AGH

AKADEMIA GÓRNICZO-HUTNICZA
IM. STANISŁAWA STASZICA W KRAKOWIE

PL GRID

Modeling of advanced nuclear systems

Dr inż. Przemysław Stanisław Stanisz
ps.stanisz@agh.edu.pl

AIRA 25.05.2023

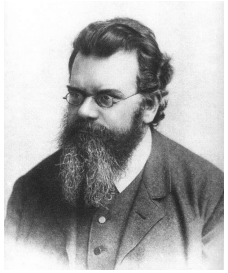
Agenda

1. History
2. Monte Carlo Methods
   - Transport
   - Variance Reduction
3. Burnup schemes
4. Fuel Evolution
   - Transmutation Trajectory Analysis
   - Trajectory Period Folding
5. Summary

Modeling of advanced nuclear systems

Two balance equations are required to describe and predict core behavior:

- Boltzmann equation for neutron distribution and spectrum (Neutron Field)
- Bateman equation for fuel evolution (nuclide field)



Ludwig Eduard Boltzmann
(1844 - 1906)

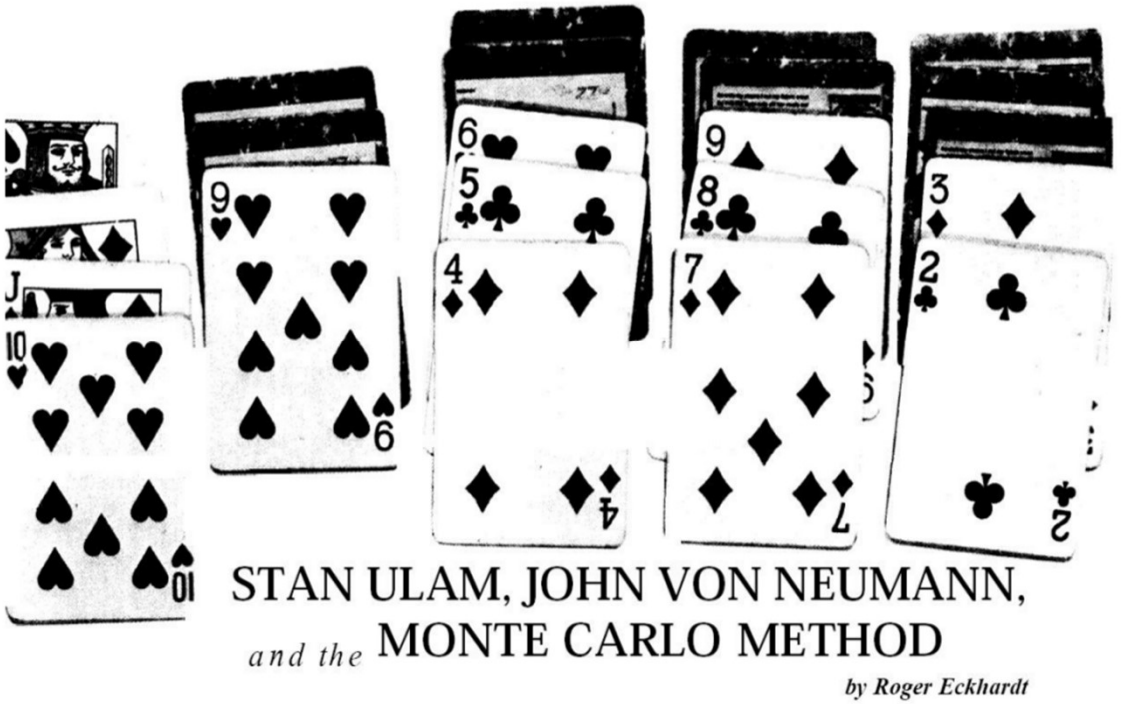
Harry Bateman
(1882 - 1946)

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \bar{\Omega}\cdot\bar{\nabla}\psi + \Sigma(\vec{r},E)\psi(\vec{r},E,\bar{\Omega},t) = \int_0^\infty dE' \int_{4\pi} d^2\bar{\Omega}'\Sigma_s(\vec{r},E'\rightarrow E,\bar{\Omega}\cdot\bar{\Omega}')\psi(\vec{r},E',\bar{\Omega}',t) + s(\vec{r},E,\bar{\Omega},t)$$

$$\frac{dN_i(t)}{dt} = \sigma_{c,k}N_k(t)\phi + \lambda_j N_j(t) + \sigma_{(n,2n),l}N_l(t)\phi - \left[\sigma_{a,i}N_i(t)\phi + \lambda_i N_i(t)\right]$$

History

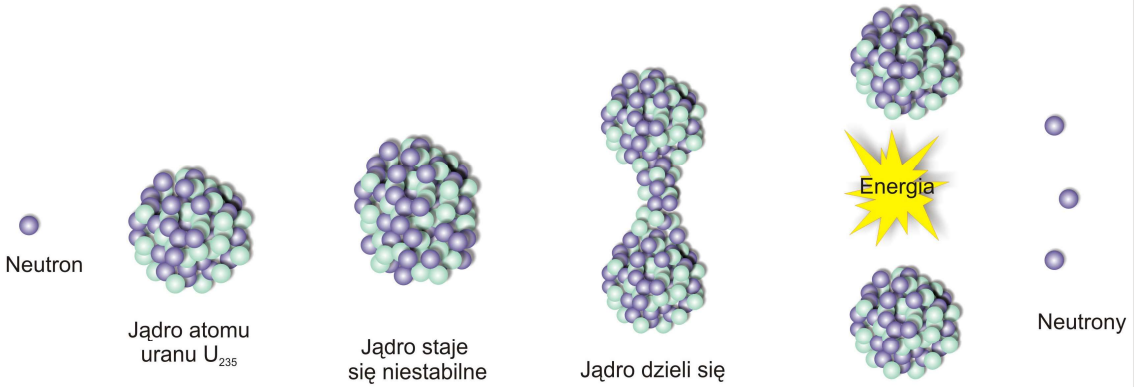
The development of the use of Monte Carlo methods in radiation transport simulations began at the Los Alamos laboratories during World War II.

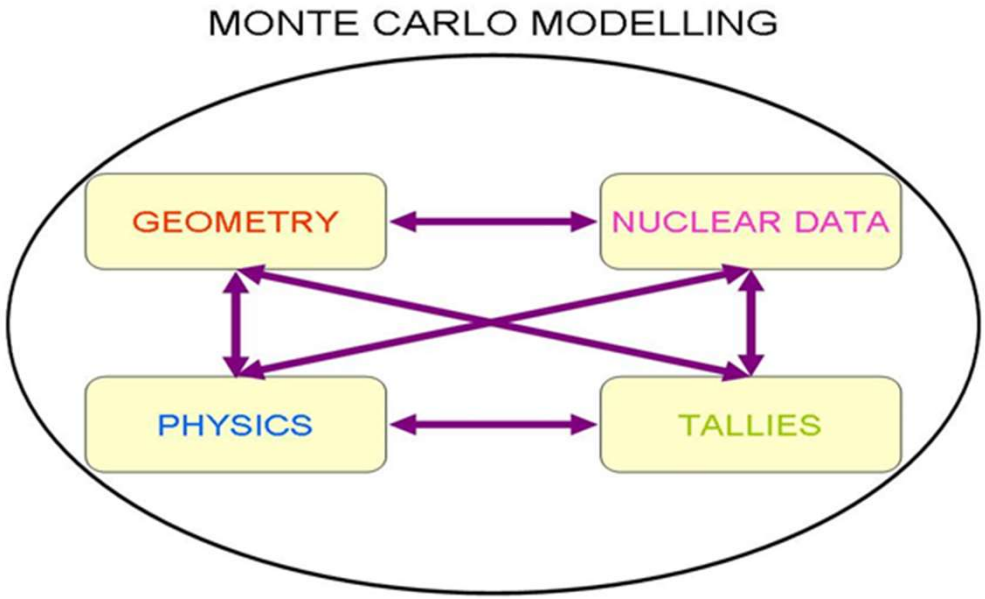


Pioneers in the development of Monte Carlo methods were:
Stanisław Ulam, John von Neumann, Nicholas Metropolis

Monte Carlo Methods

- Easy to start
- Counts the responses of the operators to the Boltzmann equation
- Calculation precision << 1% (required for reactivity level calculations)
- The importance of Monte Carlo methods has increased with the development of supercomputers

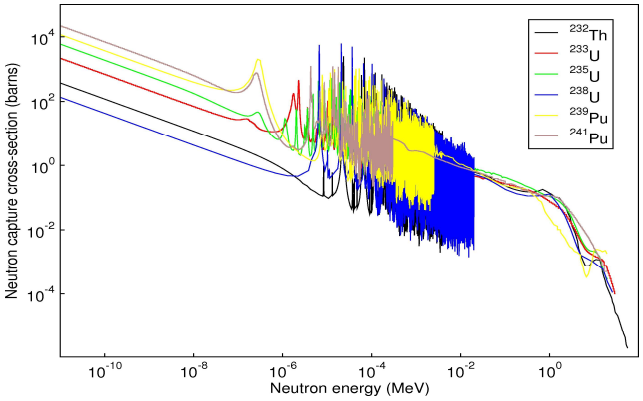




The use of neutron transport simulations using MC methods

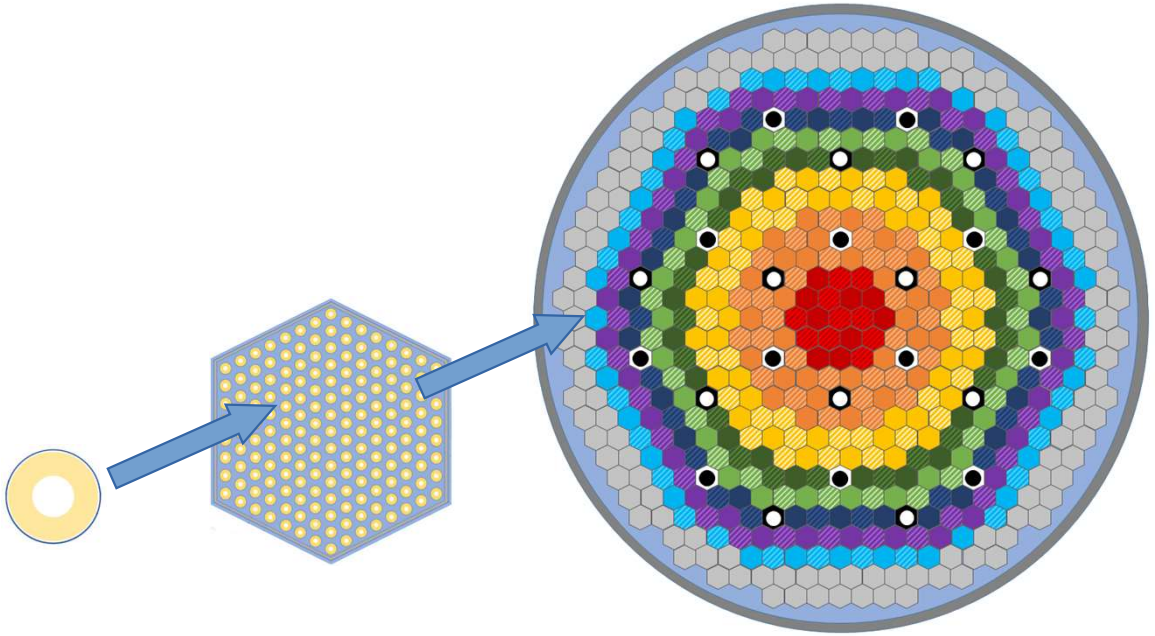
Usage:

- reactors
- detectors
- radiation protection
- subcritical systems
- critical systems
- fuel cycles
- exposure of samples
- dosimeter



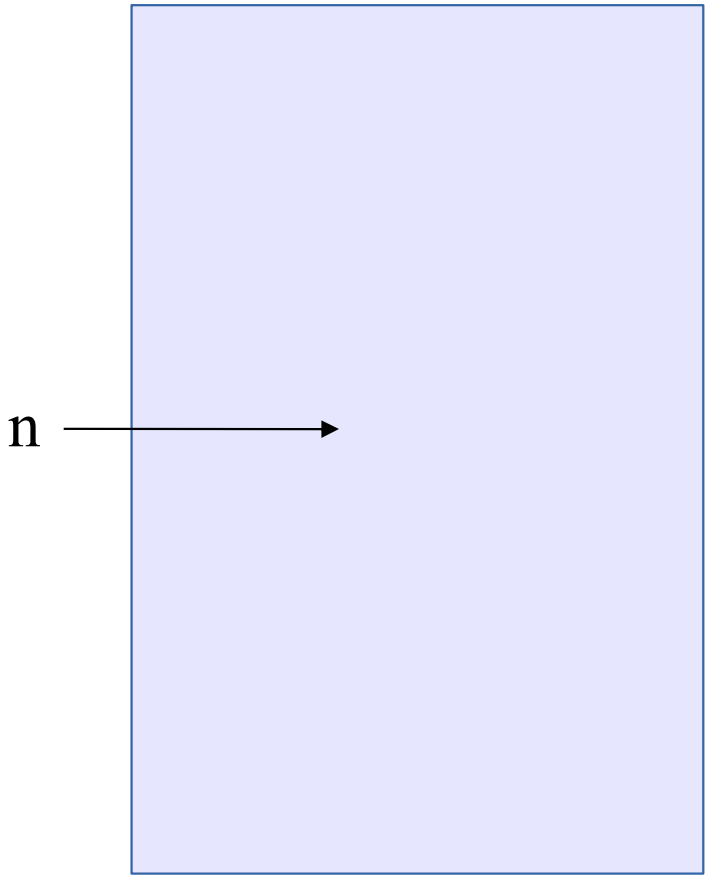
The user prepare:

- geometry,
- material (data tables),
- Localization and characteristic of the initial source
- tailling



MC Transport – Introduction (i)

Numbers between 0 and 1 are randomly assigned to determine the reaction (if any) of the neutron with the material at the simulated location. These events are based on the physical phenomena and probabilities that govern these processes, as well as the nuclids that make up given materials.

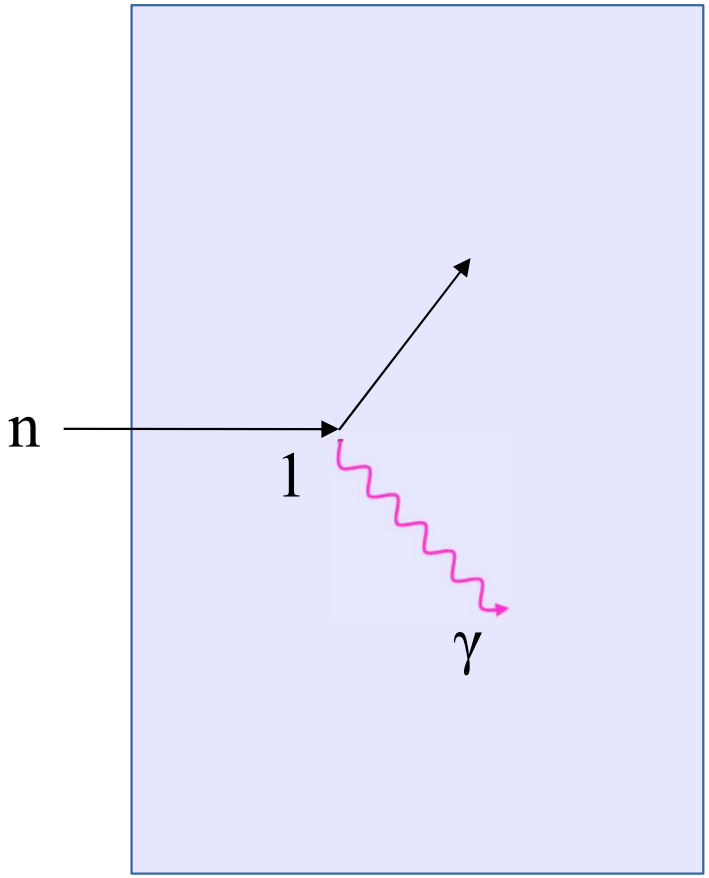


MC Transport – Introduction (ii)

In the example in point 1, a neutron collides with the material.

The neutron is scattered in the direction indicated by the second arrow. The direction is randomly chosen from the physical scattering distribution on the given nuclide with which the interaction took place.

The photon is also produced, its energy is stored, and its location is stored for later analysis.

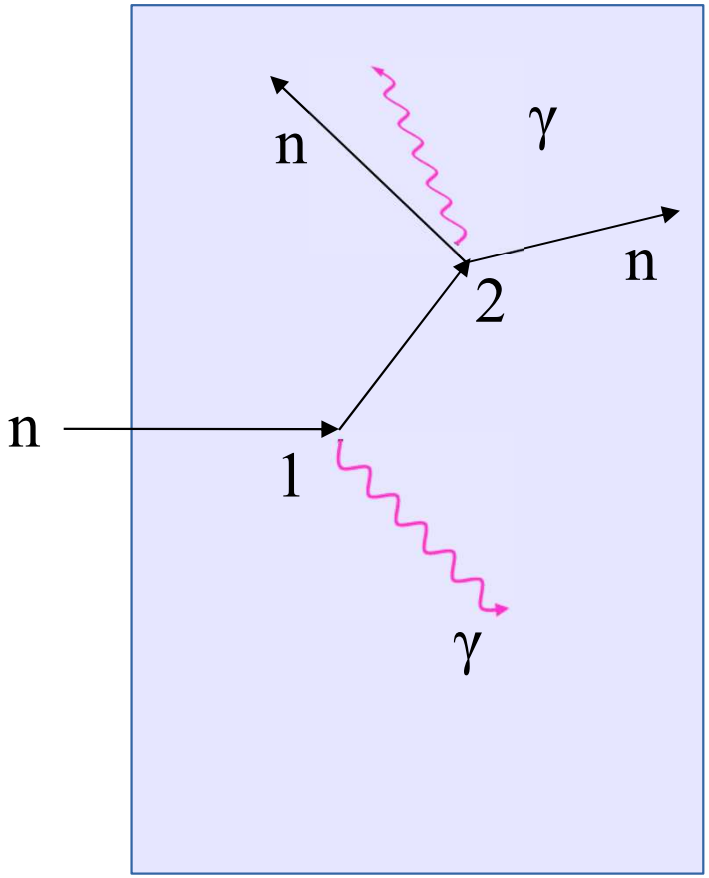


MC Transport – Introduction (iii)

In step 2. The fission reaction was drawn, ending the neutron simulation.

As a result of the fission, energy in the form of a gamma photon and two new neutrons have been randomly generated from the existing nuclear data.

