they will emit 5.3 delayed neutrons per 10,000 fissions.

Transient Monte Carlo simulations

Recapitulación de la inclusión de precursores individuales

Quantity	6- or 8-group structure	This work (50 individual)
Relative abundance	a_j with 1 < j < 6 (or 8) Groups	$(CY_i P_{n,i})/\nu_d$ with 1 < i < 50 Individual
Decay constants	λ_j with 1 < j <6 (or 8) Groups	λ_i with 1 < i < 50 Individual
Delayed neutron energy	$\chi_j(E)$ with 1 < j <6 (or 8) Groups	$\bar{\chi}_i(E)$ with 1 < i < 50 Individual

Although in this work 50 individual precursors were used to perform the simulations, all 269 individual precursors could be used should need arise.

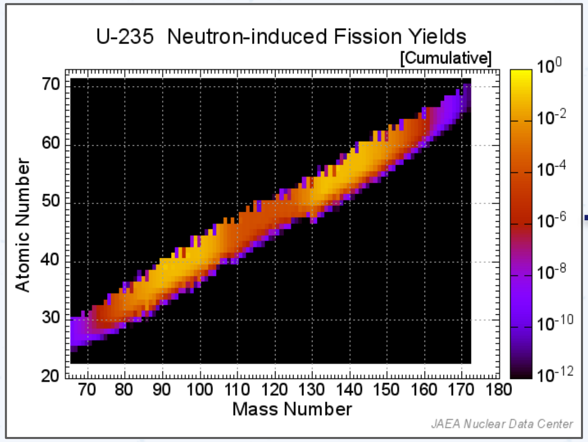
Mean energies were used because only 34 precursors have measured energy spectra*.

*Brady, M.C. "Evaluation and application of delayed neutron precursor data". PhD thesis, Los Alamos National Laboratory, USA (1989).

Transient Monte Carlo simulations

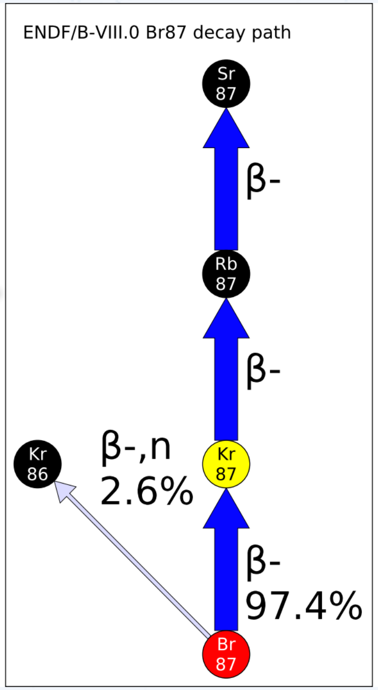
Recapitulación de la inclusión de precursores individuales

Included , in a MC simulation, β-delayed neutron emission from individual precursors, instead of using the precursor group structure.



$$I_i \equiv \frac{CY_i \, P_{n,i}}{\nu_d}$$

$$\nu_d = \sum_i^N CY_i \, P_{n,i}$$



Transient Monte Carlo simulations

Pruebas de OpenMC(TD) en sistema simple

Purpose: test OpenMC(TD) capabilities in a simple system.

- Monoenergetic fissile system
- Rectangular box of (10x12x20) cm^3
- Constant cross-sections
- 1-group precursor structure.

Configurations:
1.- Subcritical
2.- Slightly supercritical
3.- Reactivity insertion

Input: Σ_a
Observables: k_{eff} and $n(t)$

Calculated reactivity is obtained from: $\rho = \frac{\Delta k}{k}$

Compared with fitted reactivity from:

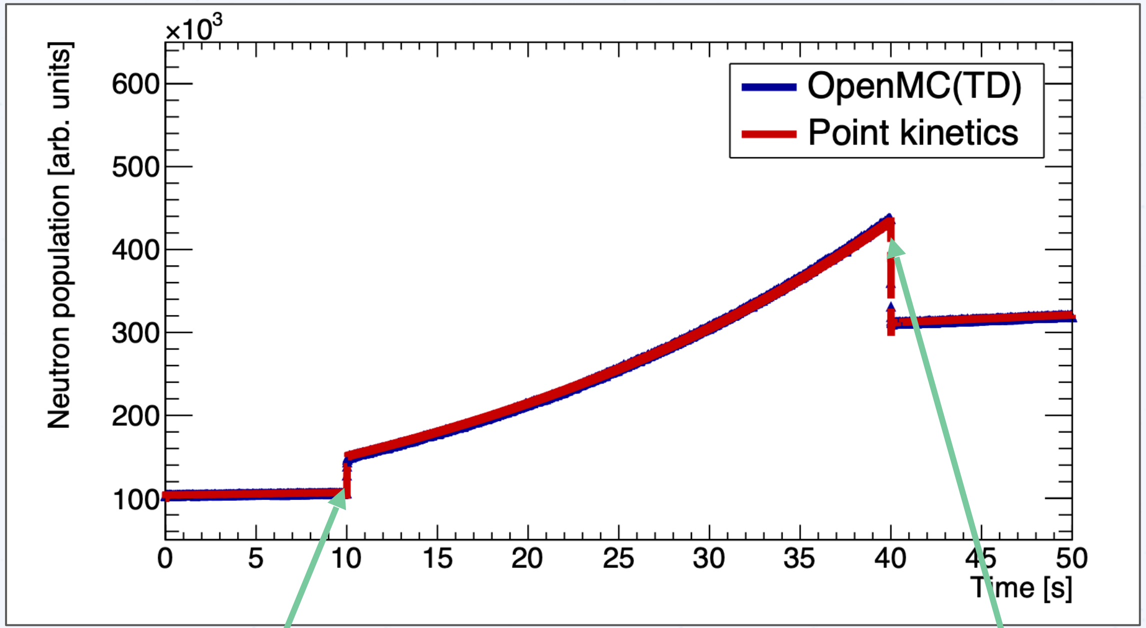
$$n(t) = n_0 \left[\frac{\rho}{\rho - \beta} \exp\left(\frac{\rho - \beta}{\bar{\Lambda}}\right) - \frac{\beta}{\rho - \beta} \exp\left(\frac{\lambda \rho}{\rho - \beta}\right) \right]$$

Parameter	Value
β	0.00685
λ (s^{-1})	0.0784
ν	2.5
Σ_t (cm^{-1})	1.0
Σ_f (cm^{-1})	0.25
Σ_a (cm^{-1})	0.5882
Σ_s (cm^{-1})	0.4118
v (cm/s)	2.2×10^4

Transient Monte Carlo simulations

Resultados de pruebas de OpenMC(TD) en sistema simple

Simulation results were compared to 1-group point kinetics equation



+211 pcm
[Σ_a = 0.5870 cm^{-1}]

Back to slightly-supercritical
[Σ_a = 0.5882 cm^{-1}]

Batches	25
Simulation time (s)	50
No. time intervals	5000
Time interval length (ms)	10

Simulation parameters

Transient Monte Carlo simulations

Pruebas de OpenMC(TD) en sistema más realista

Purposes: Test OpenMC(TD) capabilities in a more realistic system, and whether it can solve fast changes in the neutron flux.

- Energy dependent fissile system
- rectangular box of (10x12x20) cm^3
- ^{235}U cross sections
- Different group structures

β_{eff} and Λ obtained from adjoint flux calculation using MCNP

Configurations:

1.- Subcritical, n_{U235}=4.4362x10^{-2} (atoms/b cm) → k_{eff}=0.98956(3)

2.- Supercritical, n_{U235}=4.511x10^{-2} (atoms/b cm) → k_{eff}=1.00271(3)

Input: n_{U235}, delayed neutron energy and precursor structure.

Observables: k_{eff} and $\phi(t)$

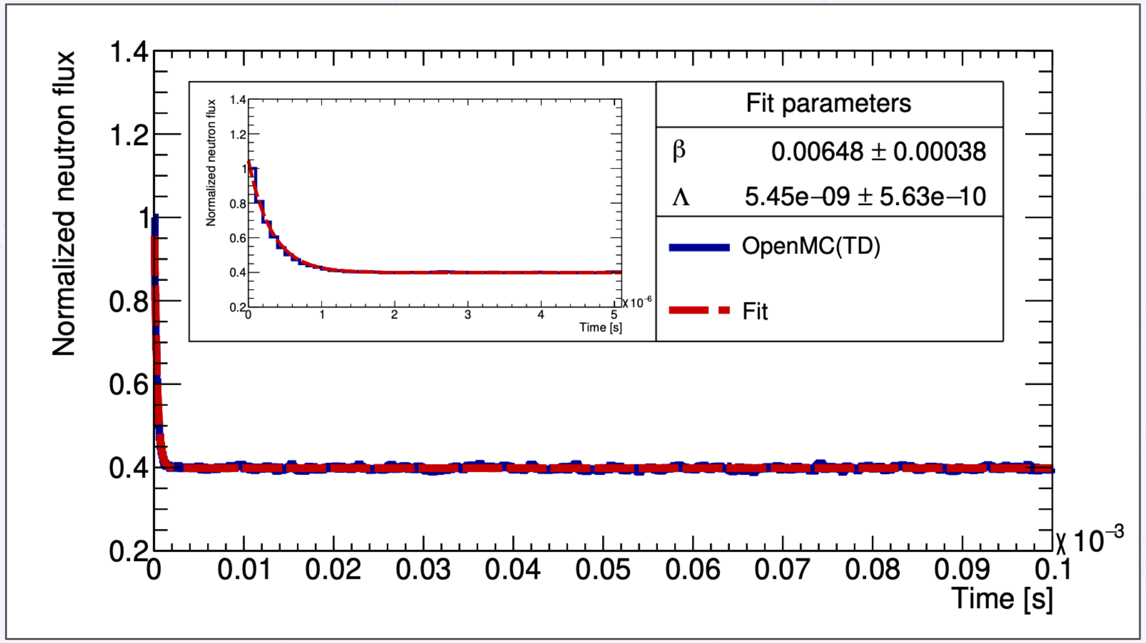
Precursor structure	Delayed neutron energy	Library
1-group	$\chi_1(E)$	JEFF 3.1.1
1-group	E_{1g}	JEFF 3.1.1
1-group	E_{6g}	ENDF-B/VIII.0
8-group	$\chi(E)$	JEFF 3.1.1
6-group	E_i	ENDF-B/VIII.0
50 individual	E_i	ENDF-B/VIII.0