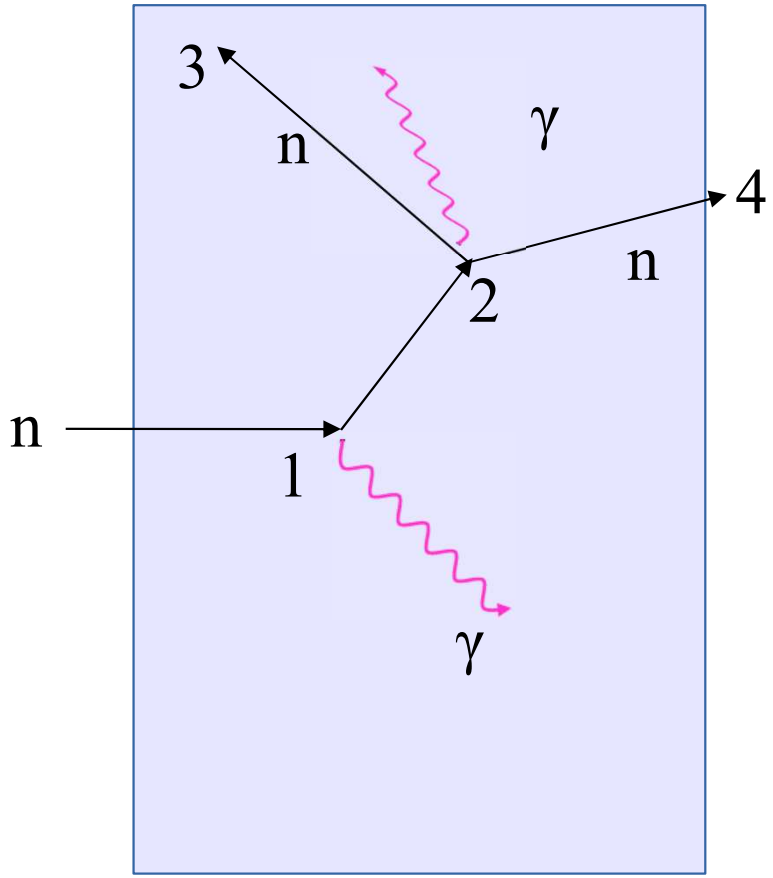
One neutron and one photon are stored for later analysis.



MC Transport – Introduction (iv)

The previously saved neutron is loaded and simulated further, ending the simulation outside the simulated area 4.

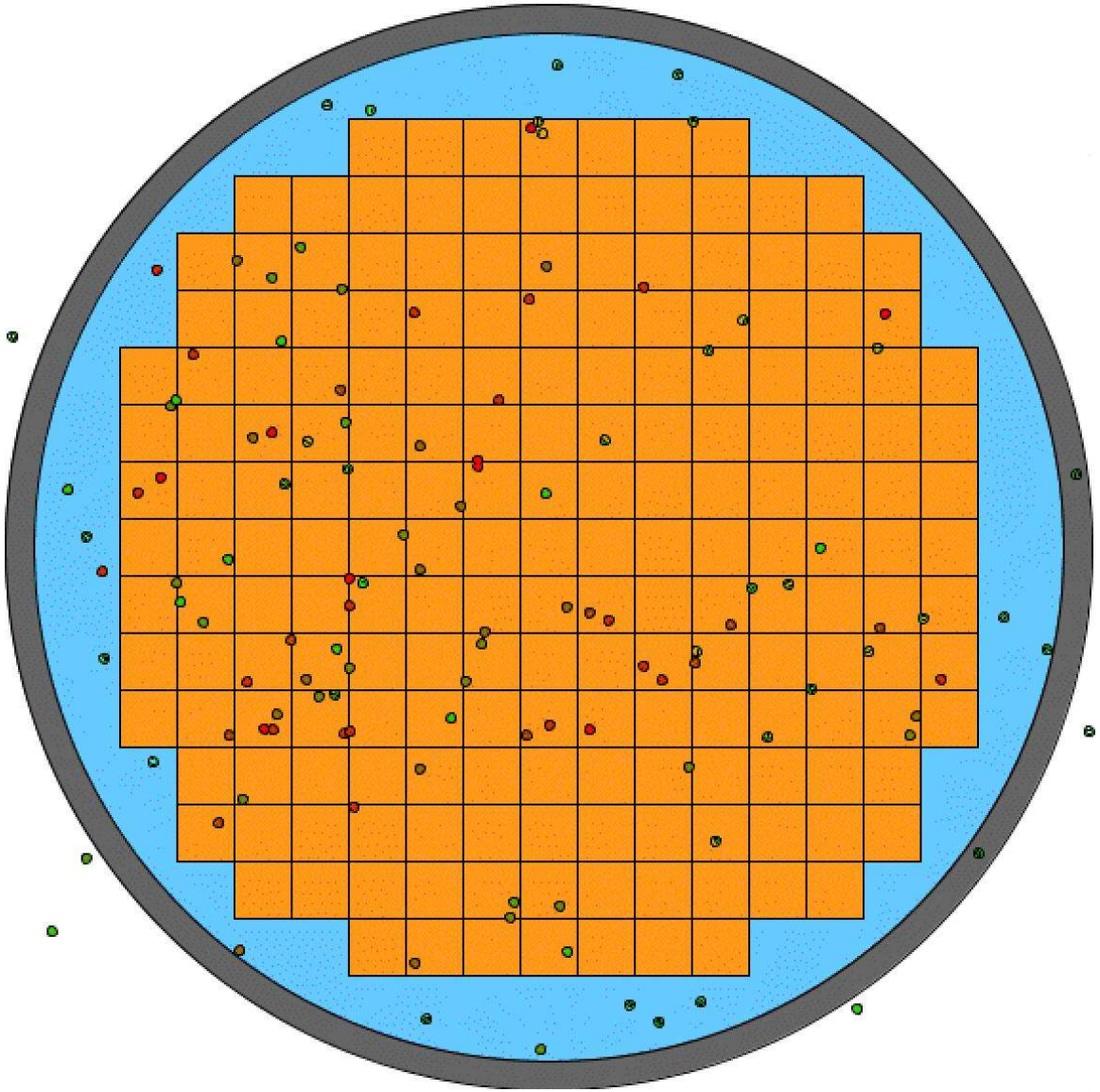
The second neutron is absorbed at point 3 and the simulation is stopped.



Modeling the whole nuclear core

Monte Carlo Simulations

- For each event, a random value is selected from the prepared probability function ranges;
- The model is computed based on statistics;
- Calculated values are given with their uncertainties;
- The accuracy of the results increases with the number of particles simulated;
- Typical Monte Carlo transport calculations for the entire core use over 100,000 neutrons per cycle.
- The results are used to describe the simulated model.



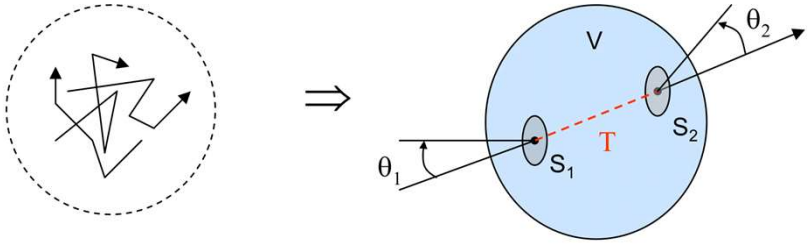
Tailling in Monte Carlo Transport

Two fundamental estimators:

- **Track length estimator.** The length of the track in a given cell or through a given surface is counted.

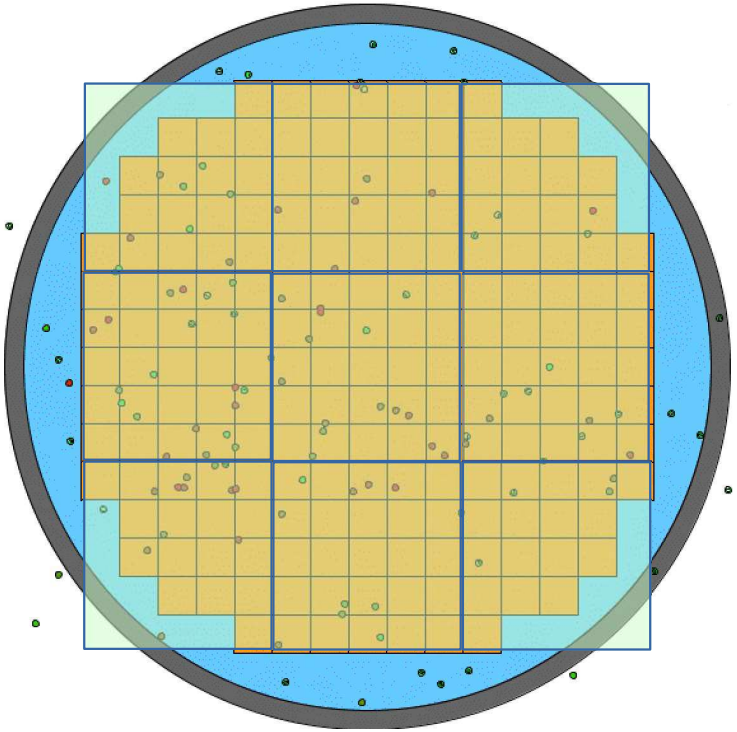
N – total numer of simulated particles

n – the numer of particle paths passing through the cell V



$$F_p(i,j) <= w \cdot s$$

$$\phi(V_i, E_j) = \frac{F_p(i,j)}{n \Delta V_i \Delta E_j}$$

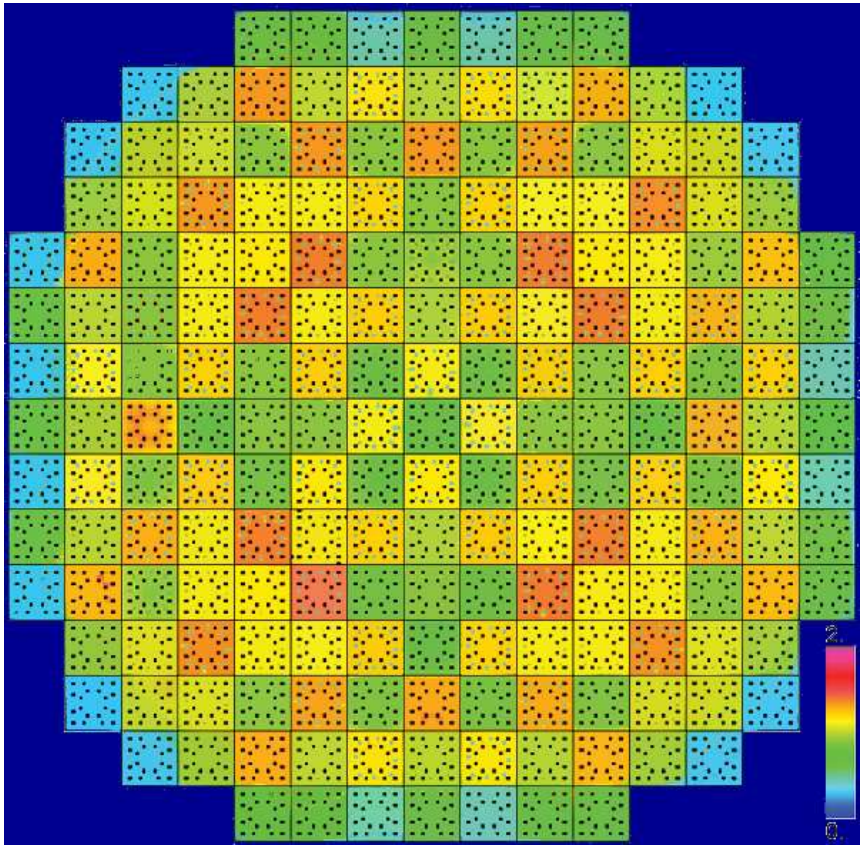


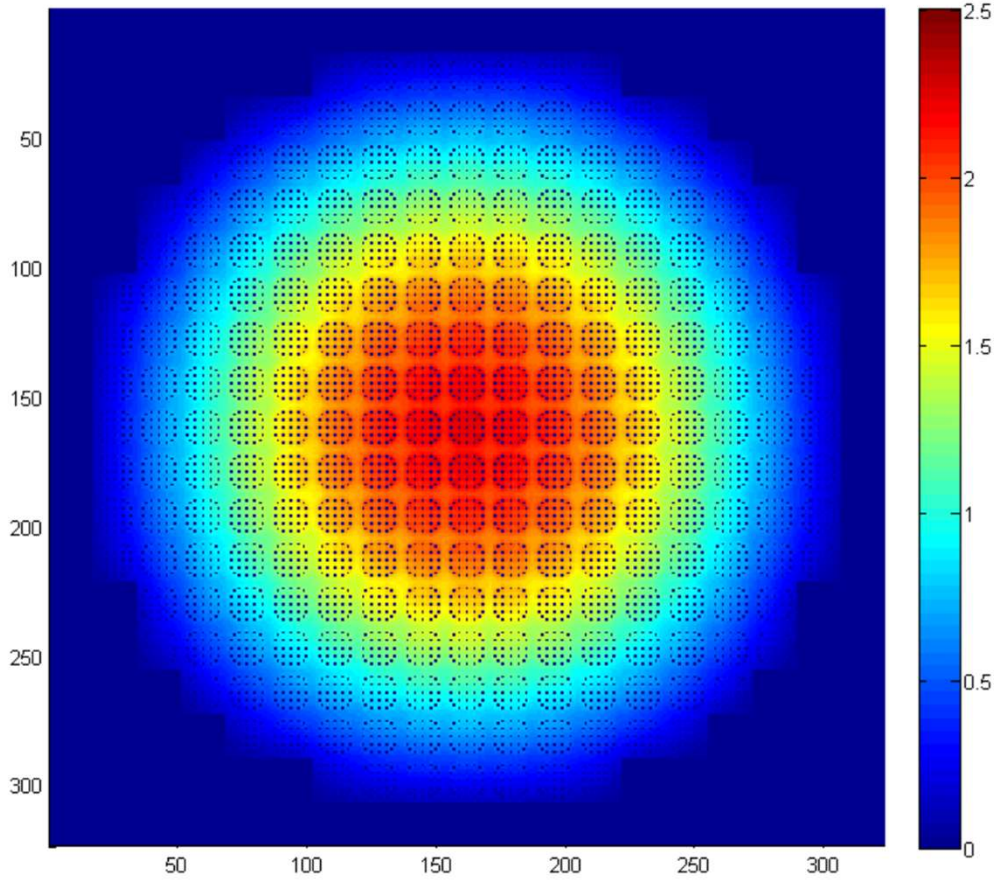
- **Collision estimator**. A less accurate but faster model based on counting the number of events in the volume under measurement.

$$F_c(i,j) <= \frac{w}{\Sigma_t(E_j)}$$

$$\phi(V_i, E_j) = \frac{F_c(i,j)}{n \Delta V_i \Delta E_j}$$

Model discretization



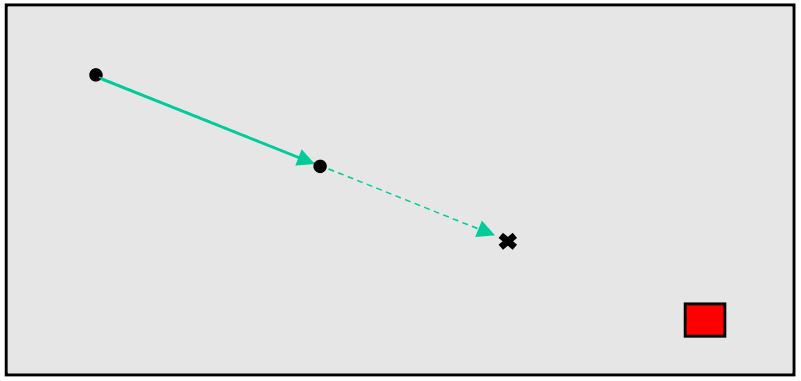


Averaging over **hundreds/thousands** of cells (on the fuel assembly level)

Averaging over **millions** of cells (on the fuel rod level)

Wariance Reduction: Exponential transform

Change sampling rules.
Biases distances between subsequent collision get larger in the direction towards the region of interest and shorter in opposite direction



Oryginal Transition Kernel $T = \Sigma_{tot} e^{-\Sigma_{tot} \cdot s}$

Projection of particle $\mu = \overrightarrow{\Omega} \cdot \overrightarrow{\Omega}_d \sim cos\alpha$

Biased Total CrossSection $\Sigma'_t = \Sigma_t - \mu \cdot c$

Biased Transition Kernel $T' = \Sigma' \cdot e^{-\Sigma'_t s}$

Due to bias, kernel distance is sampled $s = -\frac{ln(\xi)}{\Sigma_t - c\mu}$

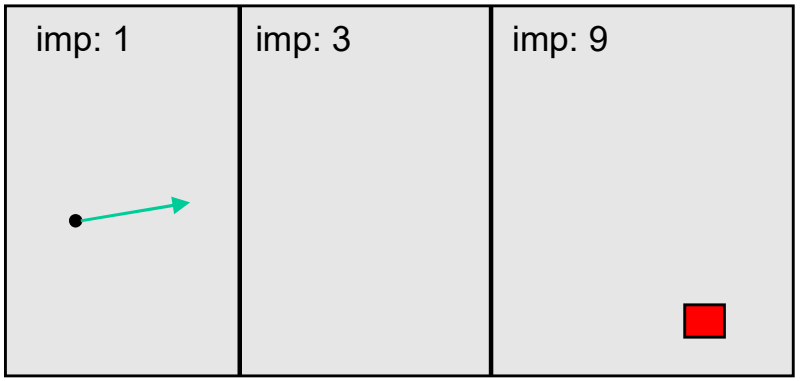
New weight $w' = w\frac{T}{T'}$

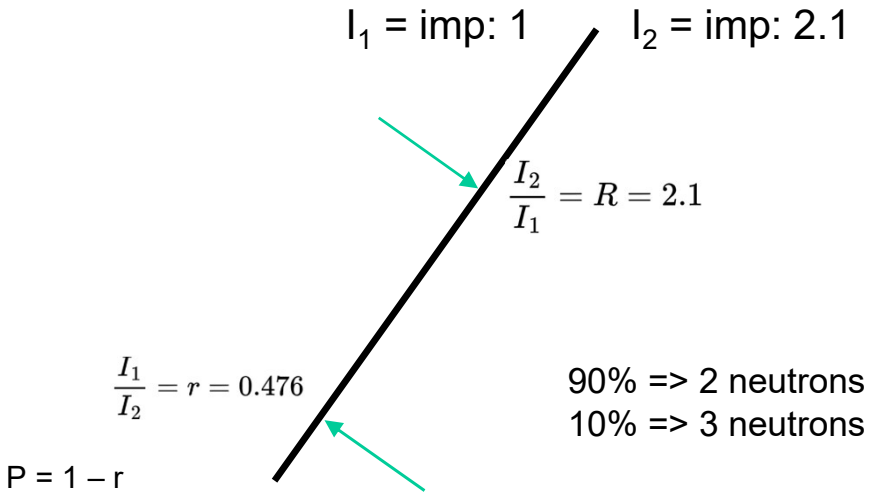
Wariance Reduction: Geometry Splitting

Each region has assigned importance.

User need define those importance based on his prior knowledge

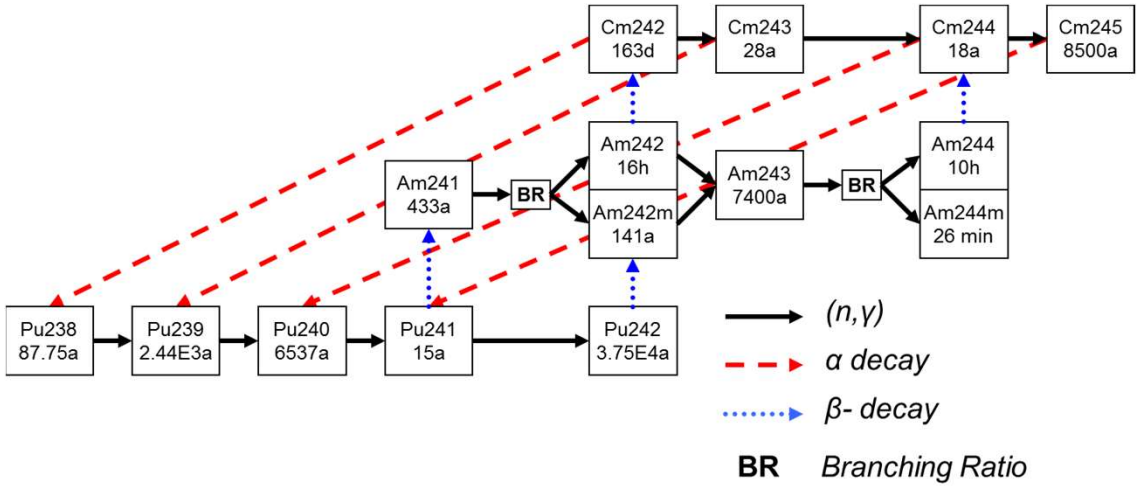
In some calculations, certain energies may be more important than others. Then we may split neutrons when their energies enter the important Energy rang, similarly as we split them in geometrical splitting

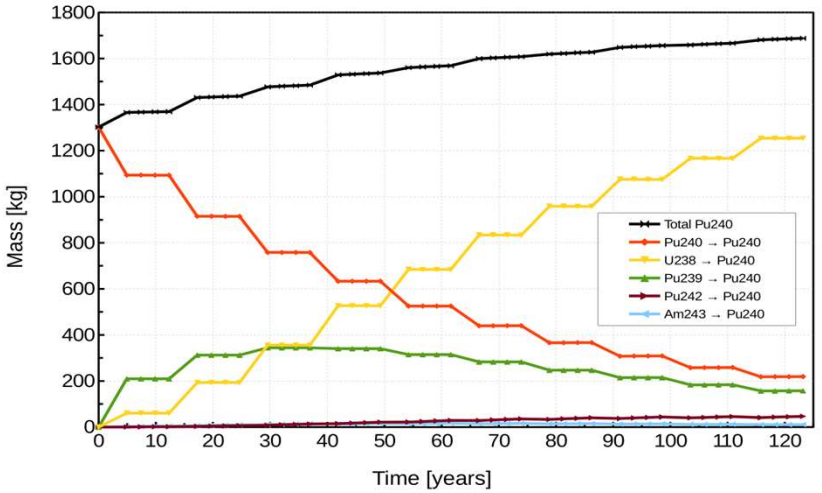




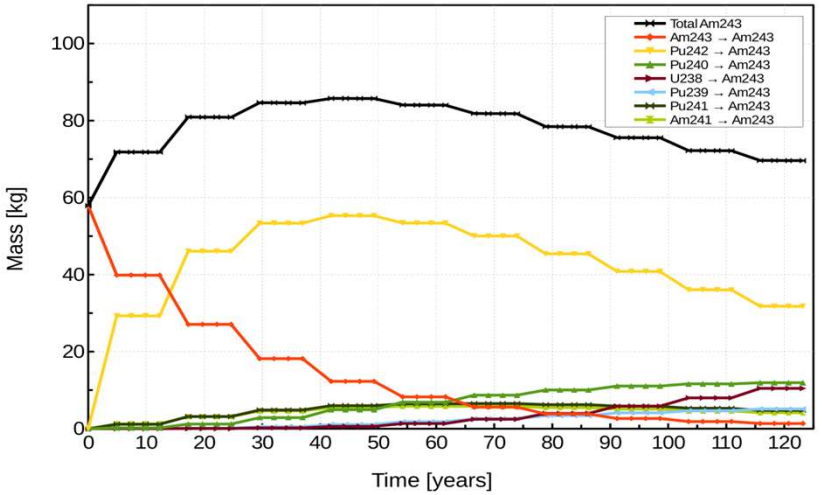
Fuel evolution

$$\frac{dN_i}{dt} = production\ rate - absorbtion\ rate - decay\ rate$$





Ewolucja Pu240 z wyszczególnonym udziałem nuklidów tworących



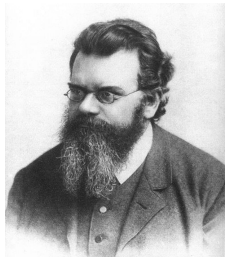
Ewolucja Am243 z wyszczególnonym udziałem nuklidów tworących

Modeling of the fuel evolution for the reactor core

Two main methodologies required to describe and predict nuclear core behavior

MCNP Monte Carlo N-Particle Transport Code is used to describe **Boltzmann equation.** Describe neutron distribution and spectrum

Bateman equation solved by **CRAM** (Chebyshev Rational Aproximation Method) or **TTA** Transmutation Trajectory Analysis analyzes nuclide density by solve**.** Describe fuel evolution



Ludwig Eduard Boltzmann
(1844 - 1906)

Harry Bateman
(1882 - 1946)

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \vec{\Omega}\cdot\vec{\nabla}\psi + \Sigma(\vec{r},E)\psi(\vec{r},E,\vec{\Omega},t) = \int_0^\infty dE' \int_{4\pi} d^2\vec{\Omega}\,\Sigma_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\psi(\vec{r},E',\vec{\Omega}',t) + s(\vec{r},E,\vec{\Omega},t)$$

$$\vec{\Phi} = M\vec{C}(\vec{N})$$

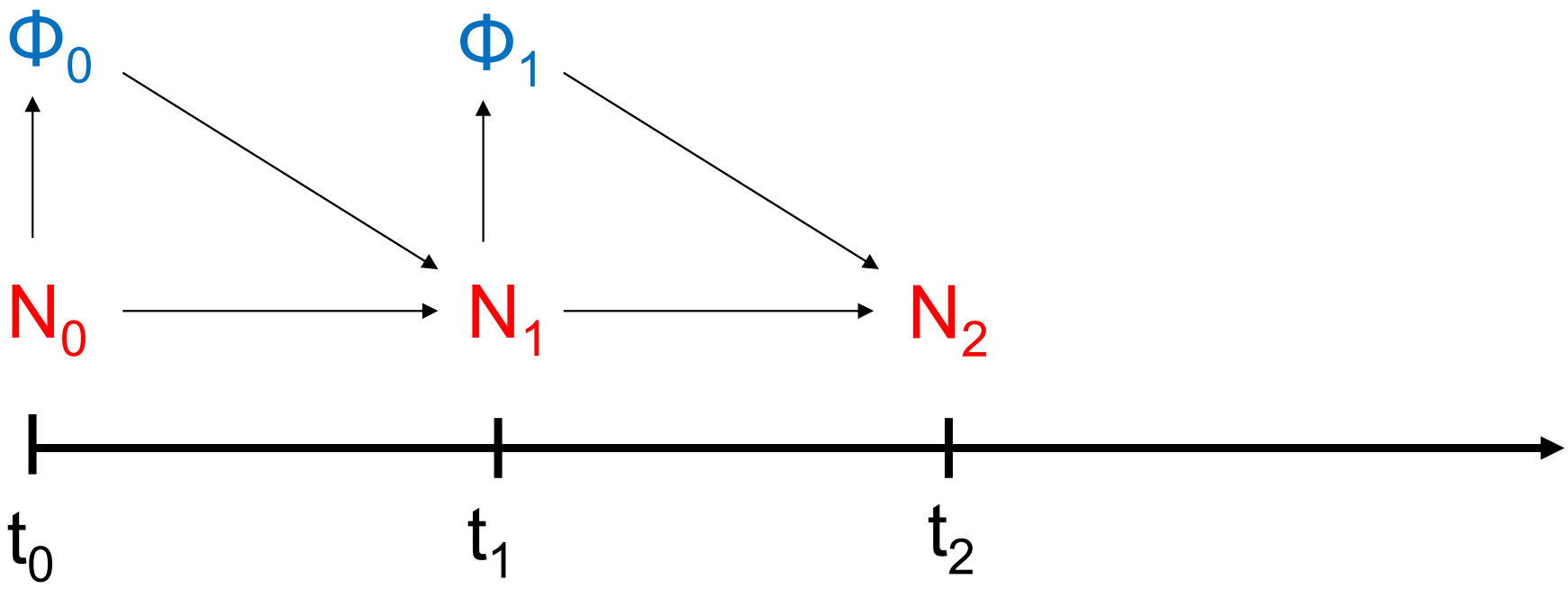
$$\frac{dN_i(t)}{dt} = \sum_k c_{ik} N_k(t)\phi + \lambda_j N_j(t) + \sigma_{n,2n,i} N_j(t)\Phi - [\sigma_{a,i} N_i(t)\phi + \lambda_i N_i(t)]$$

$$\vec{N} = \vec{N_0} e^{M(\Phi)\cdot(t-t_0)}$$

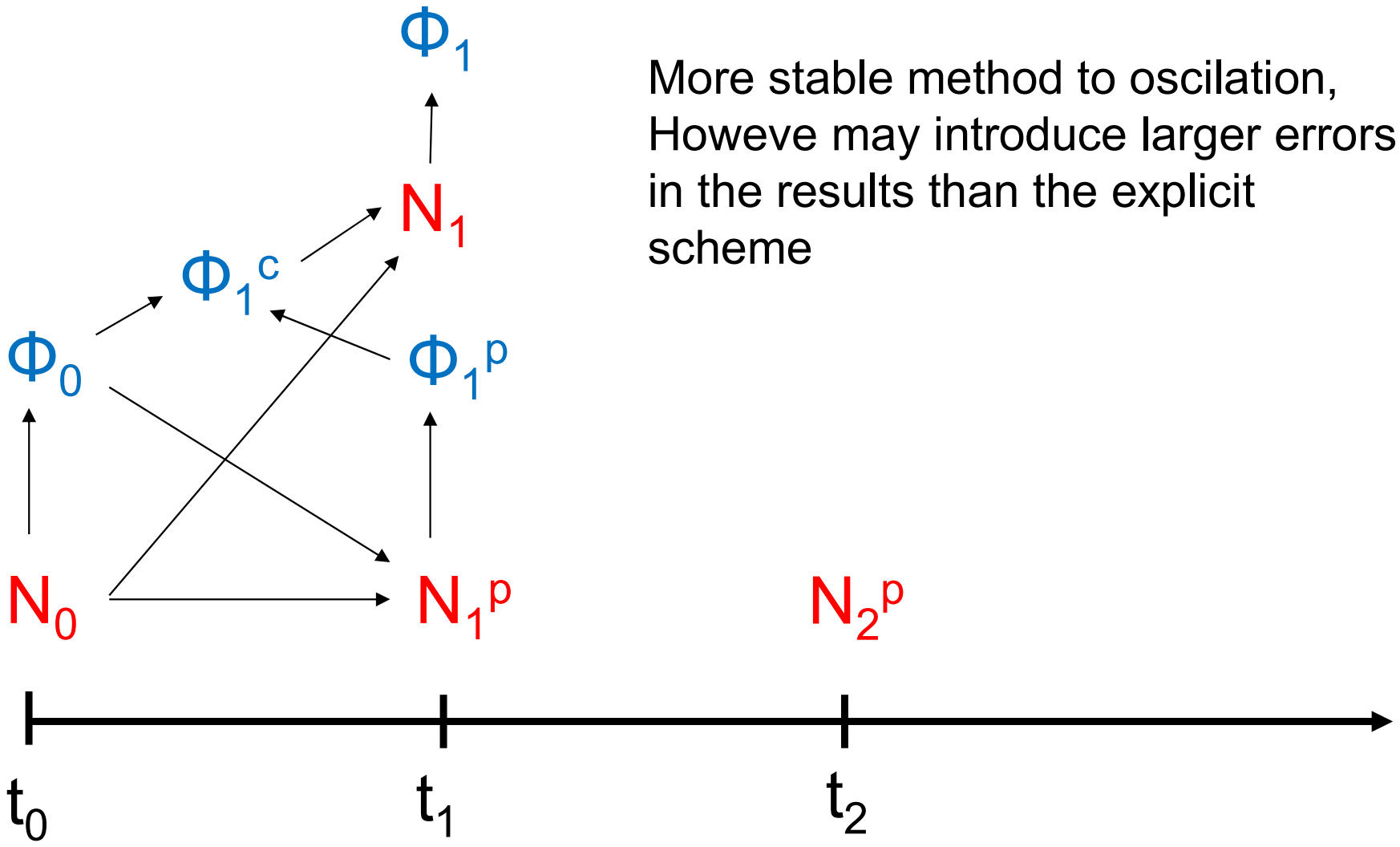
Explicit Euler Based Coupling Scheme

Burnup solver assume that neutron flux does not change through time
This can be true for small steps

Beginning-of-step constant flux approximation coupling scheme

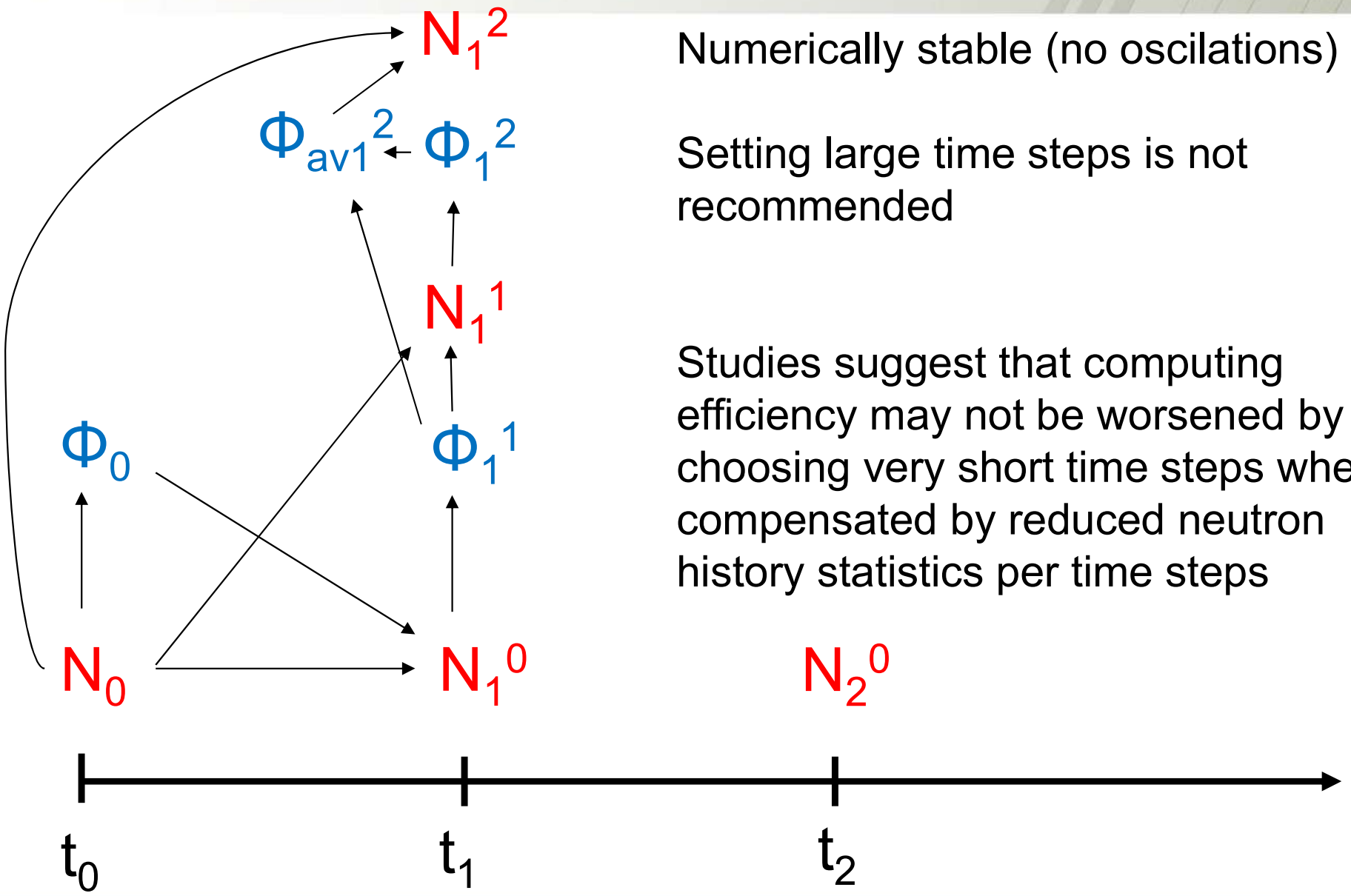


The Predictor-Corrector scheme



More stable method to oscilation, Howeve may introduce larger errors in the results than the explicit scheme

Implicit Euler Based Coupling Scheme



Numerically stable (no oscilations)

Setting large time steps is not recommended

Studies suggest that computing efficiency may not be worsened by choosing very short time steps when compensated by reduced neutron history statistics per time steps

AGH

The Monte Carlo Continuous Energy Burn-up Code

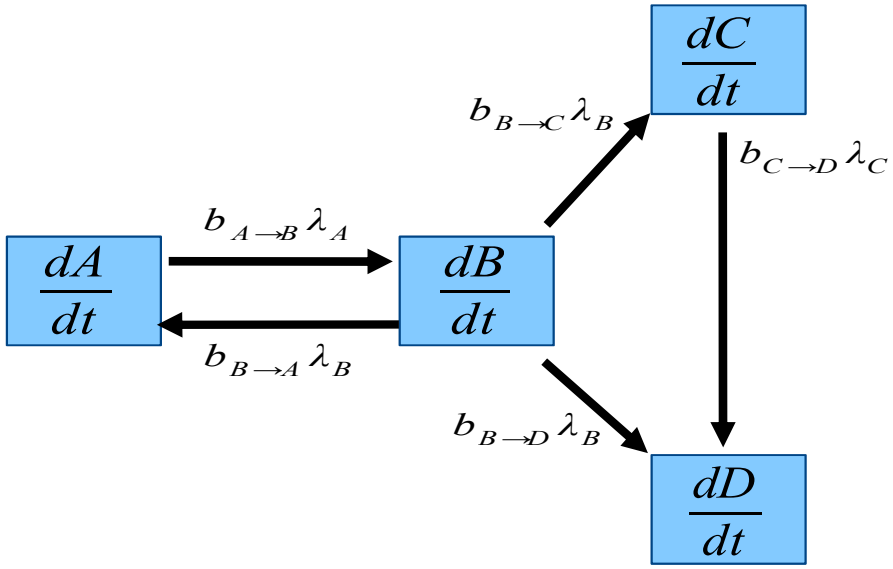
MCB = MCNP + TTA

MCNP Monte Carlo N-Particle Transport Code
The code provides results such reaction rates and heating per nuclide for each burnable zone. Results are obtained from the Monte Carlo simulation in order to provide neutron distribution and spectrum.