Compared with fitted parameters from:

$$\phi(t) = \phi_0 \left[\frac{\rho}{\rho-\beta} \exp\left(\frac{\rho-\beta}{\bar{\Lambda}}\right) - \frac{\beta}{\rho-\beta} \exp\left(\frac{\lambda\rho}{\rho-\beta}\right) \right]$$

Transient Monte Carlo simulations

Resultados de pruebas de OpenMC(TD) en sistema más realista

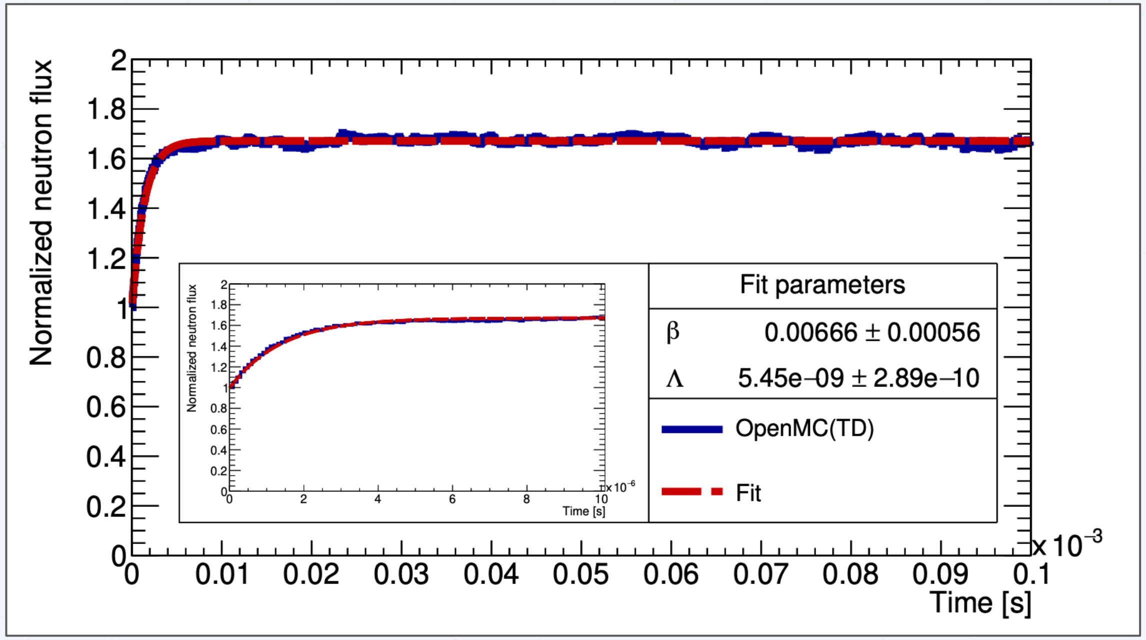


Case	1st precursor group from JEFF-3.1.1
Batches	22
No. time intervals	1000
Time interval length (ns)	100
Simulation time (ms)	0.1
Wall-clock time (h)	44.32

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	5.74(1)	5.45(56)	5.1%
β_{eff} [pcm]	644(6)	648(38)	1%

Transient Monte Carlo simulations

Resultados de pruebas de OpenMC(TD) en sistema más realista



Case	1st precursor group from JEFF-3.1.1
Batches	10
No. time intervals	1000
Time interval length (ns)	100
Simulation time (ms)	0.1
Wall-clock time (h)	52.45

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	6.00(1)	5.45(57)	9.2%
β_{eff} [pcm]	651(6)	666(56)	<1%

Transient Monte Carlo simulations

Pruebas de OpenMC(TD) en sistema termalizado

Purposes: Test OpenMC(TD) capabilities in a moderated system and explore the effect of reducing the number of precursors.

- Energy-dependent fissile system
- Box surrounded by a 4.29 cm thickness light-water moderator.
- ^{235}U cross sections
- 50 individual precursors

Configuration:
1.- Slightly supercritical, n_{U235}=3.2671x10^{-2} (atoms/b cm)

Input: n_{U235}, delayed neutron energy and precursor structure.
Observables: k_{eff} and $\phi(t)$

Criticality calculation to assess the system reactivity

	6-groups	50 precursors	Difference
k_{eff}	1.00025(3)	1.00032(3)	7(4)

Effective multiplication factors obtained for the light-water moderated system

Then, transient calculations were performed with different precursor structures.

Transient Monte Carlo simulations

Pruebas de OpenMC(TD) en sistema termalizado

$\phi(t)$ tallied during 4 seconds and 3 configurations were studied:

1. 50 precursors
2. 6-group structure
3. 10 precursors with the largest *relative importances* I_i removed

Precursor	Importance
^{137}I	0.1617
^{89}Br	0.1125
^{94}Rb	0.0915
^{88}Br	0.0740
^{90}Br	0.0733
^{85}As	0.0478
^{138}I	0.0471
^{98m}Y	0.0417
^{139}I	0.0401
^{95}Rb	0.0357

10 most *important* precursors **removed** from the list of 50 precursors

A good approximation of the decrease of the neutron flux is given by

$$\phi(t) \sim e^{\alpha_D t}$$

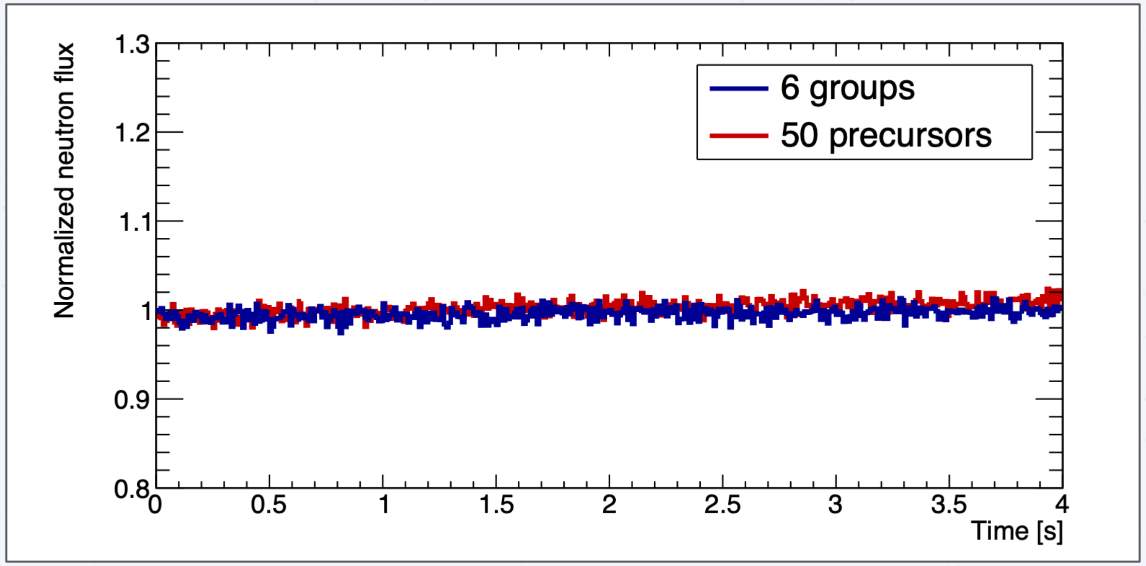
$$\alpha_D = \frac{\bar{\lambda}\rho}{\beta_{eff} - \rho}$$

Calculated reactivity from criticality calculation was compared to fitted reactivity obtained as a fitted parameter from the tallied neutron flux $\phi(t)$.

Keepin et al.. Delayed neutrons from fissionable isotopes of uranium, plutonium and thorium. Journal of Nuclear Energy (1954), 6(1):2 – 21, 1957.

Transient Monte Carlo simulations

Resultados pruebas de OpenMC(TD) en sistema termalizado

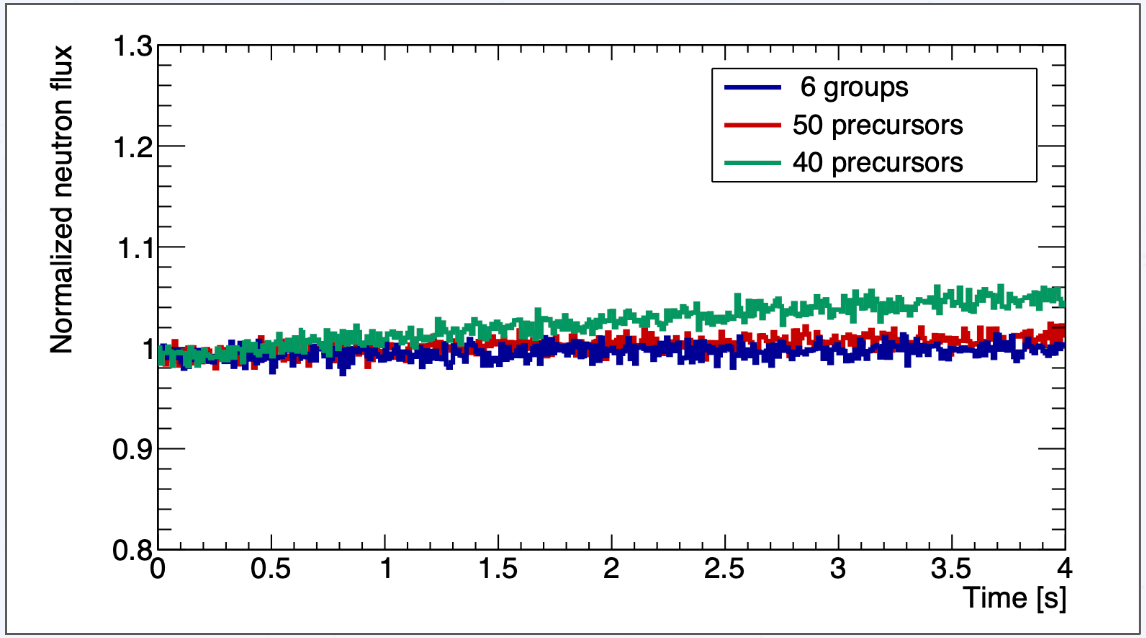


Parameter	6-group structure	50 individual precursors
ρ [pcm]	25(3)	32(3)
ρ_{fit} [pcm]	17(368)	35(347)