TTA Transmutation Trajectory Analysis
The code provides evolution of the nuclides concentration through numerical solution based on the oryginal Bateman solution.

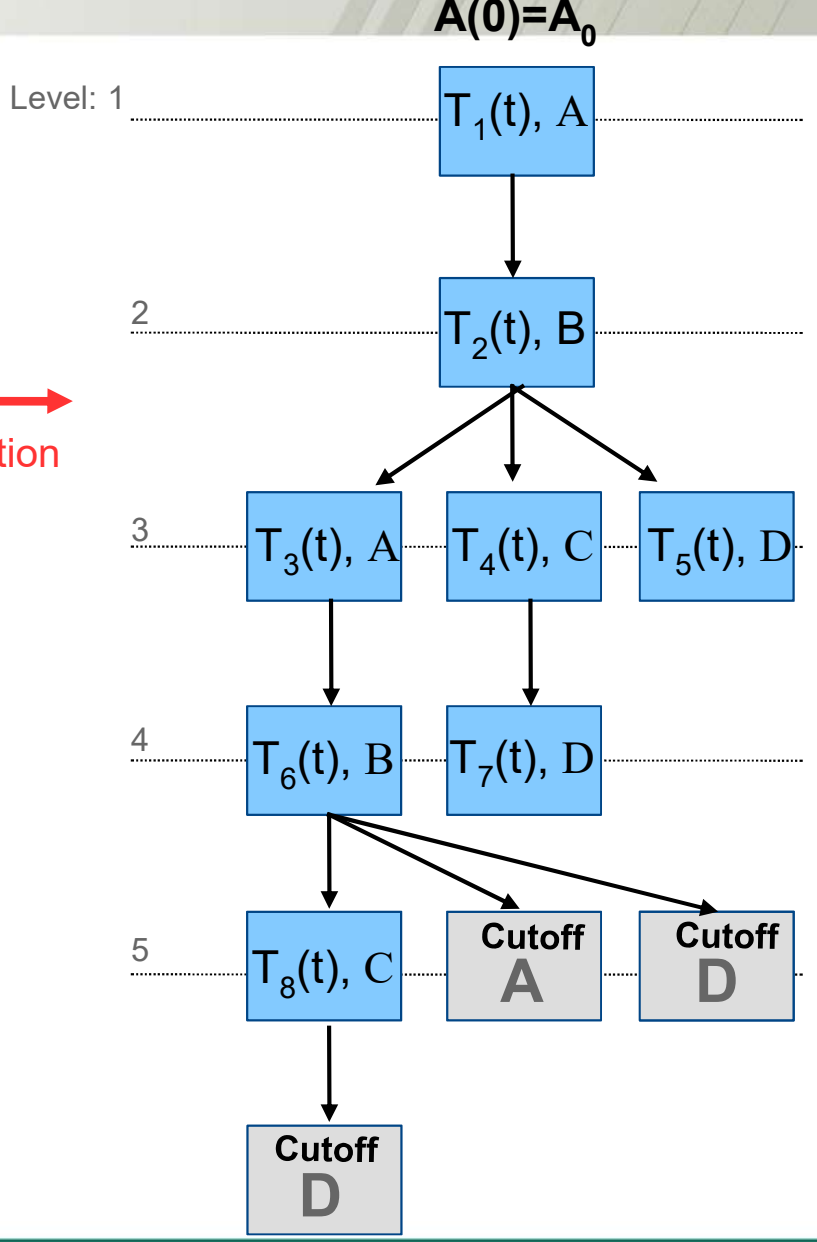
MCB has features:
- an integrated burn-up calculation code (calculations are integrated in one code)
- deals with the complexity of the burn-up process (i.e predictor-corrector method)
- deals withthe complexity of the fuel cycle process (i.e automatization shuffling and reloading of fuel)
- calculations include continuous energy representation of cross-section, spatial effects of full core reactor model and
- nuclide production in all possible reaction or decay channels.

The Transmutation Trajectory Analysis



TTA

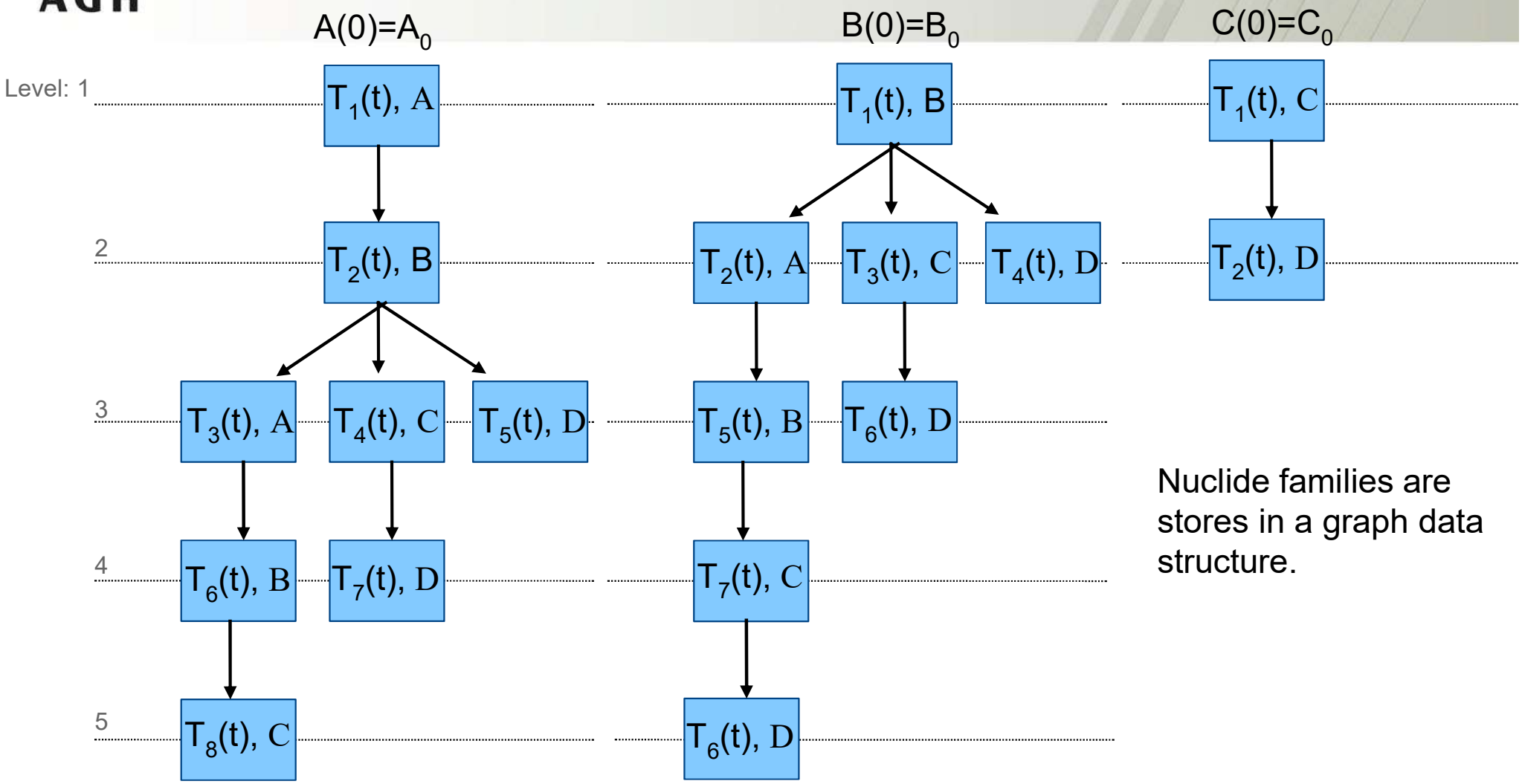
decomposition



The Bateman equations for transmutation trajectory

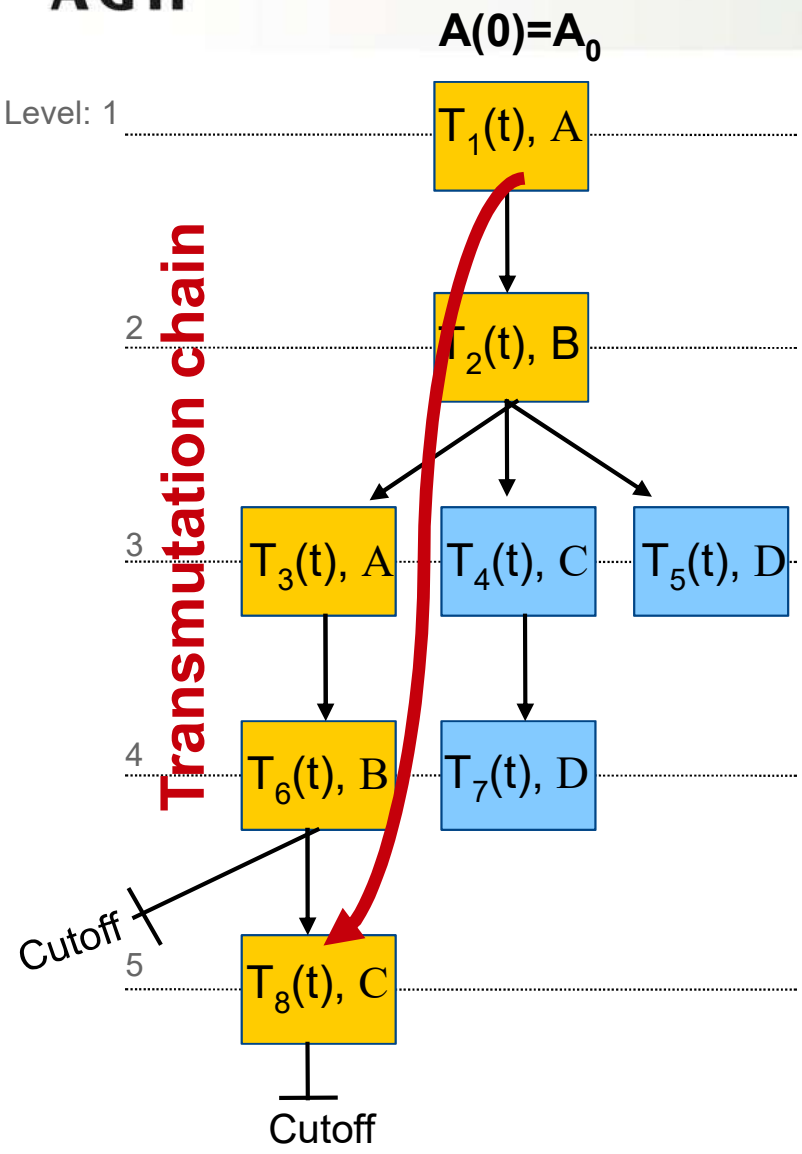
$$\frac{dN_i}{dt} = production\ rate - \ destruction\ rate$$

The Families



Nuclide families are stores in a graph data structure.

Transmutation chain vs Trajectories



Trajectories

$T_1(t)$: A (survival)

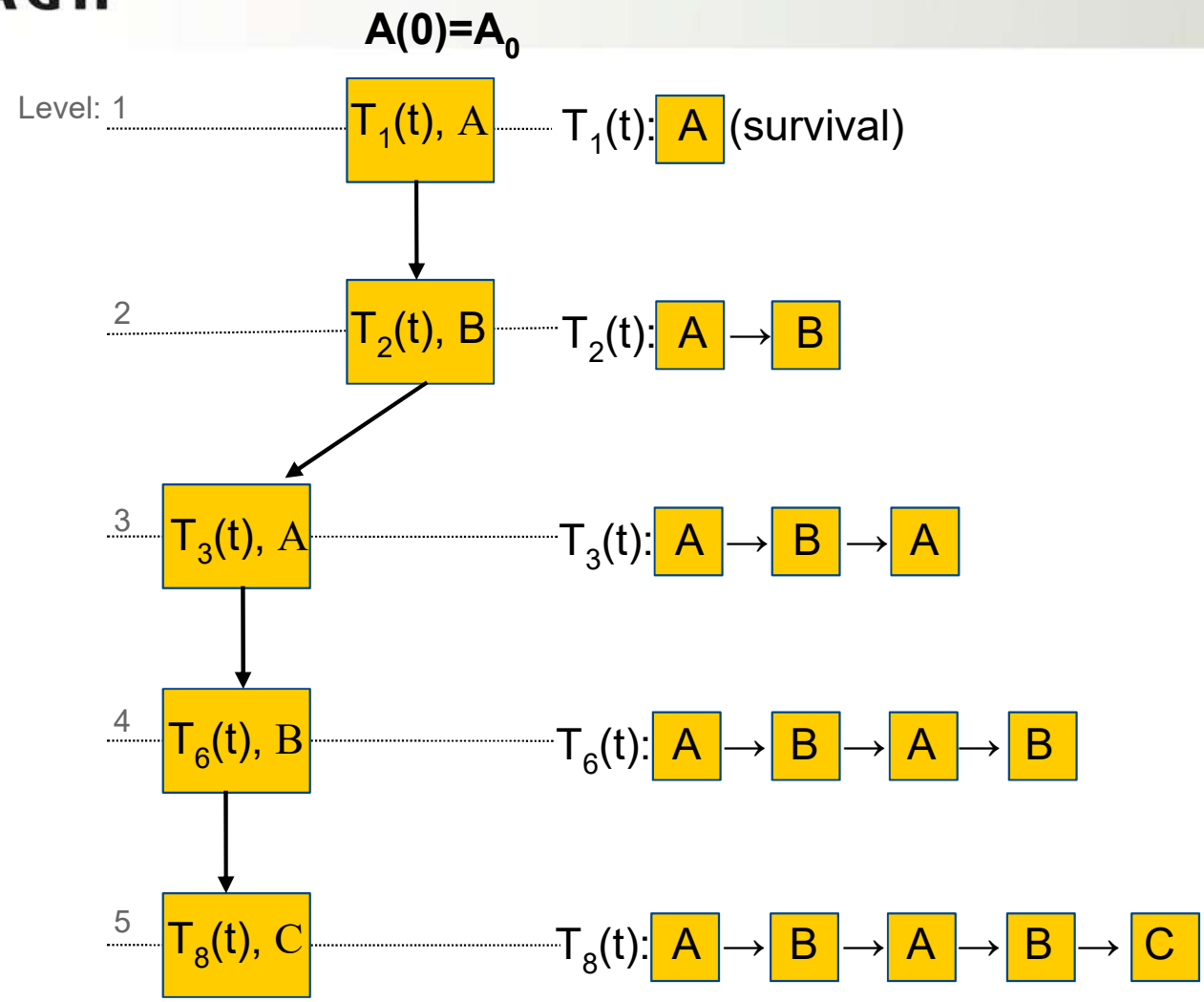
$T_2(t)$: A → B

$T_3(t)$: A → B → A

$T_6(t)$: A → B → A → B

$T_8(t)$: A → B → A → B → C

Transmutation chain vs Trajectories



The Transition and The Pasage Function

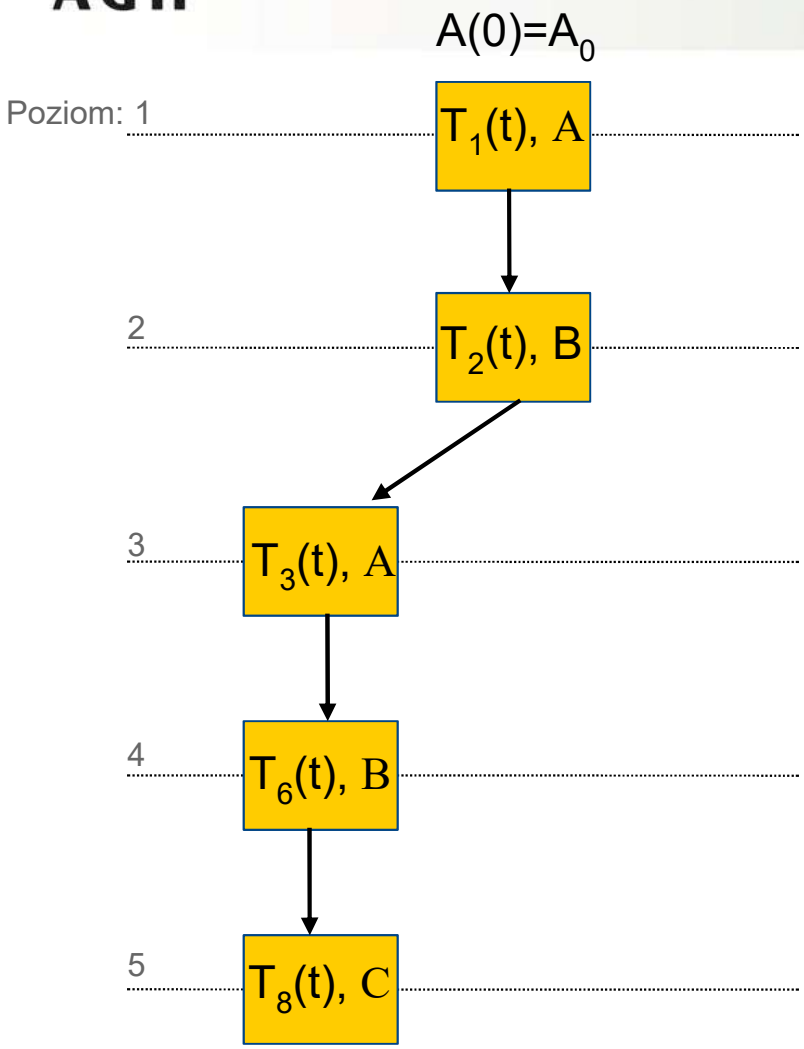
The trajectory transition calculate the number density that goes from initial nuclide to the formed nuclide for a given time t.