Batches	2
Simulation time (s)	4
No. time intervals	400
Time interval length (ms)	10
Wall-clock time 6-group precursors (h)	260.05
Wall-clock time 50 individual precursors (h)	410.76

Transient Monte Carlo simulations

Resultados pruebas de OpenMC(TD) en sistema termalizado



Batches	2
Simulation time (s)	4
No. time intervals	400
Time interval length (ms)	10
Wall-clock time 40 individual precursors (h)	319.65

Parameter	6-group structure	50 individual precursors	40 individual precursors
ρ_{fit} [pcm]	17(368)	35(347)	111(270)

Combined precursor decay probability

$$p_{combined}(t) = \sum_i \Gamma_i \, \lambda_i \, e^{-\lambda_i (t - t_0)} \, \theta(t - t_0)$$

$$\Gamma_i = \begin{cases} \frac{\beta_i}{\beta}, & \text{for precursor group} \\ I_i, & \text{for individual precursor.} \end{cases}$$

β-delayed neutron emission

$$w_d(t) = w_c \sum_i \Gamma_i \, \lambda_i \, e^{-\lambda_i (t - t_0)} \, \theta(t - t_0)$$

“Physical” statistical weight of delayed neutrons

$$P_i(t) = \frac{\Gamma_i \, \lambda_i \, e^{-\lambda_i (t - t_0)}}{\sum_i \Gamma_i \, \lambda_i \, e^{-\lambda_i (t - t_0)}}$$

β-delayed neutron emission

Precursor weight at a given time t

$$w_p(t) = w_c \sum_i \Gamma_i e^{-\lambda_i (t - t_0)}$$

$$w_{d,av} = w_c \sum_i \Gamma_i \left(e^{-\lambda_i (t - t_0)} - e^{-\lambda_i (t_1 + \Delta t - t_0)}\right)$$

Precursor forced decay

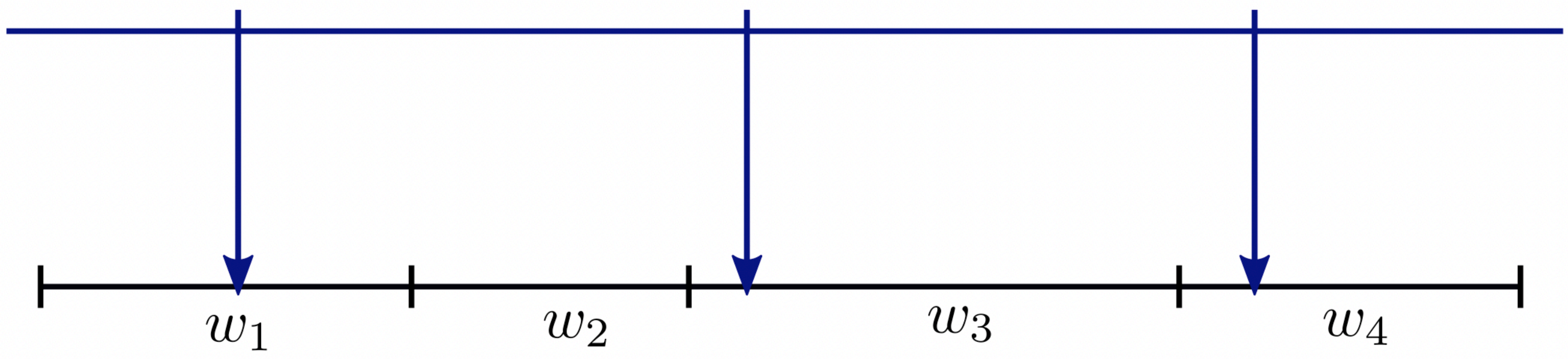
Biased decay probability

$$\bar{p}(t) = \frac{1}{t_{j+1} - t_j} = \frac{1}{\Delta t}$$

$$w_d(t) = \frac{p(t)}{\bar{p}(t)} = w_c\, \Delta t \sum_i \Gamma_i \lambda_i e^{-\lambda_i (t - t_0)} \quad \text{with} \quad t_j < t < t_{j+1}$$

$$w_p(t_{j+1}) = w_c \sum_i \Gamma_i e^{-\lambda_i (t_{j+1} - t_0)}$$

Population control



If there are K particles at the end of a time interval and the objective is to comb them to M, these K particles will be combed into M using a comb with M teeth.

After combing each particle has weight $w_i' = W/M$ and since there are M particles, total weight is preserved.

In this work, the neutrons and precursors were combed separately.

Branchless collisions

$$P_c = \frac{\nu_p \Sigma_f}{\nu_p \Sigma_f + \Sigma_s}$$

Fission probability

$$P_s = \frac{\Sigma_s}{\nu_p \Sigma_f + \Sigma_s}$$

Scattering probability

$$P_p = w_n \frac{\nu_d \Sigma_f}{\Sigma_t}$$

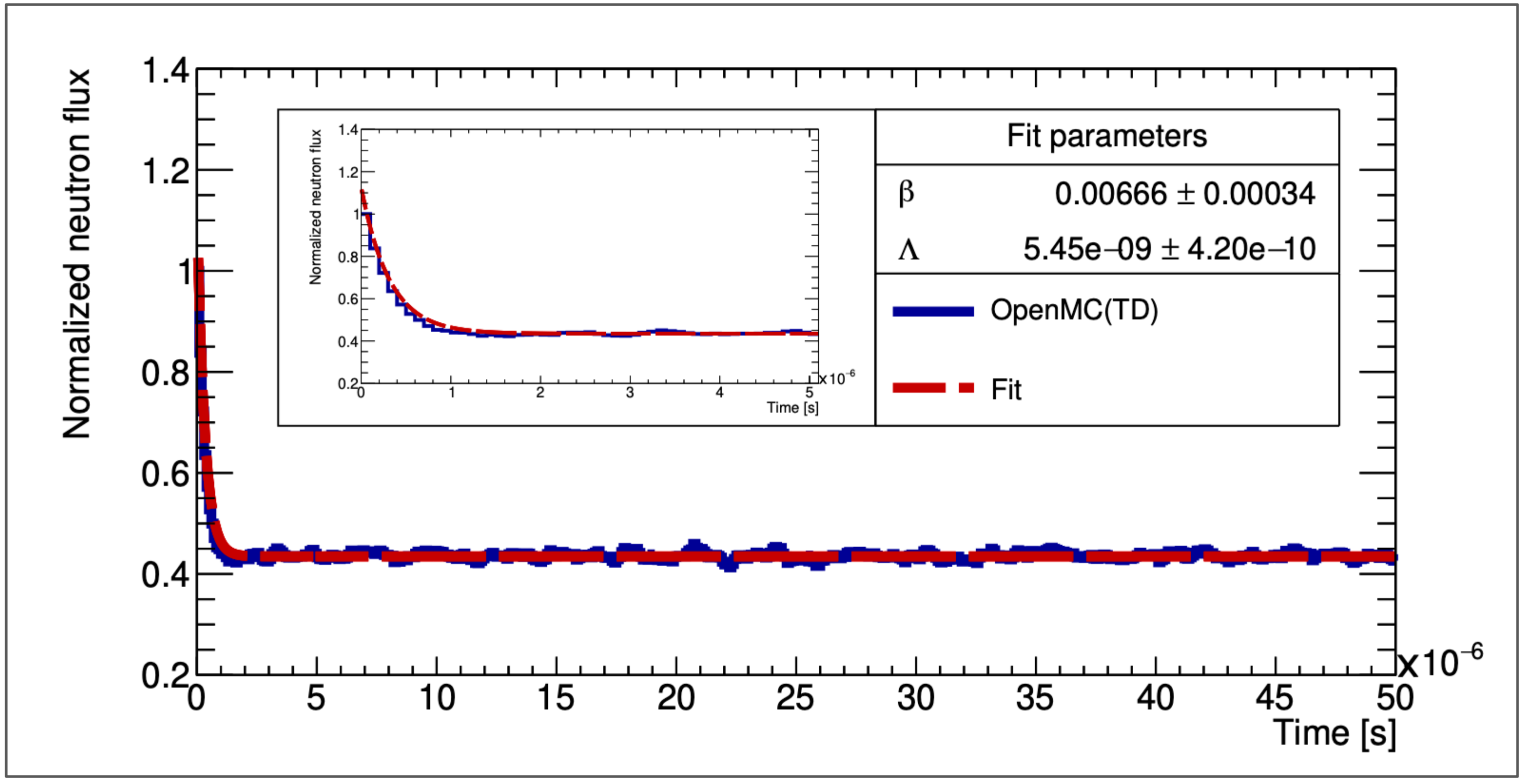
Probability generating a precursor

$$w_n' = w_n \frac{\nu_p \Sigma_f + \Sigma_s}{\Sigma_t}$$

Statistical weight of neutron

B. Sjenitzer and E. Hoogenboom, "Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations," Nuclear Science and Engineering, vol. 175, no. 1, pp. 94–107, 2013.

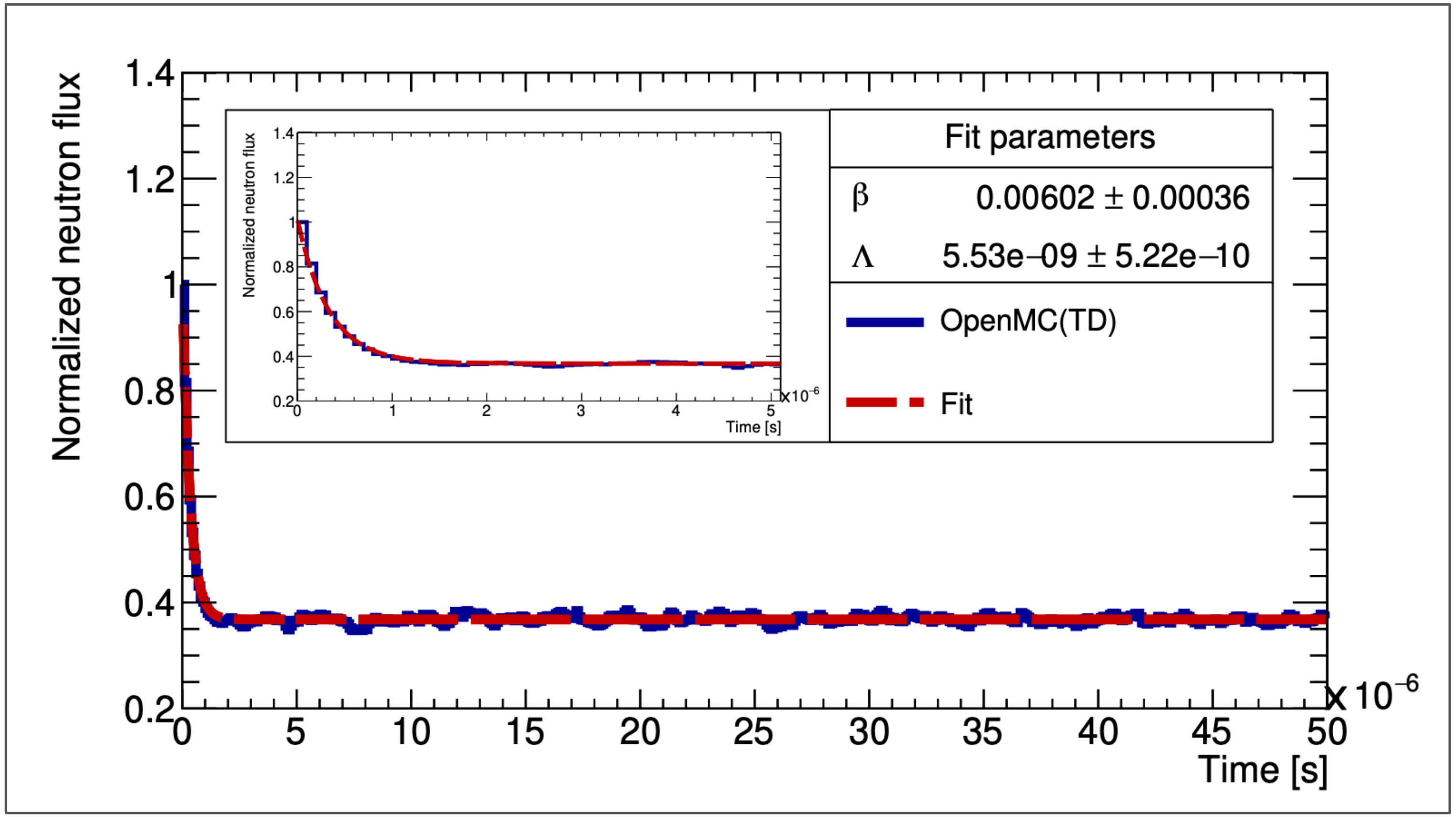
Energy-dependent ^{235}U system: Subcritical configuration case ii



Case	First group with average energy from JEFF-3.1.1
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	3.51

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	5.74(1)	5.45(42)	5.1%
β_{eff} [pcm]	644(6)	666(34)	3.4%

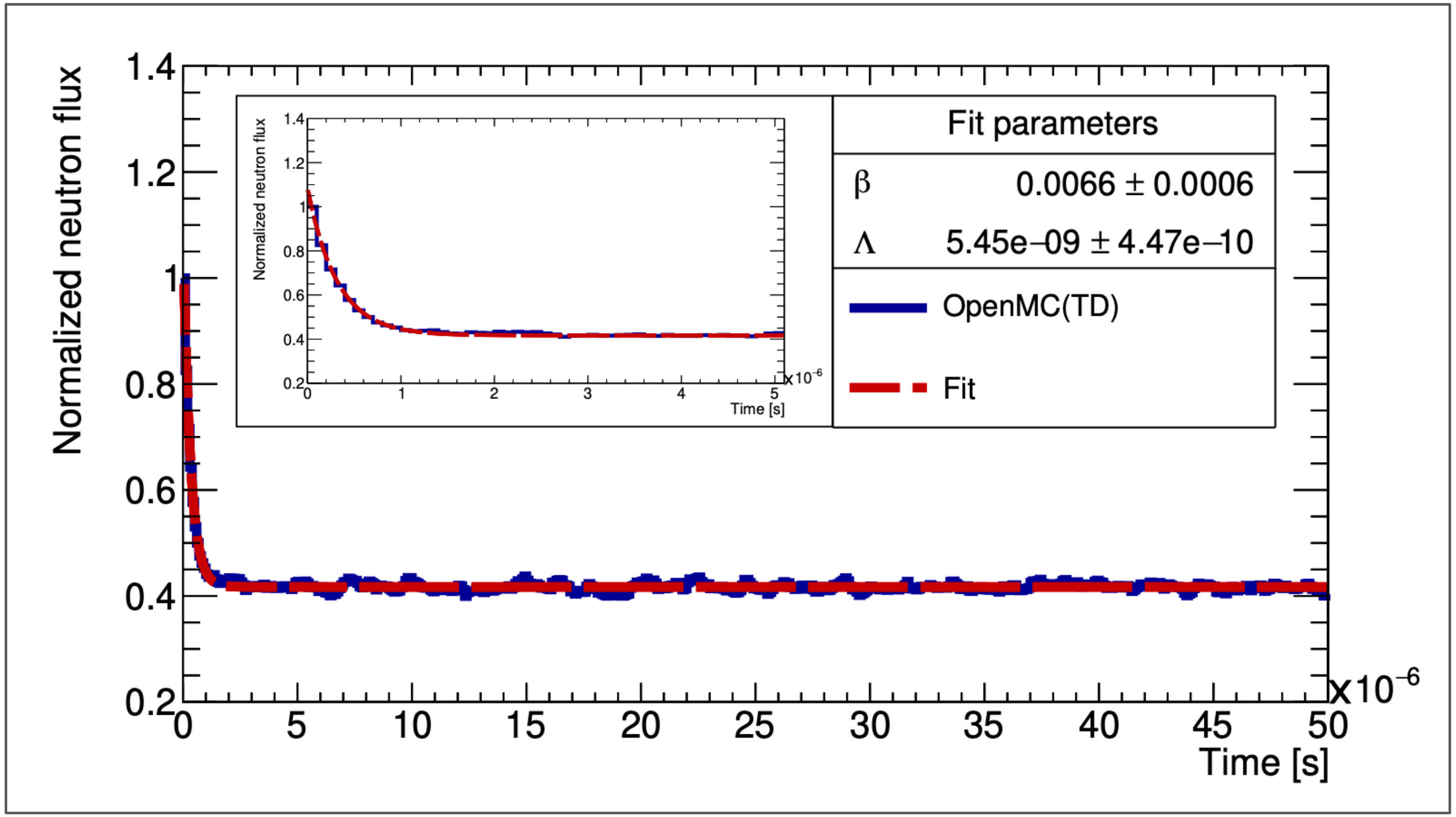
Energy-dependent ^{235}U system: Subcritical configuration case iii



Case	1 group with average energy from ENDF-B/VIII.0
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	3.49

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	5.74(1)	5.53(52)	3.7%
β_{eff} [pcm]	644(6)	602(36)	6.5%

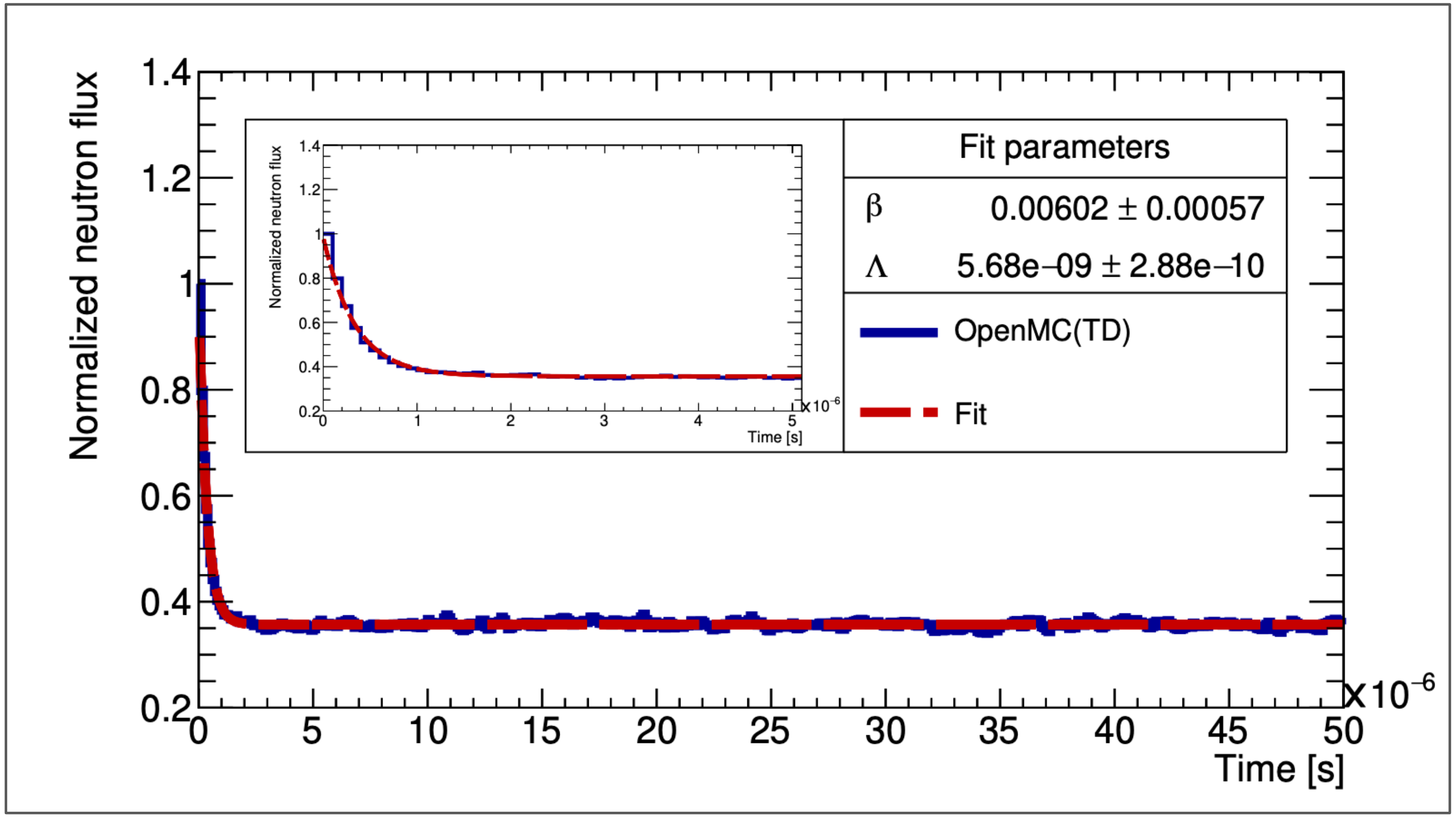
Energy-dependent ^{235}U system: Subcritical configuration case iv