$$T_n(t) = N_n(t)/N_1(0)$$

Passage is defined as the total removal rate in the considered trajectory or a fraction of the nuclides in a chain that passed beyond n nuclide and is assigned (or not) to following nuclides in the chain for the considered period.

$$P_n(t) = I_n(t)/N_1(0)$$

Transition and Pasage Function in trajectory



$P_1(t)$: A

=

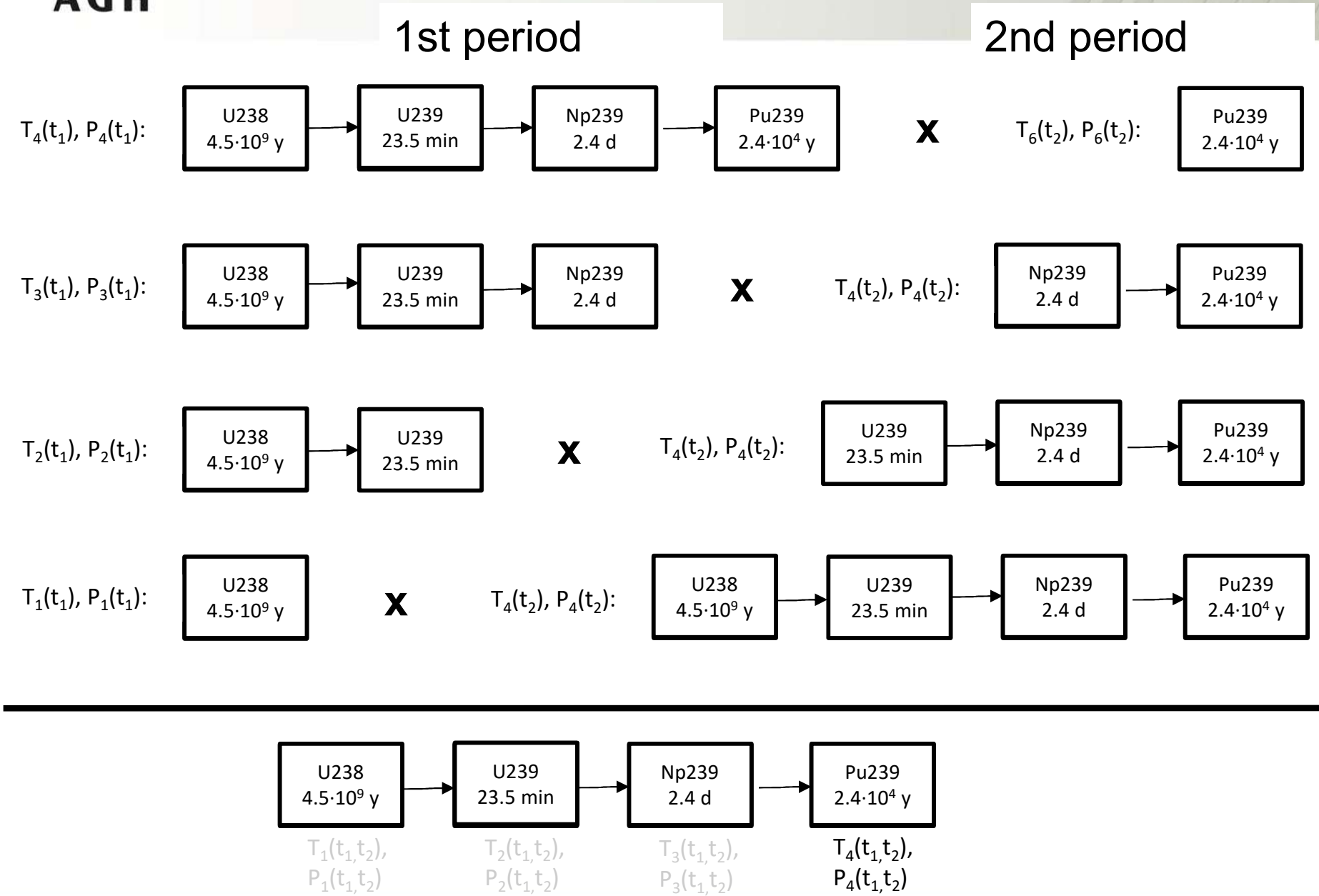
$T_2(t)$: A → B

$T_3(t)$: A → B → A

$T_6(t)$: A → B → A → B

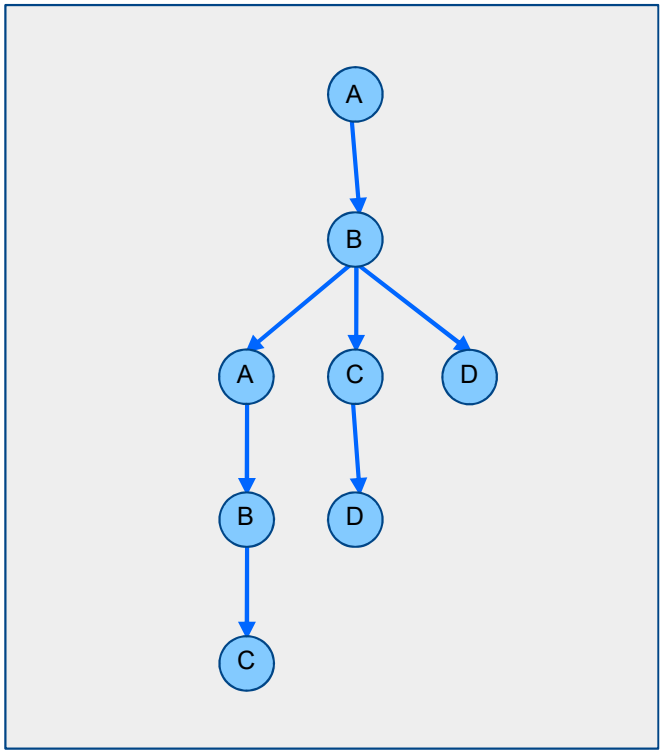
$T_8(t)$: A → B → A → B → C

The Trajectory Period Folding Method

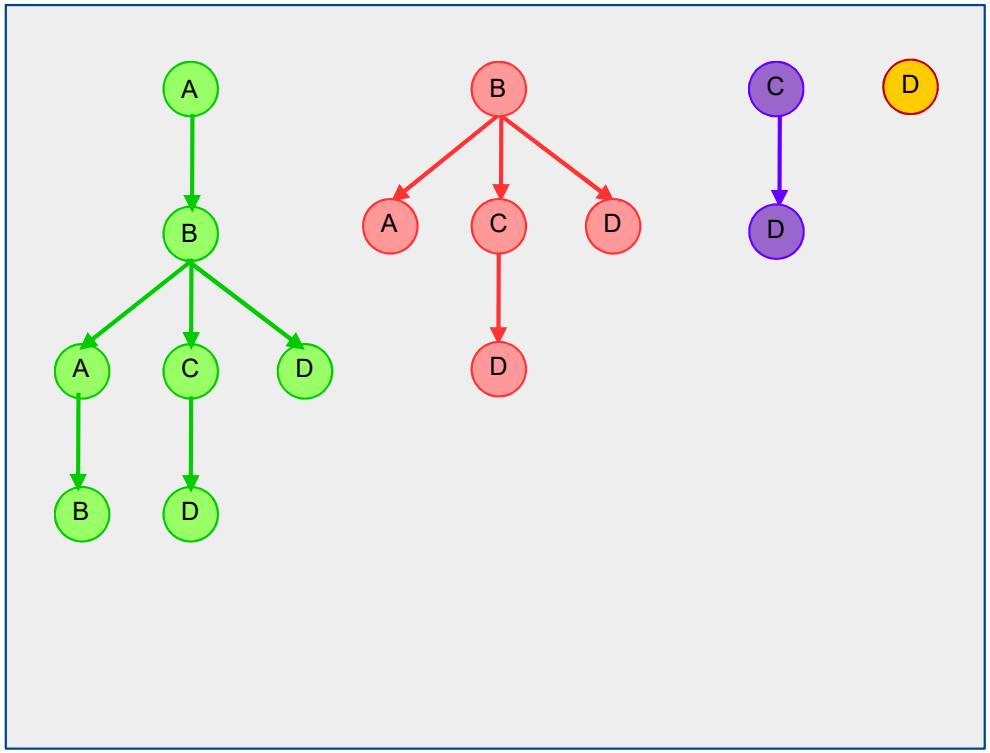


The Parent Pointer Tree Folding

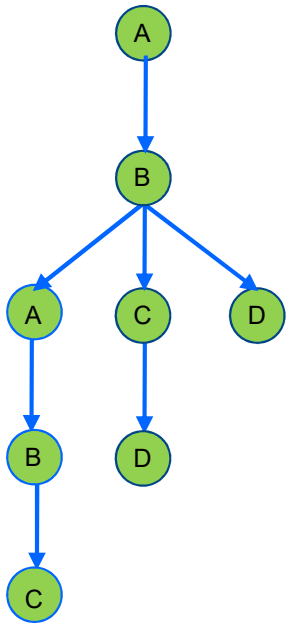
Period 1



Period 2



The Parent Pointer Tree Folding



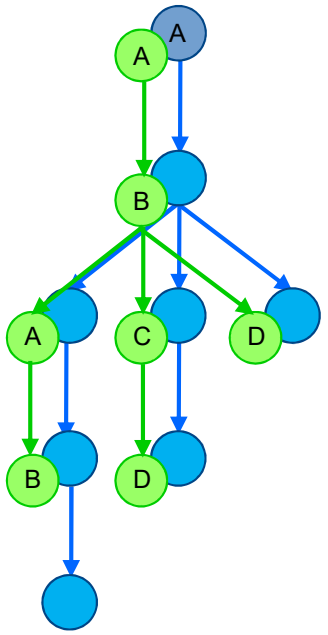
Folded trajectories

⇐ (1, A) * (1,A)

⇐ (1, A) * (2,B)

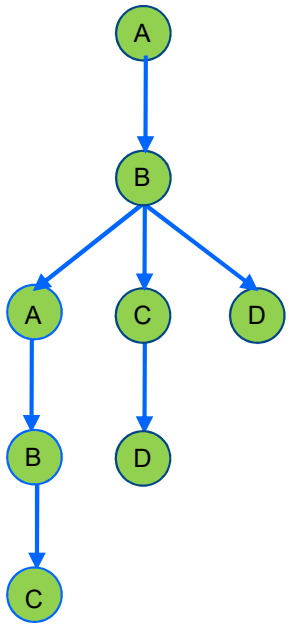
⇐ (1, A) * (3,A)
⇐ (1, A) * (4,C)
⇐ (1, A) * (5,D)

⇐ (1, A) * (6,B)
⇐ (1, A) * (7,D)



Trajectories at t_1 and t_2

The Parent Pointer Tree Folding

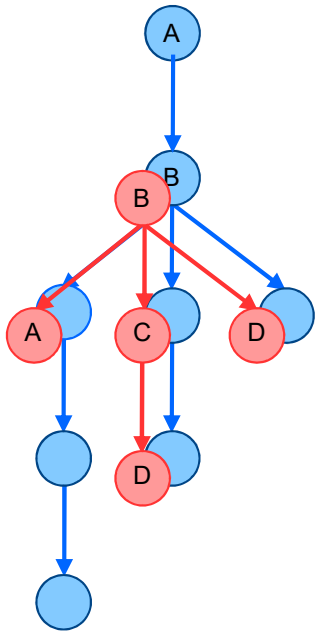


Folded trajectories

⇐ (2, B) * (1,B)

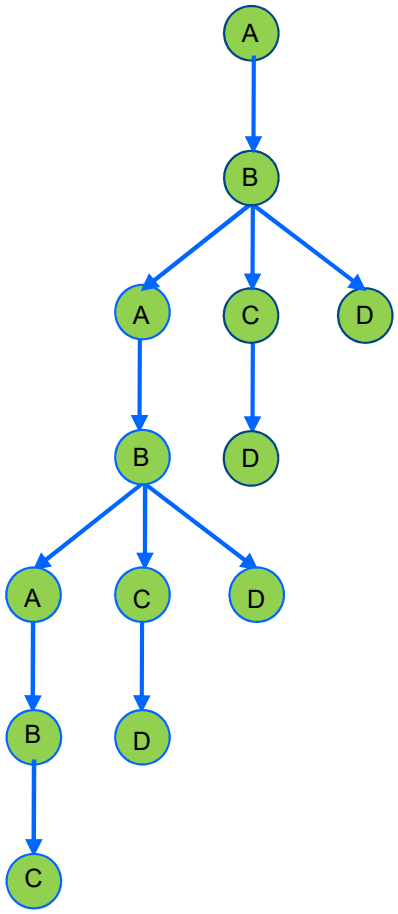
⇐ (2, B) * (2,A)
⇐ (2, B) * (3,C)
⇐ (2, B) * (4,D)

⇐ (2, B) * (5,D)



Trajectories at t_1 and t_2

The Parent Pointer Tree Folding



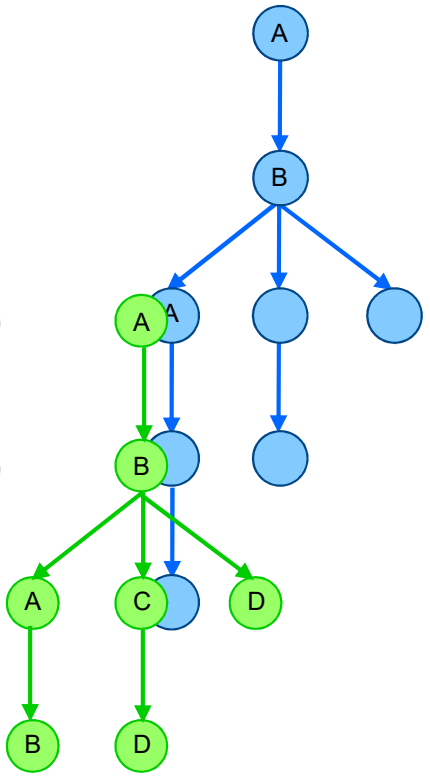
⇐ (3, A) * (1,A)

⇐ (3, A) * (2,B)

⇐ (3, A) * (3,A)
⇐ (3, A) * (4,C)
⇐ (3, A) * (5,D)

⇐ (3, A) * (6,B)
⇐ (3, A) * (7,D)

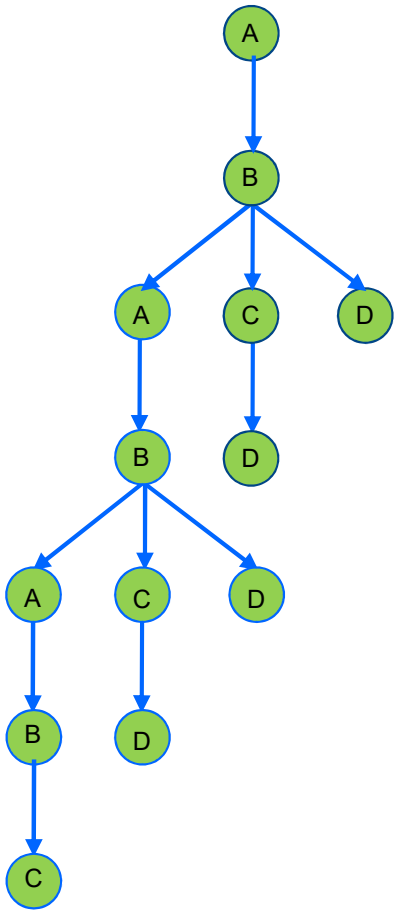
⇐ (3, A) * (8,C)



Folded trajectories

Trajectories at t_1 and t_2

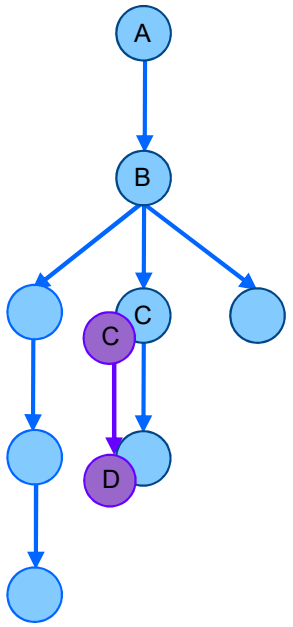
The Parent Pointer Tree Folding



Folded trajectories

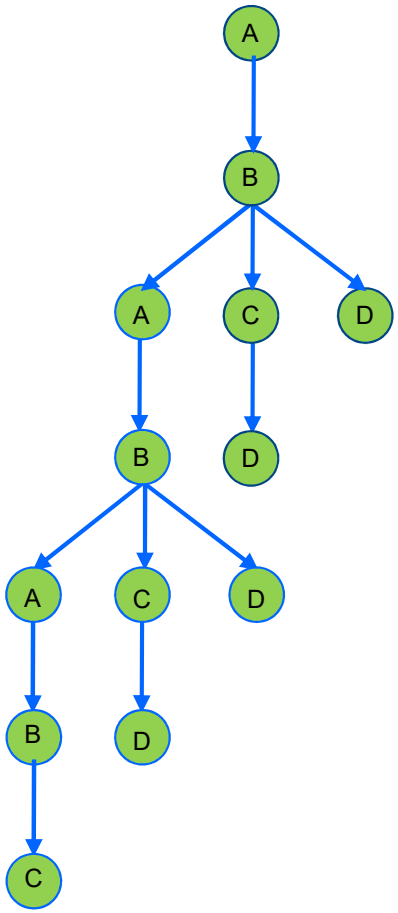
⇐ (4, C) * (1,C)

⇐ (4, C) * (2,D)