Case	8-group with energy distribution from JEFF-3.1.1.
Batches	22
No. time intervals	1000
Time interval length (ns)	100
Simulation time (ms)	0.1
Wall-clock time (h)	4.32

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	5.74(1)	5.45(45)	5.1%
β_{eff} [pcm]	644(6)	660(38)	2.5%

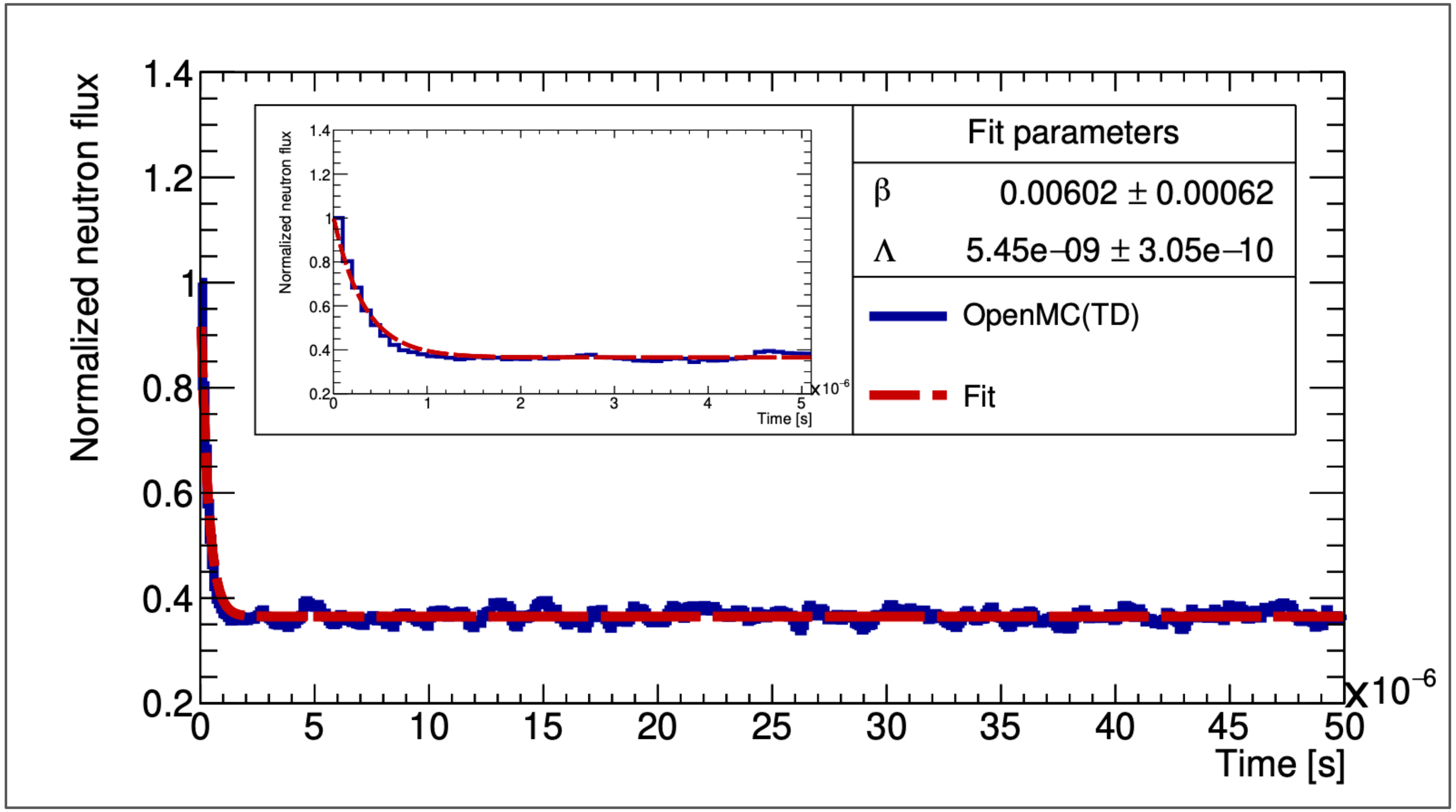
Energy-dependent ^{235}U system: Subcritical configuration case v



Case	6-group with average energy from ENDF-B/VIII.0
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	4.27

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	5.74(1)	5.68(29)	1%
β_{eff} [pcm]	644(6)	602(57)	6.5%

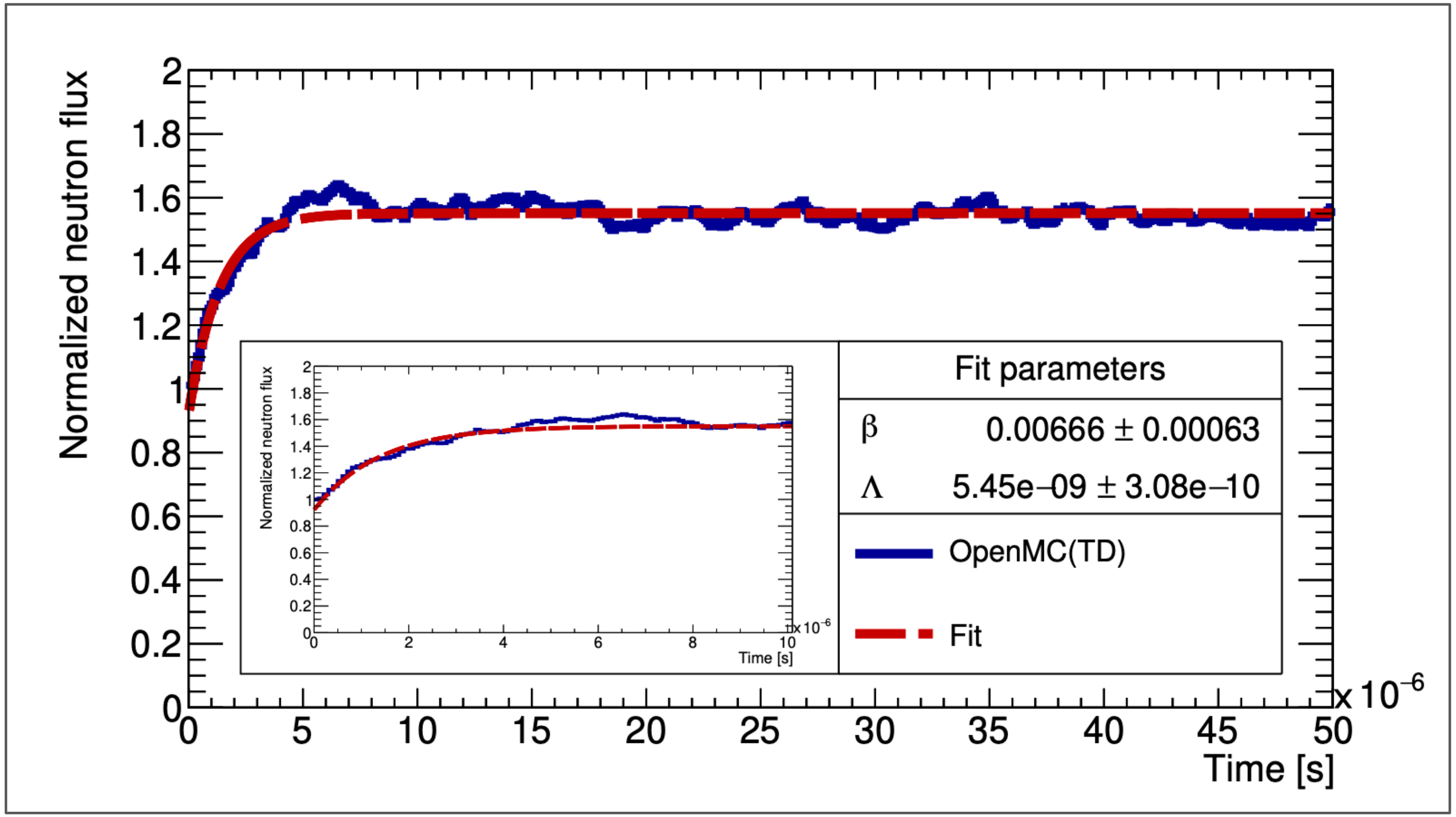
Energy-dependent ^{235}U system: Subcritical configuration case vi



Case	50 individual precursors with average energies from ENDF-B/VIII.0
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	6.43

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	5.74(1)	5.45(31)	5.3%
β_{eff} [pcm]	644(6)	602(57)	6.5%