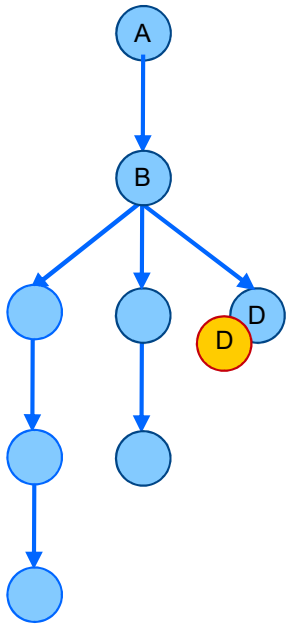


Trajectories at t_1 and t_2

The Parent Pointer Tree Folding



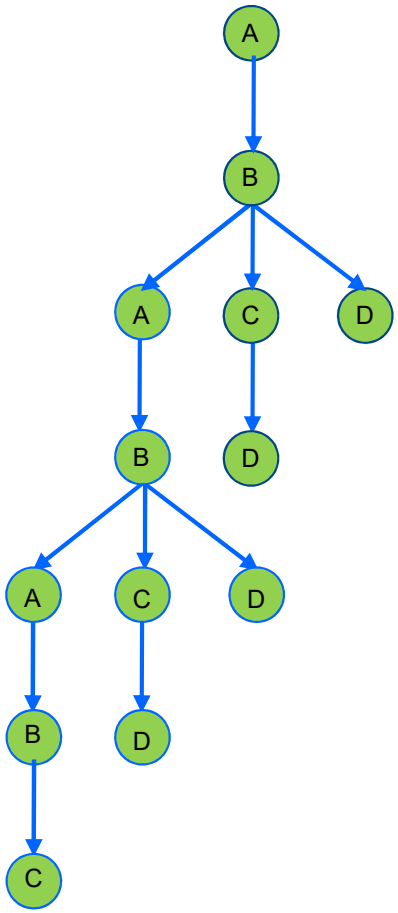
⇐ (5, D) * (1,D)



Folded trajectories

Trajectories at t_1 and t_2

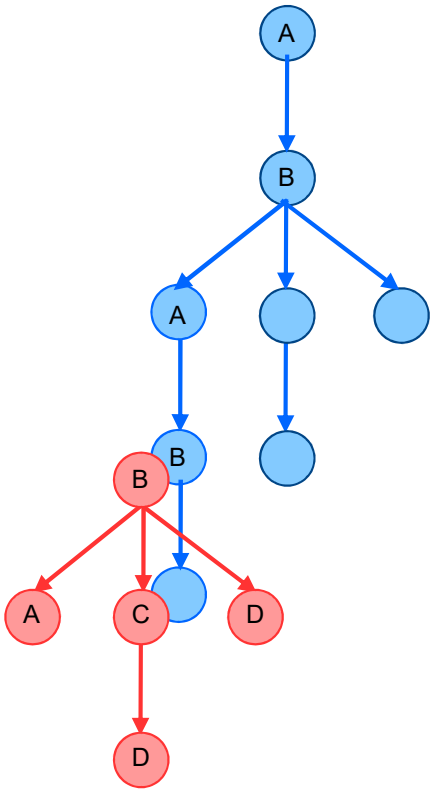
The Parent Pointer Tree Folding



⇐ (6, B) * (1,B)

⇐ (6, B) * (2,A)
⇐ (6, B) * (3,C)
⇐ (6, B) * (4,D)

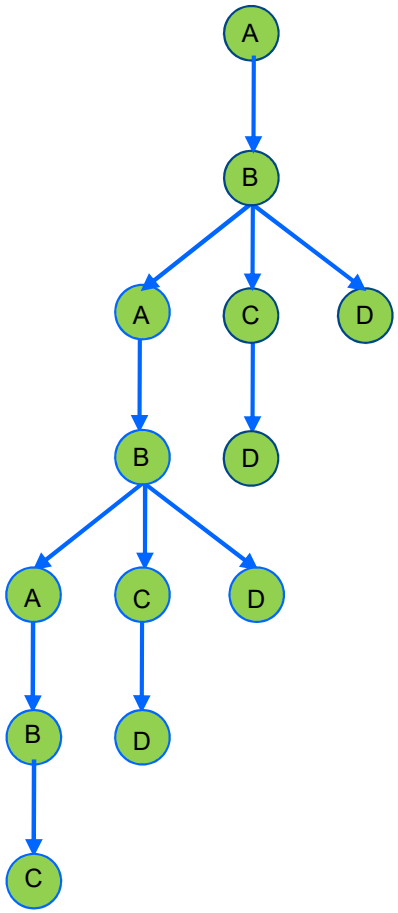
⇐ (6, B) * (5,D)



Folded trajectories

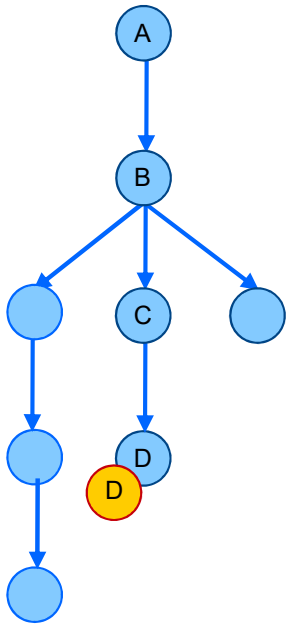
Trajectories at t_1 and t_2

The Parent Pointer Tree Folding



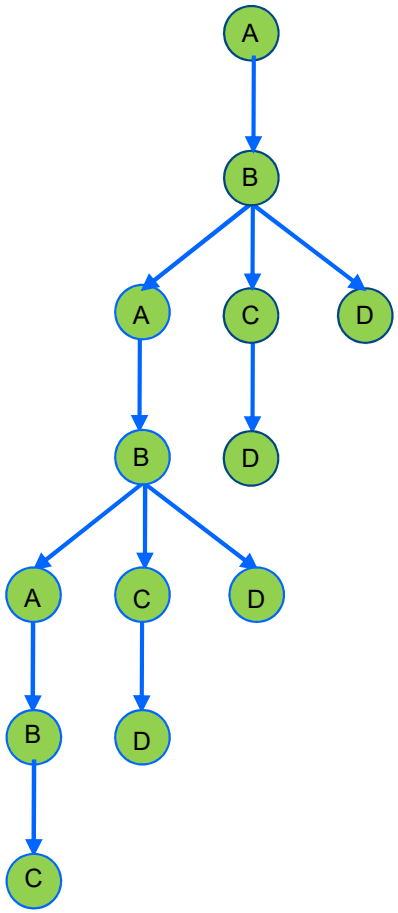
Folded trajectories

⇐ (7, D) * (1,D)



Trajectories at t_1 and t_2

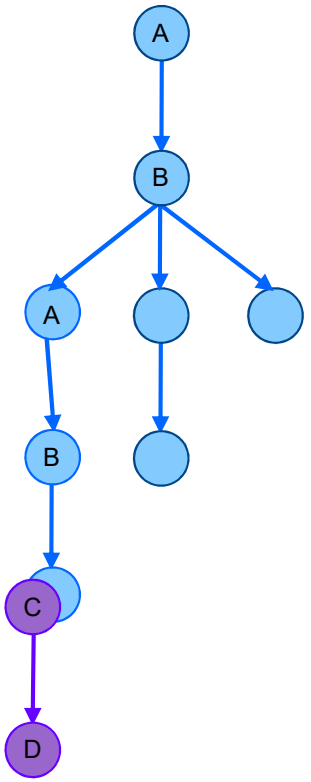
The Parent Pointer Tree Folding



Folded trajectories

⇐ (8, C) * (1,C)

⇐ (8, C) * (2,D)



Trajectories at t_1 and t_2

Applications in explainability

Folded trajectories have been applied in the folowing procedures:

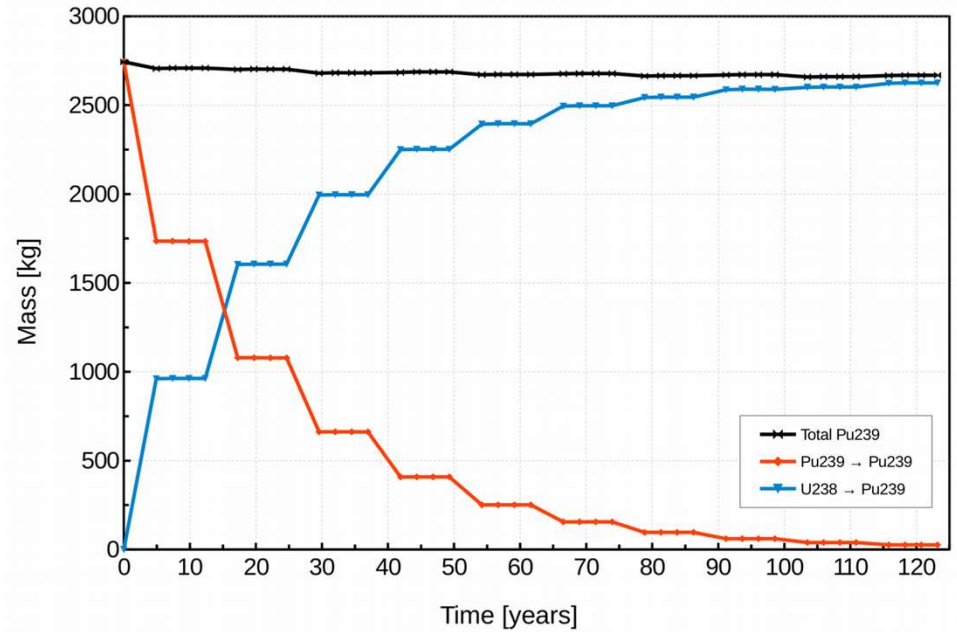
1) **The origin of the fuel.**
What amounts of final composition are formed from the initial nuclides;

2) **Trajectory evolution**
Which are the most common routes for transmutation over time;

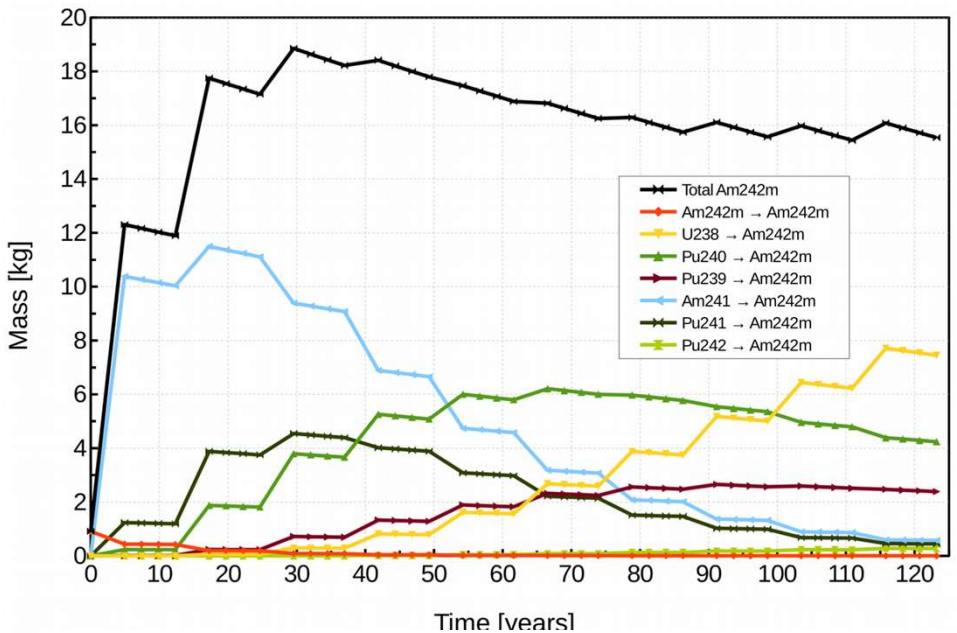
3) **The most frequent reactions**
Which trajectories are the most sensitive for the cross-sections;

The origin of the fuel

- the TTA folding time procedurę can be used to represent single nuclide evolution;
- the identification of key trajectories following to formation of transuranic elements is the crucial issues to understand formation mechanism of notably radioactive isotopes, which in turn may help to optimize handling of unloaded fuel before its reprocessing or final disposal;
- the developed numerical method of nuclear transmutation trajectories folding may be used for analysis of any critical or subcritical nuclear system during the arbitrary number of subsequent irradiation or cooling periods.



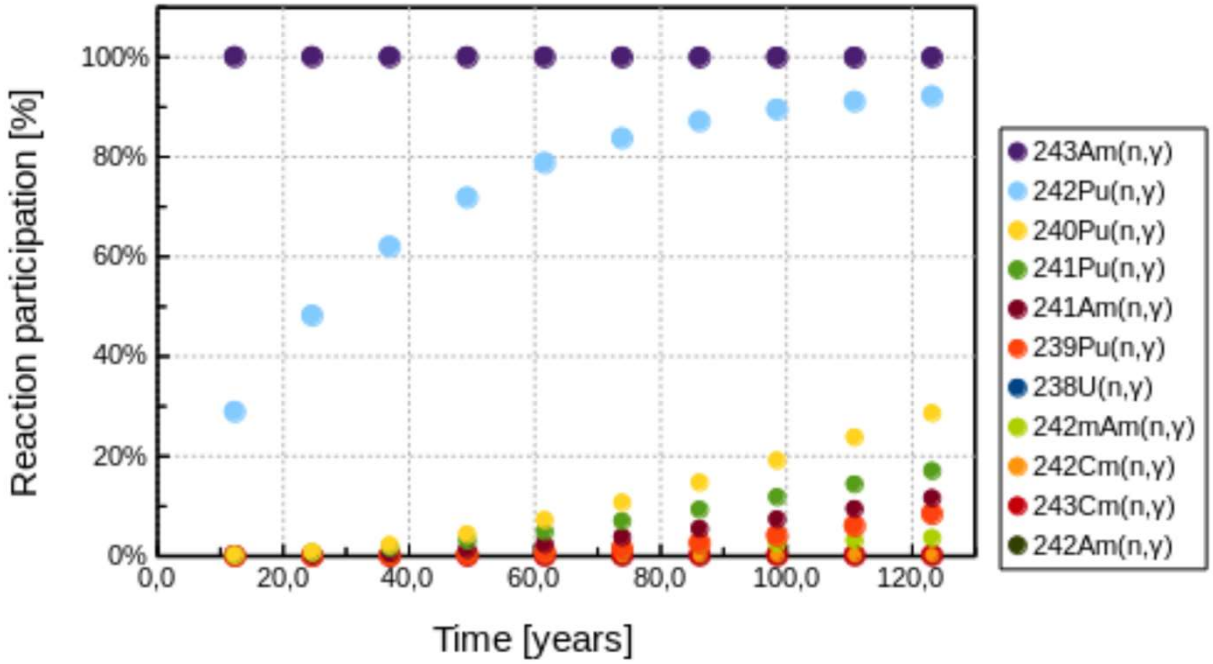
Batch mass flow of Pu239 with source distribution of the initial fuel



Batch mass flow of Am242m with source distribution of the initial fuel

The most frequent reactions

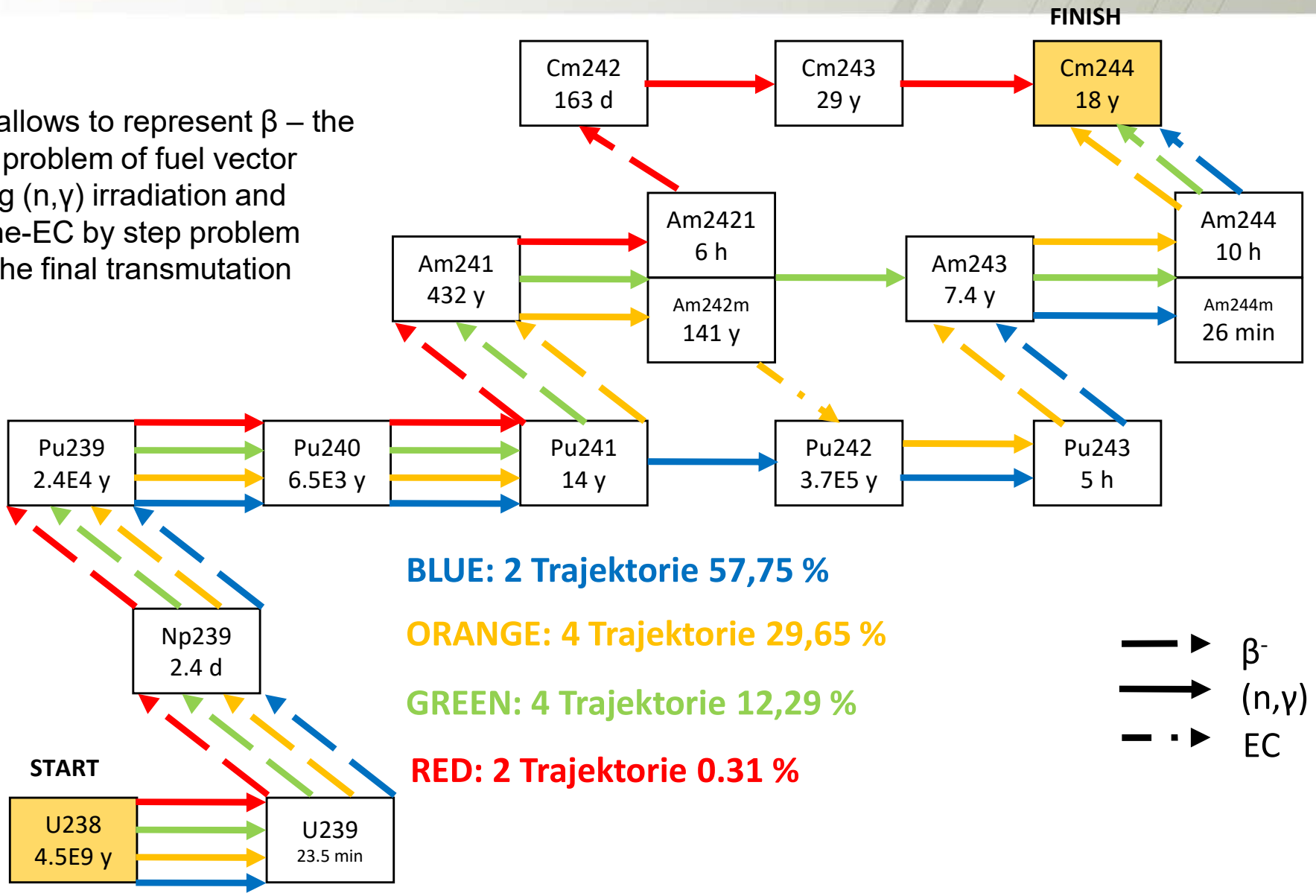
A set of period folded trajectories can be summed-up for those with the same reaction of interest. We can choose reaction which are the most important for production interested nuclides. Parametric sensitivity analysis could be the next step towards verification of nuclear data in production some rare, but crucial nuclides. Interesting reactions can be checked from the point of view of their influence on the transmutation dynamics. This analysis finally should indicate reaction with the highest influence.



The reactions taking part in Cm244 production

Trajectory evolution

The approach allows to represent β – the the multi-cycle problem of fuel vector evolution during (n,γ) irradiation and cooling as a one-EC by step problem characterized the final transmutation chain system.