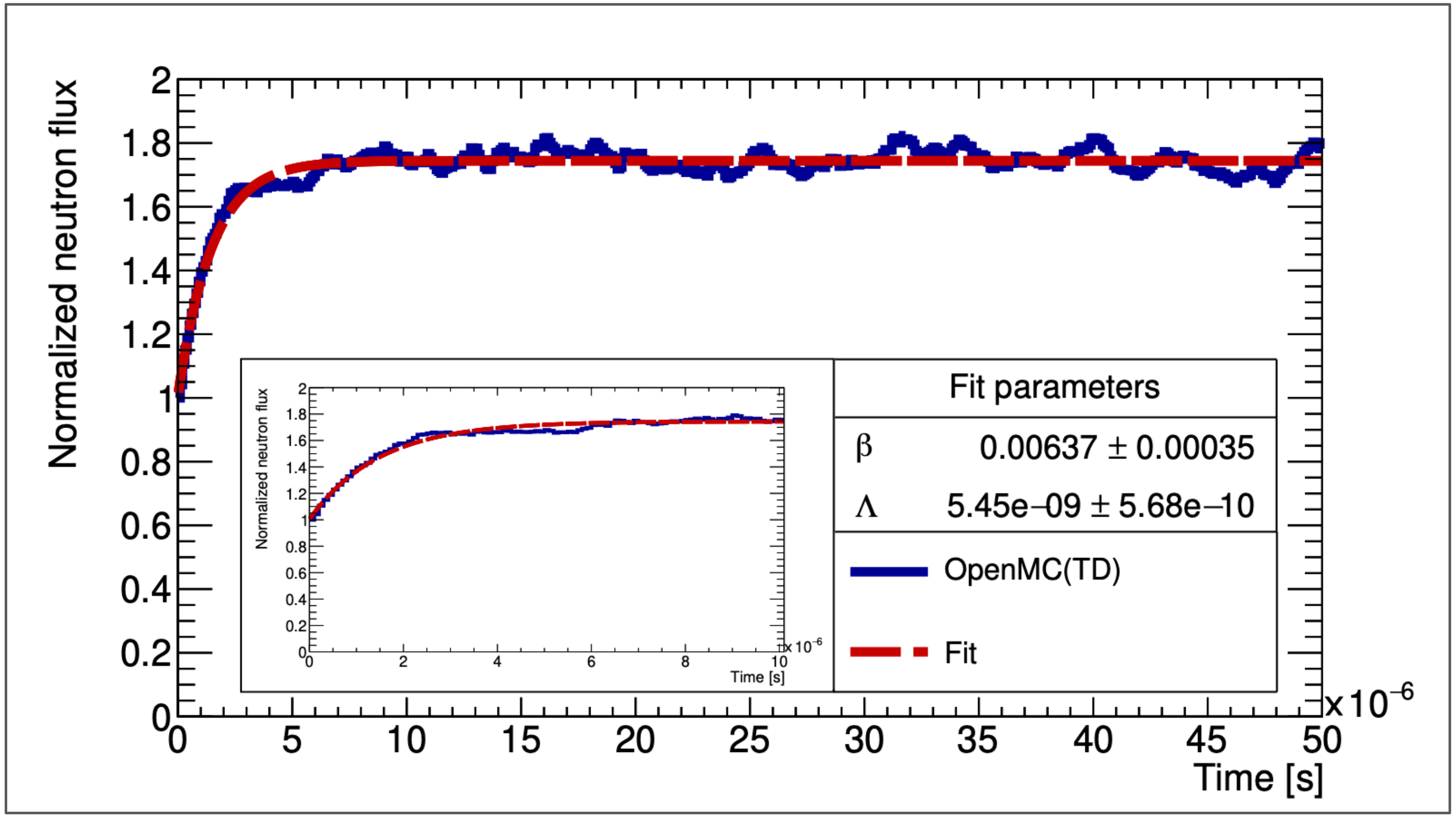
Energy-dependent ^{235}U system: Supercritical configuration case ii



Case	First group with average energy from JEFF-3.1.1
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	7.84

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	6.00(1)	5.45(31)	9.2%
β_{eff} [pcm]	651(6)	666(63)	2.3%

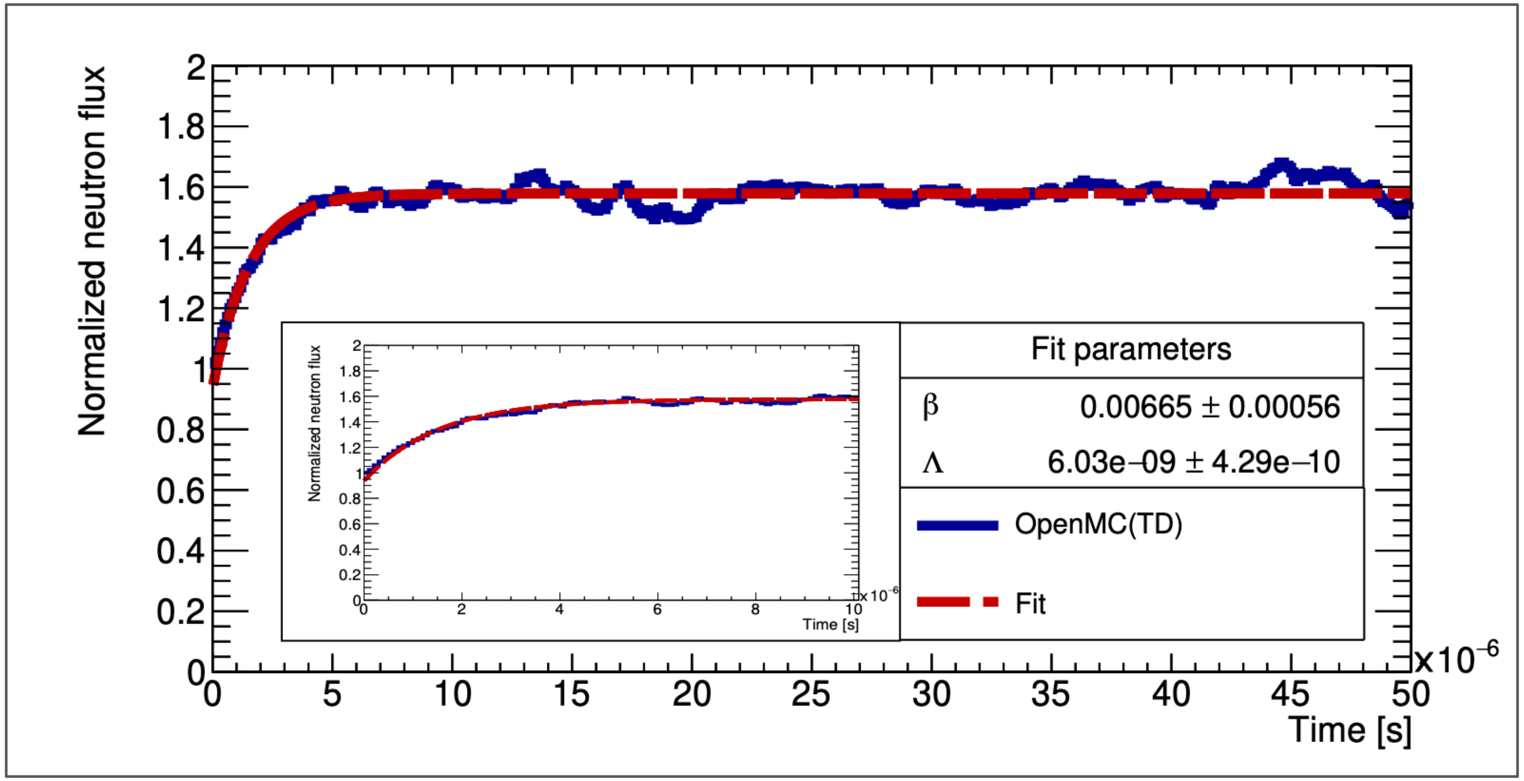
Energy-dependent ^{235}U system: Supercritical configuration case iii



Case	1-group with average energy from ENDF-B/VIII.0
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	7.81

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	6.00(1)	5.45(57)	9.2%
β_{eff} [pcm]	651(6)	637(35)	2.2%

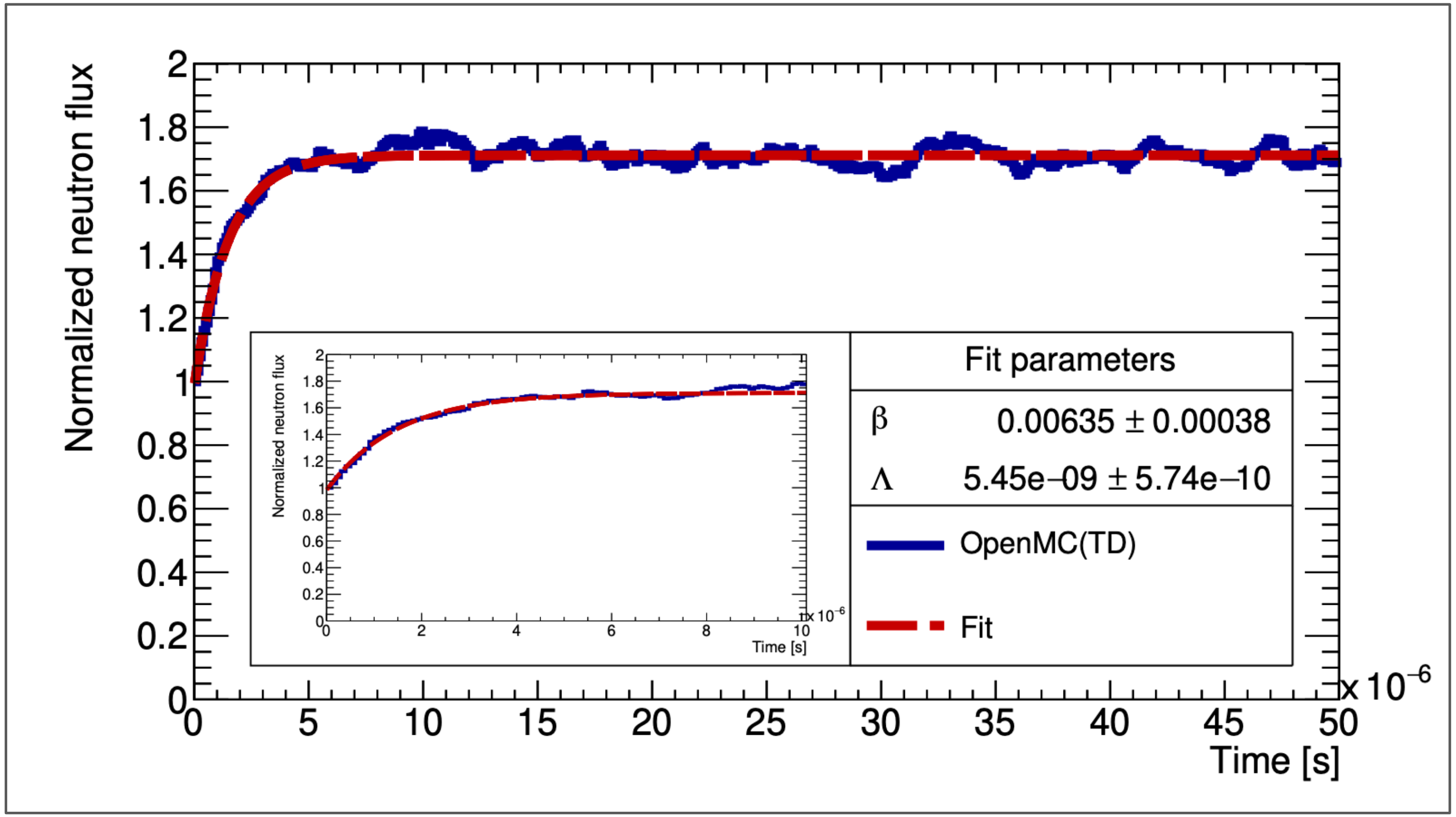
Energy-dependent ^{235}U system: Supercritical configuration case iv



Case	8-group with energy distribution from JEFF-3.1.1
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	11.19

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	6.00(1)	6.00(43)	< 1%
β_{eff} [pcm]	651(6)	665(35)	2.2%

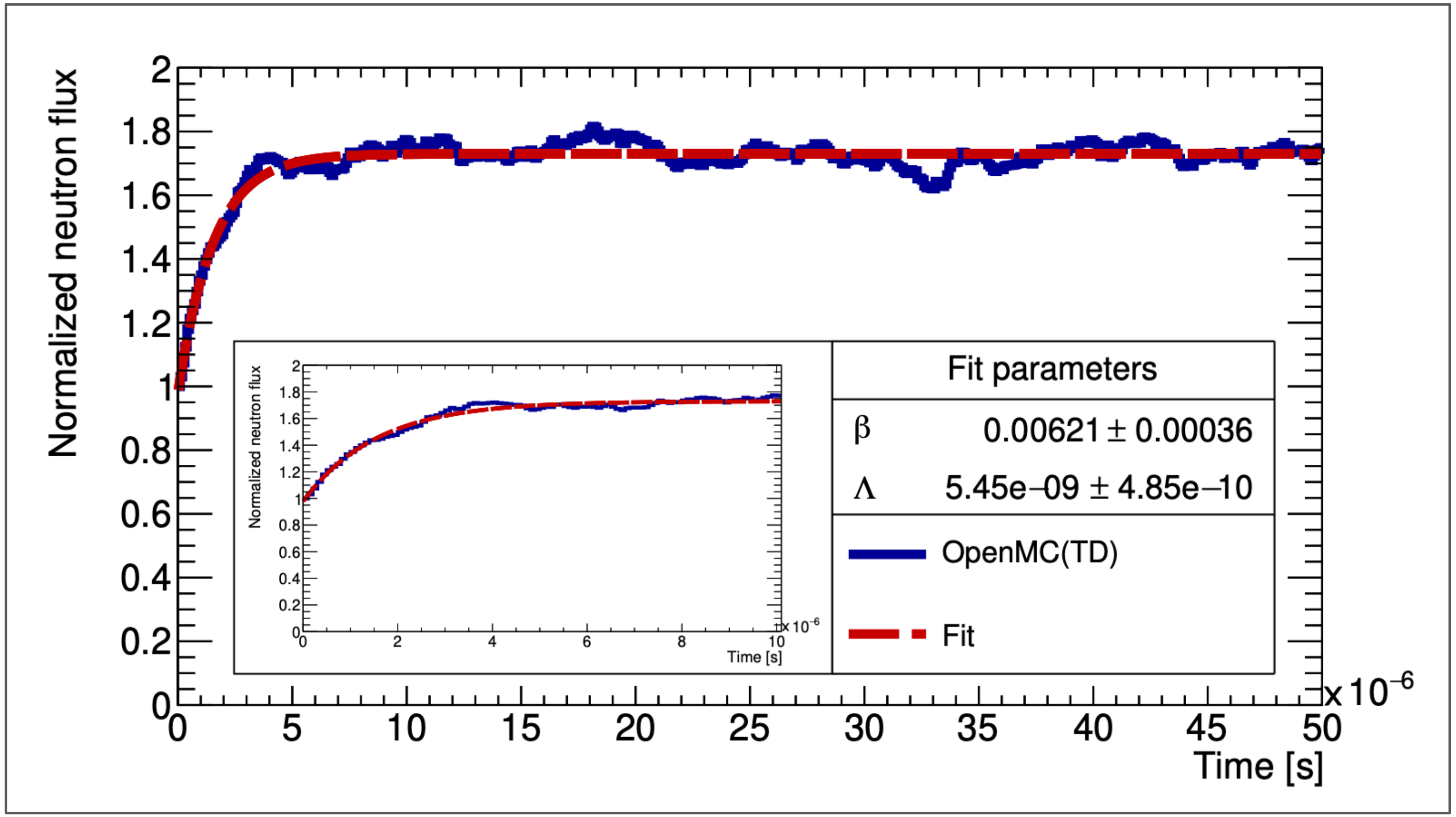
Energy-dependent ^{235}U system: Supercritical configuration case v



Case	6-group with average energy from ENDF-B/VIII.0
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	11.03

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	6.00(1)	5.45(57)	9.2%
β_{eff} [pcm]	651(6)	635(38)	2.5%

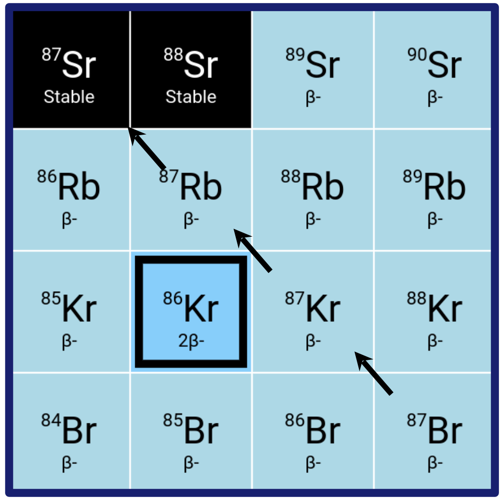
Energy-dependent ^{235}U system: Supercritical configuration case vi

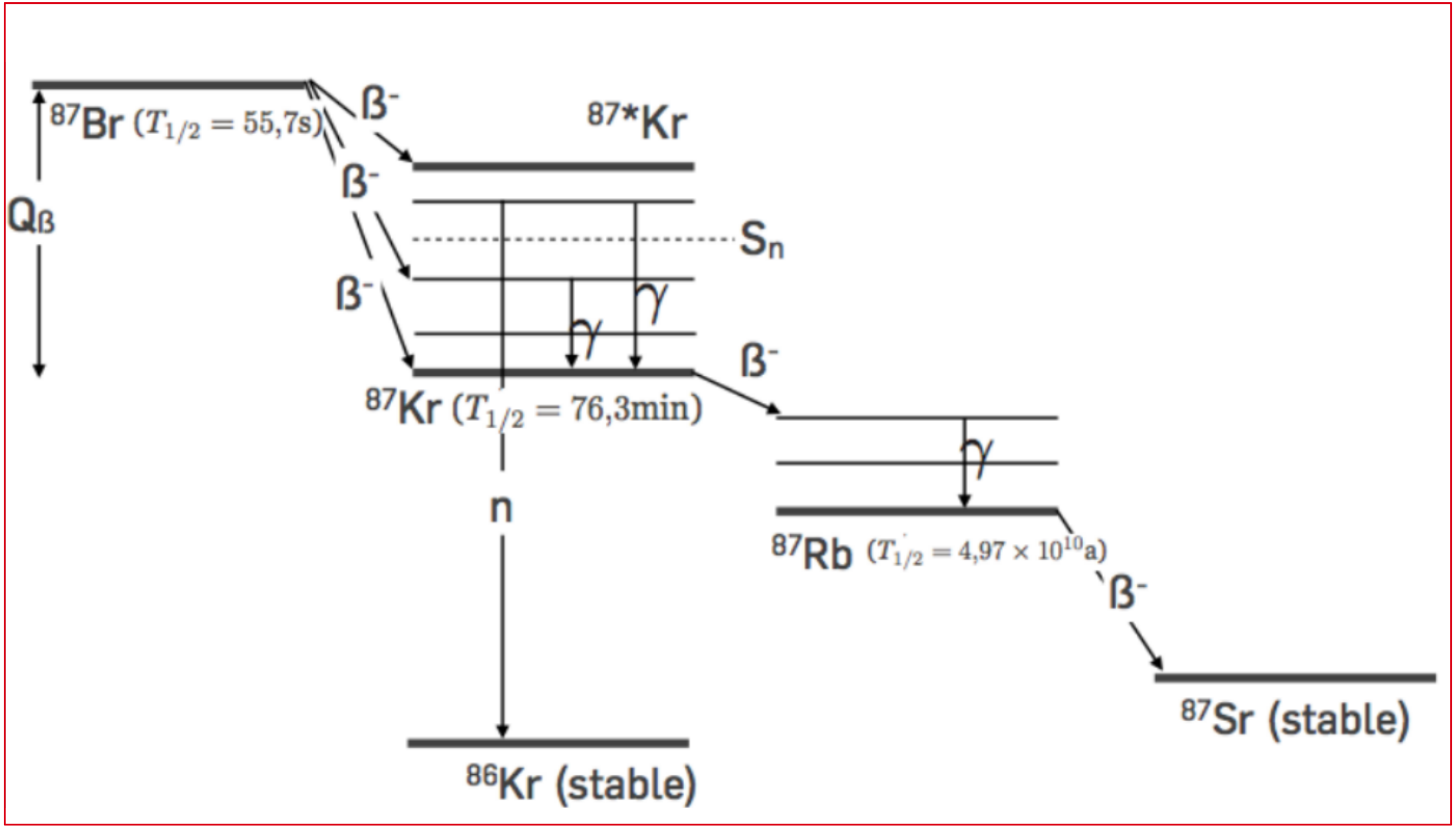


Case	50 individual precursors with average energies from ENDF-B/VIII.0
Batches	3
No. time intervals	500
Time interval length (ns)	100
Simulation time (ms)	0.05
Wall-clock time (h)	17.24

Parameter	Calculated MCNP	Fitted OpenMC(TD)	Difference
Λ [ns]	6.00(1)	5.45(49)	9.2%
β_{eff} [pcm]	651(6)	621(36)	4.6%

Example: ^{87}Br Decay scheme





Delayed neutron measurement techniques

Experiments to measure delayed neutron energy spectra are complicated because it is difficult to isolate the precursors and measure their spectrum at the same time

1. ^{3}He spectrometry: Helium-3 gas filled ionization chambers.