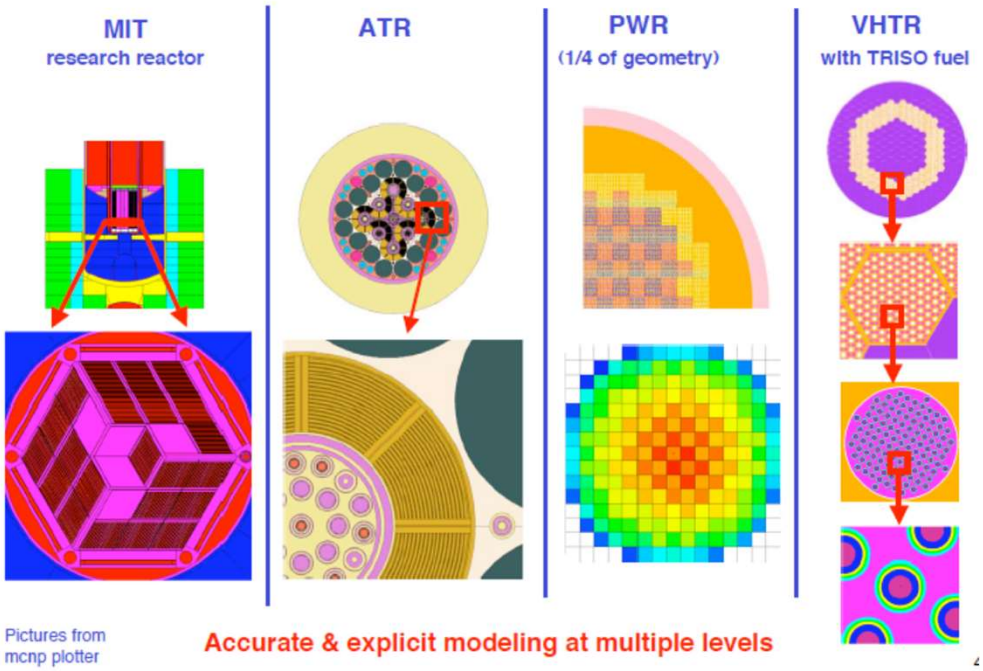
Thank You for Your Attention

Przemysław Stanisz
email: ps.stanisz@gmail.com

Podsumowanie

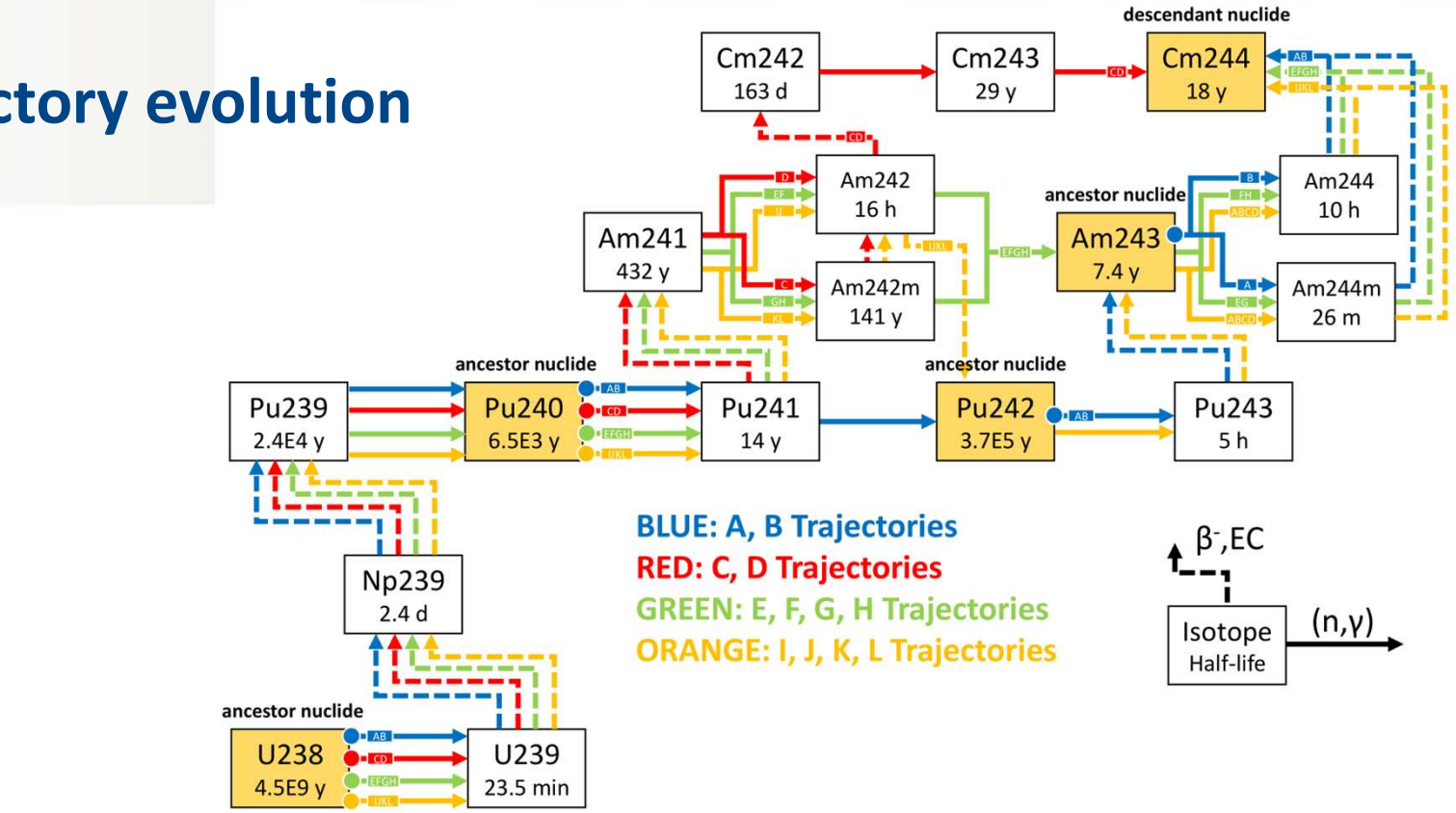
MCB The Monte Carlo Continuous Energy Burn-up Code

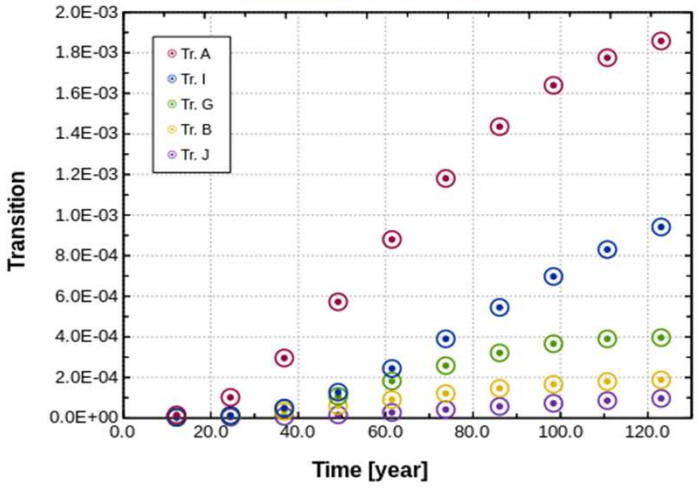
- Metody Monte Carlo są wykorzystywane i rozwijane prze Katedrę Energetyki Jądrowej na klastrze obliczeniowym Promehteus;
- Obliczenia na klastrze dla nowych urzytkowników są dostępne w ramach usługi: **Energetyka Jądrowa i CFD: MCB - System Monte Carlo do obliczeń wywołanych promieniowaniem jądrowym zmiany w materii;**
- Rozwój superkomputerów pozwala na stosowania metod Monte Carlo w analizie całych rdzeni jądrowych;
- Jest to metoda alternatywan do metod deterministycznych w wykorzystaniu badań związanymi z zagadnieniami reaktorów jądrowych;
- Wyniki otrzymywane za pomocą losowo generowanych zdażeń;
- Wyniki zbierane w kontrolnych obiętościach/płaszczyznach (Tallie).

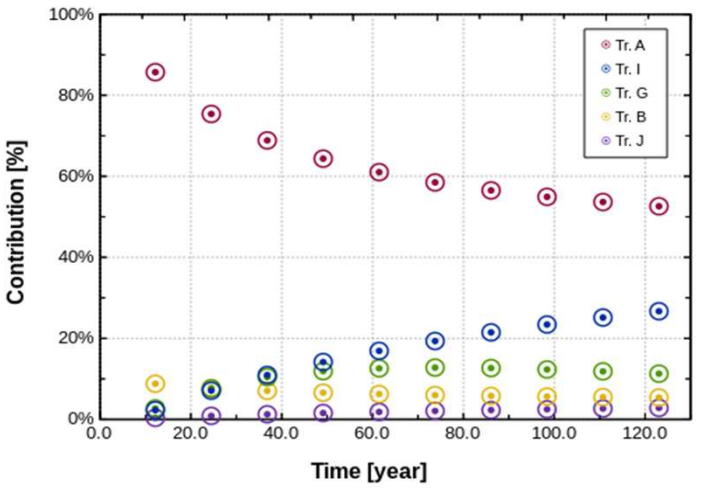


Trajectory evolution

In the proposed methodology, the mass flow of direct nuclide-to-nuclide transitions leading to nuclide transmutation chains in every step is interpreted over entire period of interest. In this way, all quantitative information about the Transmutation process for the period beyond single calculation step is preserved. The method builds sets of transmutation trajectories prepared for each computing time step and then combines them in the process of time period folding. Resulted period folded trajectories are interpreted as they would be obtained by the set of parameters from one calculation step.

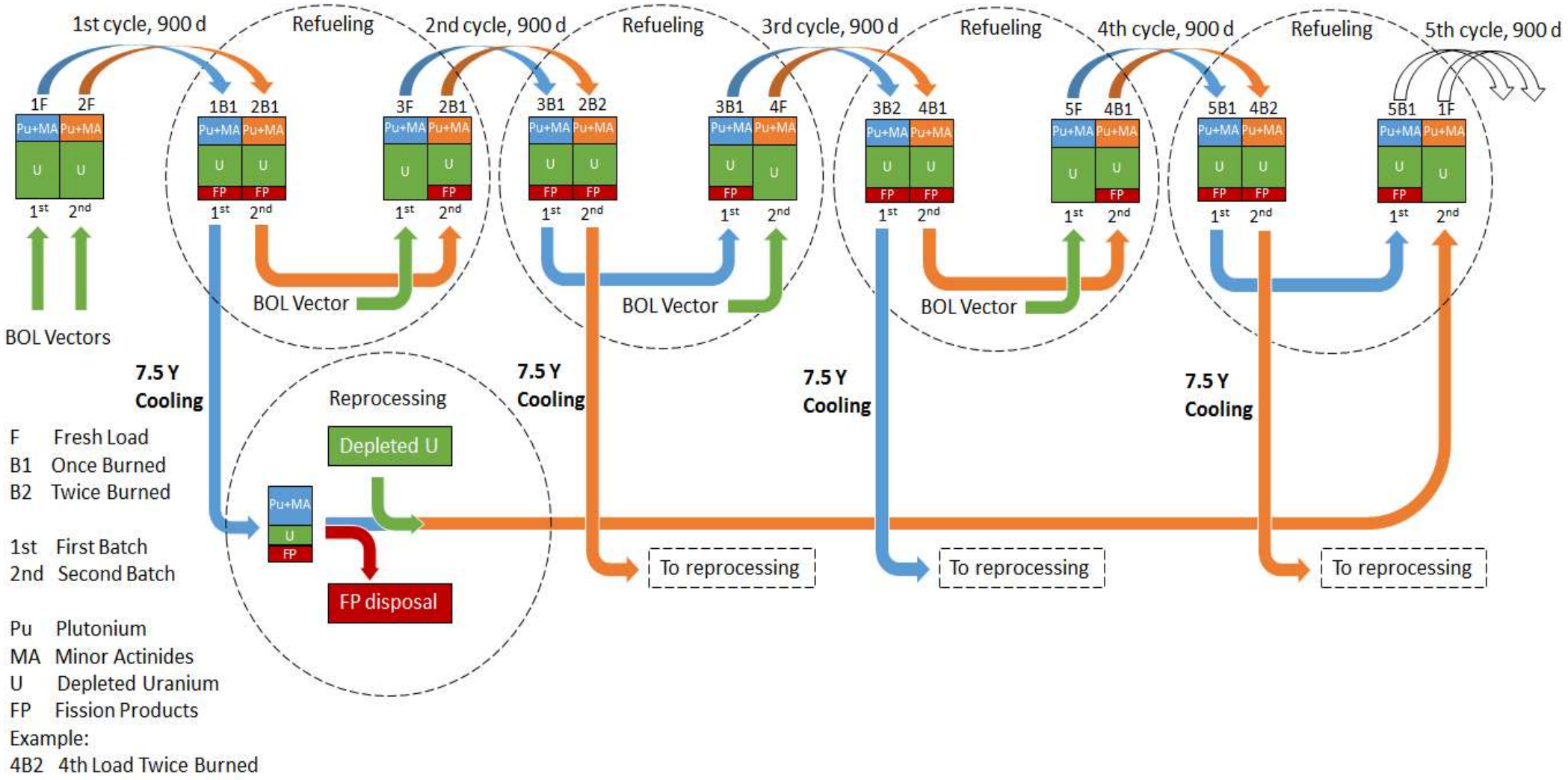






Transition value evolution for trajectories from 240Pu to 244Cm and their contribution in the transition value from 240Pu to 244Cm

The Modelling of Adiabatic Fuel Cycle



Krytyczność

$$k = \frac{\text{number of neutrons in one generation}}{\text{number of neutrons in preceding generation}}$$

$$\rho = \frac{K_{eff} - 1}{K_{eff}}$$

K_{eff}<1 układ podkrytyczny
K_{eff}=1 układ krytyczny
K_{eff}>1 układ nadkrytyczny

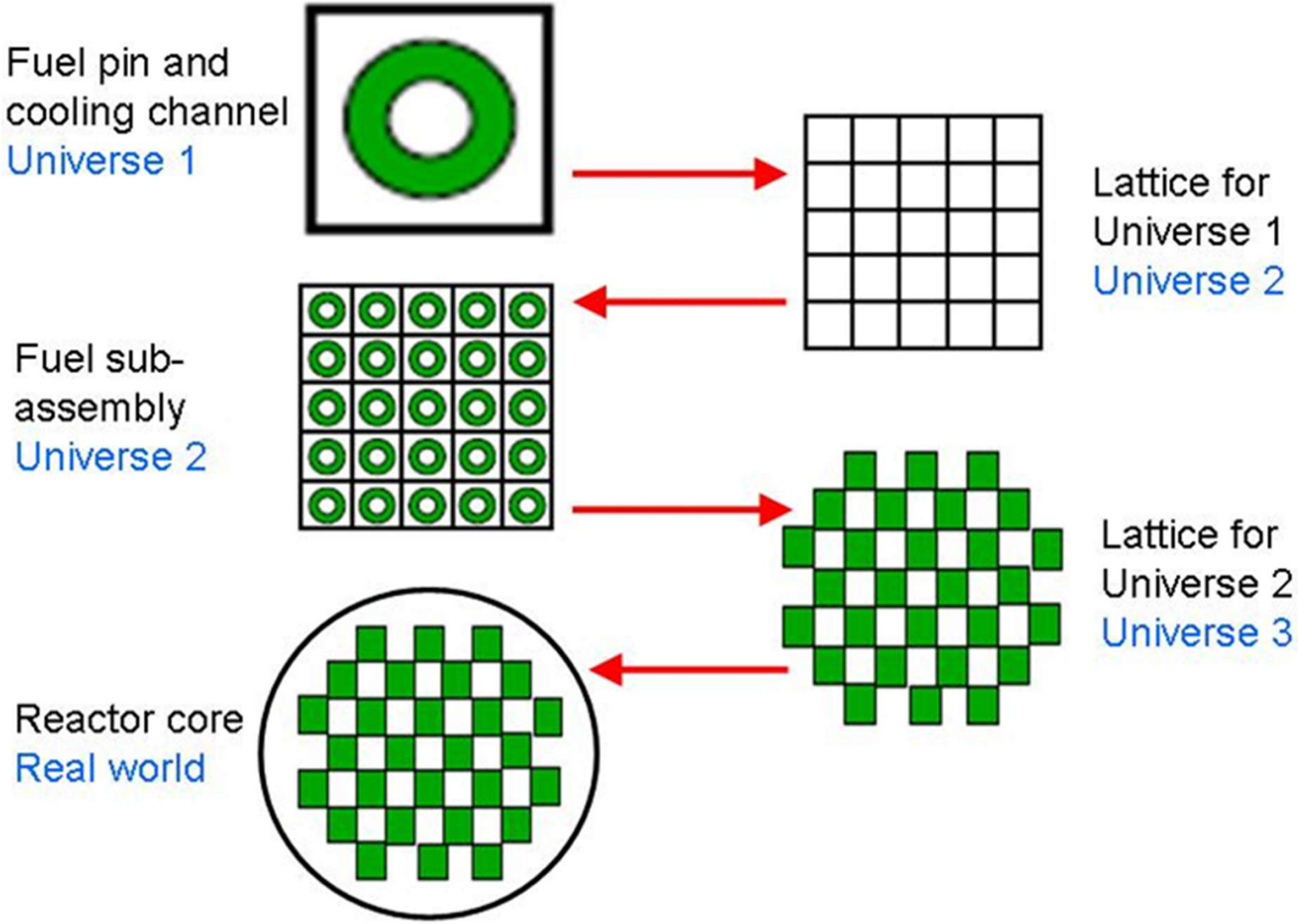
ρ<0 układ podkrytyczny
ρ =0 układ krytyczny
ρ >0 układ nadkrytyczny

K_{eff}

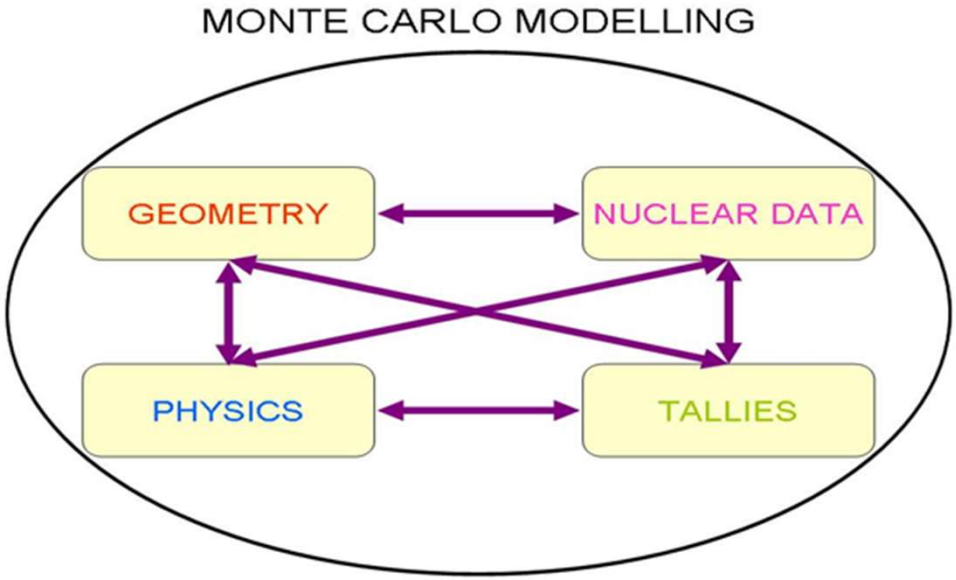
$$(L+C-S)\psi\left(\vec{r},E,\vec{\Omega}\right)=\frac{1}{K_{eff}}M\psi\left(\vec{r},E,\vec{\Omega}\right) \quad \Rightarrow \quad K_{eff}=\frac{M\psi\left(\vec{r},E,\vec{\Omega}\right)}{(L+C-S)\psi\left(\vec{r},E,\vec{\Omega}\right)}$$

- leakage operator L,
- collision operator C,
- scatter-in operator S,
- fission multiplication operator M.

Geometria


Fuel pin and
cooling channel
Universe 1
Lattice for
Universe 1
Universe 2
Fuel sub-
assembly
Universe 2
Lattice for
Universe 2
Universe 3
Reactor core
Real world

Monte Carlo



W symulacjach Monte Carlo

1. Losowa wartośc jest wybierana dla każdego zdażenia z przygotowanych zakresow estymatorow

2. Model jest obliczany bazujac na jego losowej wartosci

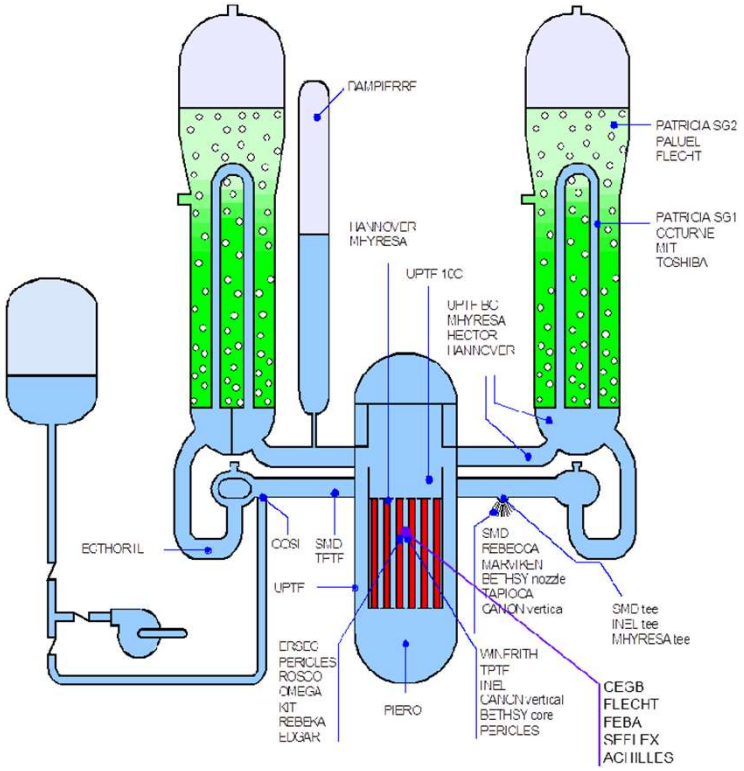
3. Resultaty modelu sa zapisywane I proces jest powtarzany

Typowe obliczenia transportu Monte Carlo obliczaniją model tysiące razy za każdym razem używając innej wartości losowej

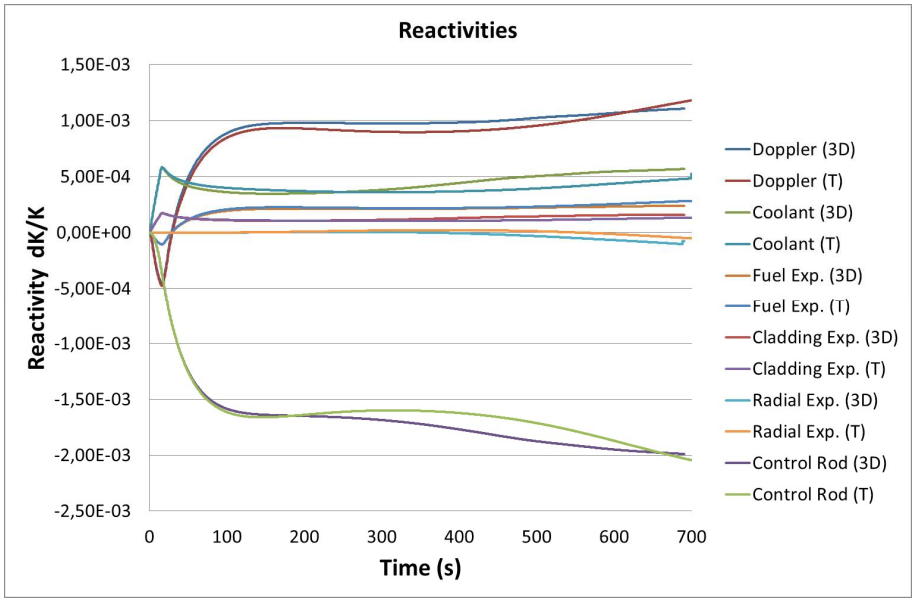
Całe obliczenia tworzą dużą baze rezultatow

Rezultaty są wykorzystywane do opisu symulowanego modelu.

Symulacje obiegów jądrowych

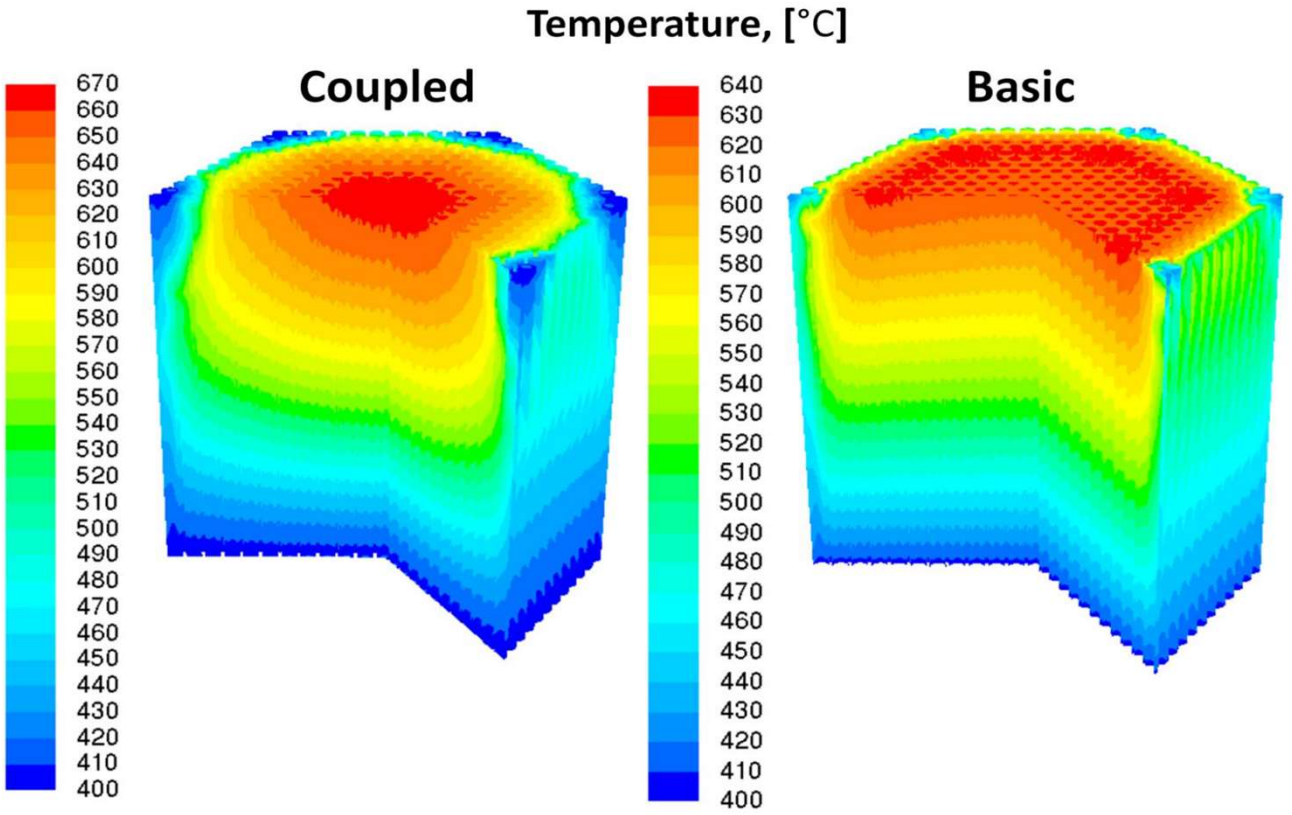


Obieg pierwotny reaktora typu PWR



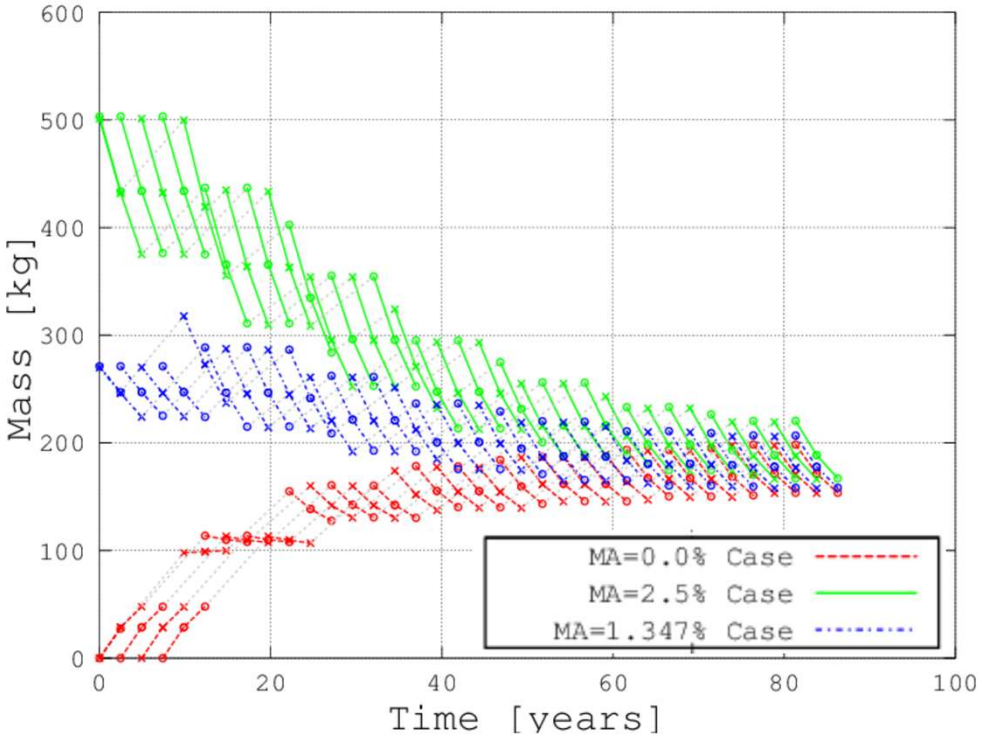
Reaktywności układu dla modelu 1D i 3D

Metoda elementów skończonych

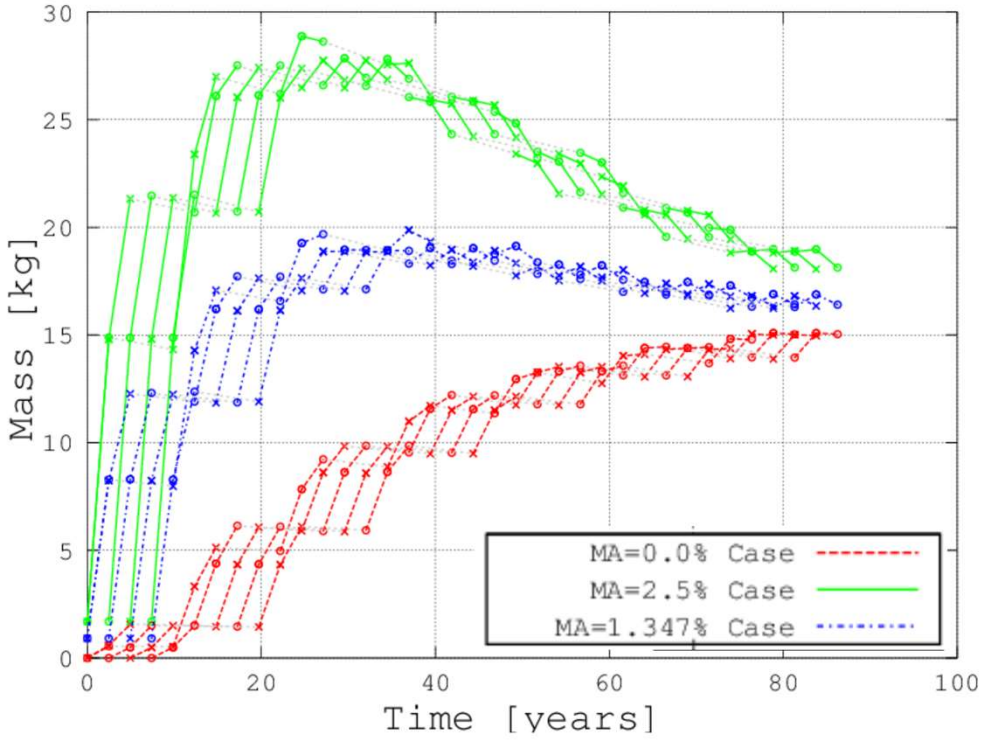


Rozkład temperatury w paliwie

The Fuel Evolution

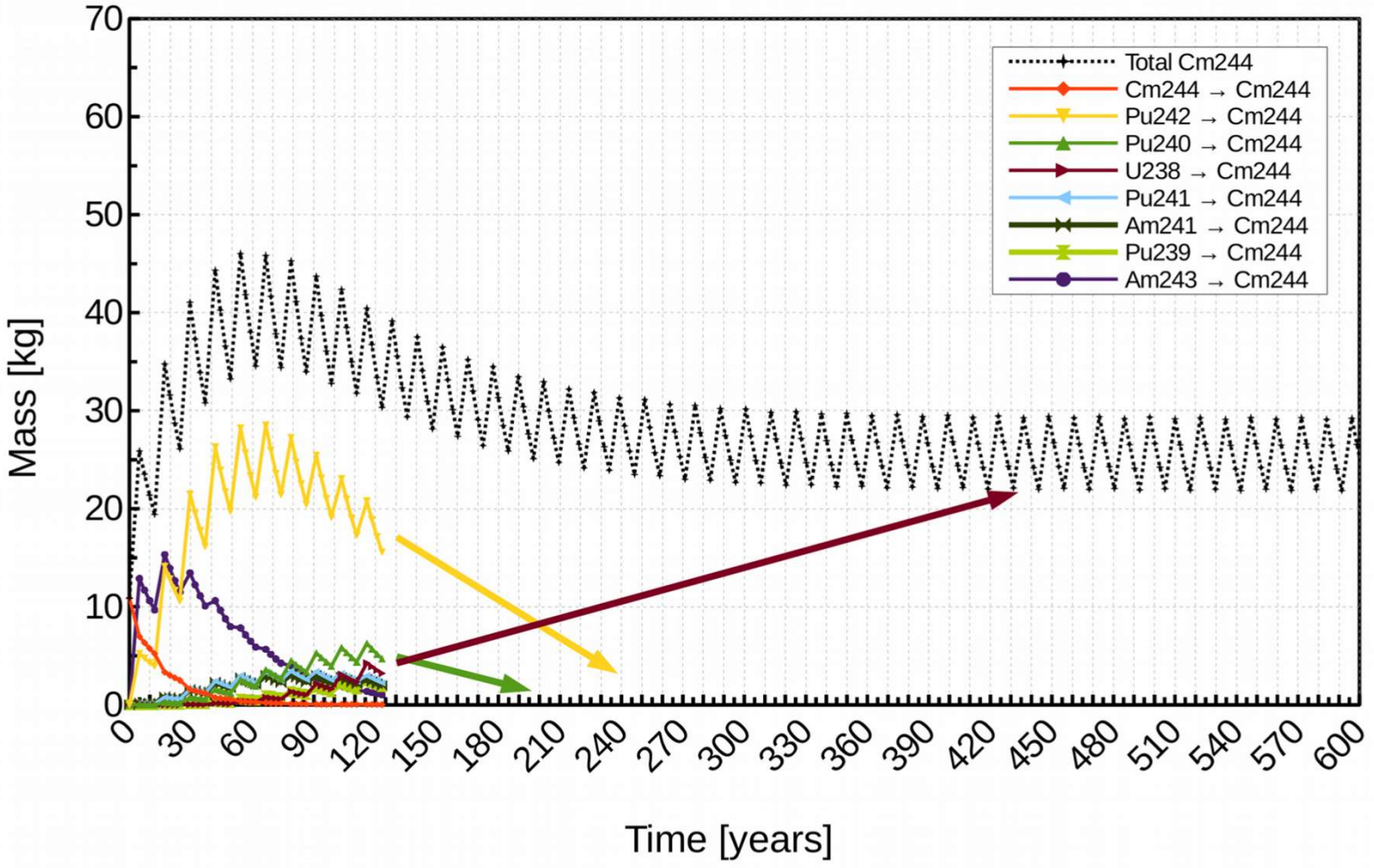


Mass flow of Am241 for one of the three cases fuel strategy option



Mass flow of Am242m r one of the three cases fuel strategy option

The origin of the fuel



Batch mass flow of Cm244 with source distribution of the initial fuel

Wariance Reduction: Weight window technique

Similar to geometry spliting.

Jeżeli urodzi się neutron z rozszczepienia to będzie miał przypisaną wagę 1

Ale okno jest 0.01 – 0.05 znaczy to że neutron będzie musiał być rozbity na 20 neutronów i każdy będzie miał w/20

This method has great potential,
but is more difficult to use.