2. Proton recoil counters: measure the energy of recoil protons which result from neutron elastic scattering from ordinary hydrogen.

3. Time of flight measurements: time of flight measured over a specified distance.

Some available Monte Carlo (MC) codes

TRIPOLI 4®

- Transient calculations*
- Grouped precursors
- Burnup calculations

MCNP6

- Fixed source subcritical calculations
- Grouped precursors
- Burnup calculations

GEANT4 A SIMULATION TOOLKIT

- Monte Carlo Toolkit
- G4Stork: transient calculations ~50 ms
- Grouped precursors

OpenMC

- Transient calculations*
- Grouped precursors
- Burnup calculations

Serpent

- Transient calculations
- Grouped precursors
- Burnup calculations

FLUKA

- I dunno

Point kinetics equations with individual precursor data

$$\frac{dn(t)}{dt} = \frac{\rho(t) - \beta}{\Lambda} n(t) + \sum_j \lambda_j P_n^j C_j(t)$$

$$\frac{dC_j(t)}{dt} = \frac{Y I_j}{\nu \Lambda} n(t) + \sum_k \lambda_k \, BF_{k \to j} C_k(t) - \lambda_j C_j(t)$$

$$k = \text{Multiplication factor} = \frac{\text{Number of neutrons in one generation}}{\text{Number of neutrons in preceding generation}}$$

$\Lambda = \frac{l}{k}$ = mean generation time between birth of neutron and subsequent absorption inducing fission

$\rho = \frac{k-1}{k}$ = reactivity

β = fraction of fission neutrons which are delayed

β_{eff} = fraction of delayed neutron that are effective at inducing fissions

Prompt chain lengths

$P_p = k_{eff}(1 - \beta)$ probability of creating a prompt neutron

$P(n) = (1 - P_p) \sum_{i=1}^{n} P_p^{(i-1)}$ probability to create a chain of length *n*

Then, the average chain length is now given by:

$$\bar{n} = \sum_{n=1}^{\infty} nP(n) = (1 - P_p) \sum_{n=1}^{\infty} nP_p^{n-1} = \frac{1}{1 - P_p}$$

International Conference on the Physics of Reactors "Nuclear Power: A Sustainable Resource"
Casino-Kursaal Conference Center, Interlaken, Switzerland, September 14-19, 2008

Scouting the feasibility of Monte Carlo reactor dynamics simulations

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The Dynamic Monte Carlo Method
for
Transient Analysis of Nuclear Reactors

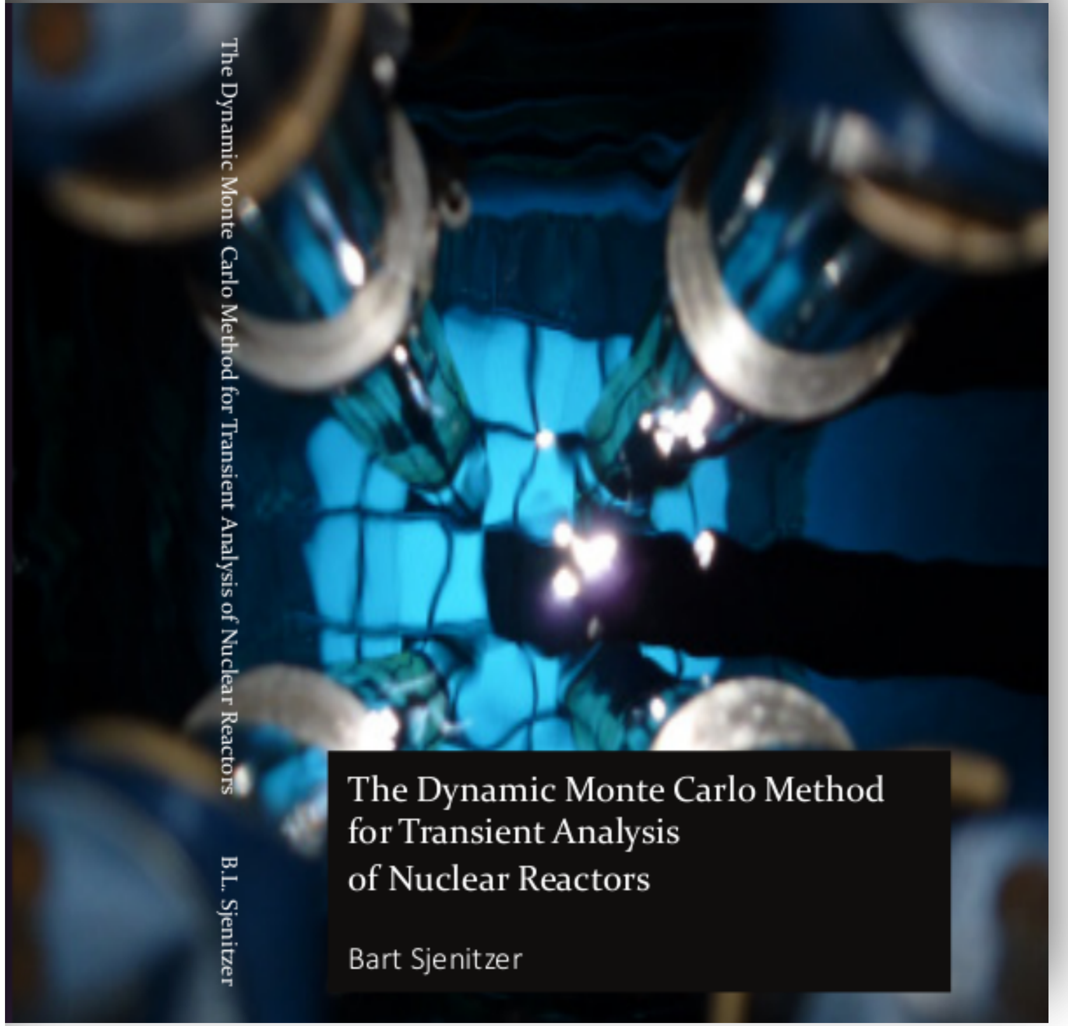
Proefschrift

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus Prof. ir. K.C.A.M. Luyben,
voorzitter van het College voor Promoties,
in het openbaar te verdedigen
op vrijdag 05 juli 2013 om 10:00 uur
door

Bart Laurens SJENITZER

Natuurkundig ingenieur

geboren te Amsterdam



STATIC AND DYNAMIC STOCHASTIC NEUTRONIC REACTOR ANALYSIS WITH THERMAL-HYDRAULIC FEEDBACK

DOCTORAL DISSERTATION

ANTONIOS G. MYLONAKIS

SUPERVISOR:
A. CLOUVAS
Professor

ATHENS, September 2017

Coupling between Monte Carlo neutron transport and thermal-hydraulics for the simulation of transients due to reactivity insertions

Thèse de doctorat de l'Université Paris-Saclay
préparée à l'Université Paris-Sud

Ecole doctorale n°576 Particules, Hadrons, Énergie, Noyau, Instrumentation, Image, Cosmos et Simulation (PHENIICS)
Spécialité de doctorat : Énergie nucléaire

Thèse présentée et soutenue à Saclay, le 18 octobre 2019, par

MARGAUX FAUCHER

Probability of creation of precursor at t<0

$$P_i = \begin{cases} \dfrac{\lambda^b}{\lambda_i} \dfrac{\beta_i}{\beta}, & \text{for precursor group} \\ \dfrac{\lambda^b}{\lambda_i} I_i, & \text{for individual precursor,} \end{cases}$$

where λ^b is the inversely weighted decay constant defined as

$$\lambda^b = \begin{cases} \dfrac{\beta}{\sum_i \dfrac{\beta_i}{\lambda_i}}, & \text{for precursor group} \\ \dfrac{1}{\sum_i \dfrac{I_i}{\lambda_i}}, & \text{for individual precursor,} \end{cases}$$

Probability of creation of precursor at t<0

$$n_0(\mathbf{r}, E) = \int_{4\pi} \frac{\psi_0(\mathbf{r}, \mathbf{\Omega}, E)}{v(E)} d\mathbf{\Omega},$$

$$C_{i,0}(\mathbf{r}) = \int_{4\pi} \int_0^\infty \frac{\beta_i(\mathbf{r}, E)\nu(\mathbf{r}, E)\Sigma_f(\mathbf{r}, E)}{\lambda_i} \psi_0(\mathbf{r}, \mathbf{\Omega}, E)\, dE d\mathbf{\Omega},$$

Relevance of delayed neutrons

$$n(t) = n_0 \exp\left(\frac{\Delta k}{l} t\right) \equiv n_0 \exp\left(\frac{t}{\tau}\right)$$

If there are no delayed neutrons, then $\Delta k = 0.0001$ means that in one second power would rise by a factor of ≈ 20000 and the reactor cannot be controlled using mechanic means.

$$l = l_p(1 - \beta_{eff}) + (T_{avg} + l_p) \approx \beta_{eff} T_{avg}$$

In this case, with delayed neutron present, reactor power would rise by a factor of ≈ 0.1 in one second, making possible to control the reactor by mechanical means.