# Introduction to Monte Carlo simulations of neutron transport in nuclear reactors

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# Outline

# Introduction

# What is the Monte Carlo method?

## What is the Monte Carlo method?

The Monte Carlo method is a way of solving a deterministic problem by a stochastic approach using random numbers.

A number $n$ of independent observations (e.g. neutron histories) are collected. The result is derived from the averaged observation.

The Monte Carlo method is commonly applied on deterministic problems that are **difficult** to solve by deterministic methods.

## Methodological position

| | | Type of the problem | |
|---|---|---|---|
| | | deterministic | stochastic |
| solution method | deterministic | numerical analysis | probability theory |
| | stochastic | **Monte Carlo** | simulation |

# General advantages and disadvantages of the MC method

## General advantages

- Complex problems can be solved without simplifications.
- Precision of the results can be improved simply by running the simulation longer (making more observations).
- Governing equations do not need to be formulated for the quantities of interest.

## General advantages

- Large computing cost to achieve a good precision of some results.
- Statistical uncertainty in the results.

# Specific advantages and disadvantages of the MC method in reactor physics

## Specific advantages

- Geometry of the nuclear reactor does not need to discretised and homogenised, as in case of deterministic methods.
- Microscopic neutron cross sections and other data can be treated with an accurate dependence on neutron energy.
- A single MC criticality code can simulate a great variety of nuclear reactors.

## Specific disadvantages

- Quantities with spatial dependence (local power or flux) are hard to compute.
- Acceleration methods common in deterministic calculations ineffective due to presence of the random noise.

# Major components of the Monte Carlo method

- Probability distribution function (pdf's) that describe the system
- Random number generator
- Sampling rules
- Scoring (tallying) the outcomes
- Error estimation
- Variance reduction techniques

# Application

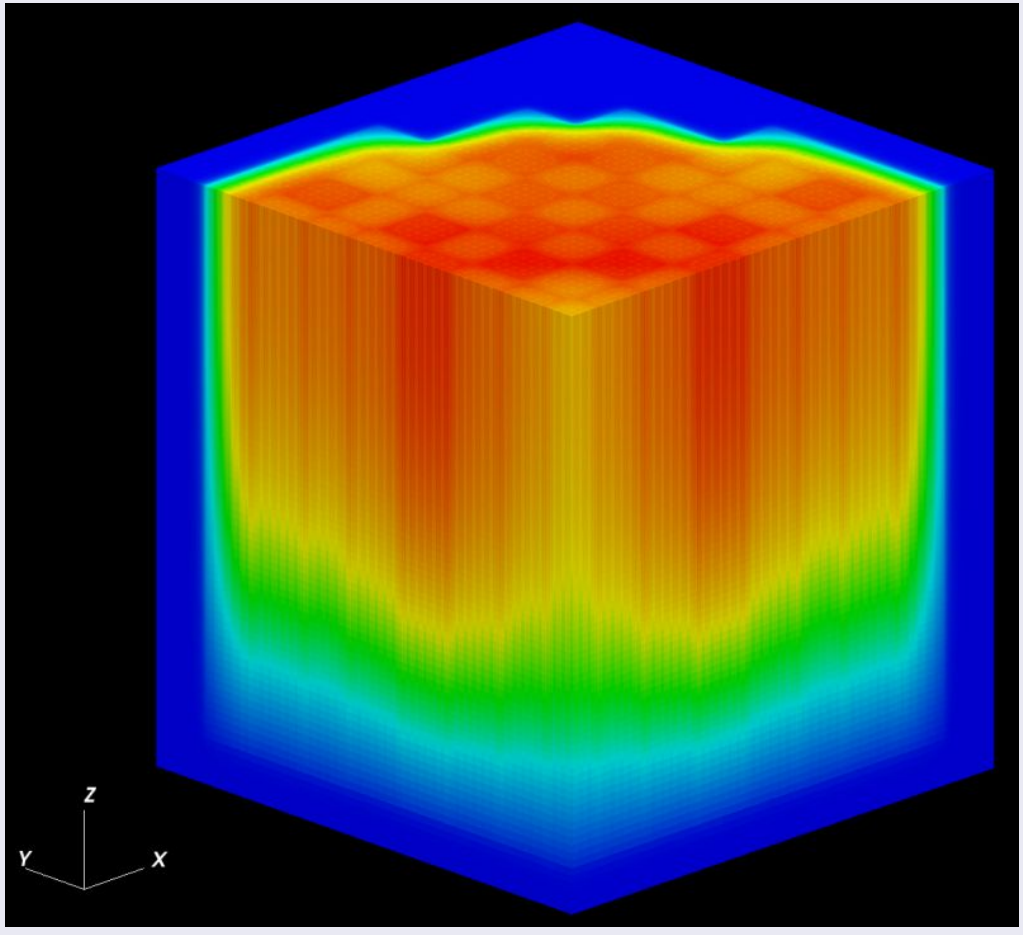
## Application in nuclear engineering

- Benchmarking of deterministic codes
- R&D of new reactors
- Computation of quantities in complex shielding and criticality problems (mainly in research), such as:
  - multiplication factor
  - neutron flux
  - reaction rates, group cross sections, etc.

## Major Monte Carlo codes for reactor physics

- MCNP - Monte Carlo N-Particle Transport Code (Los Alamos National Laboratory, USA)
- TRIPOLI (CEA, France)
- KENO (Oak Ridge National Laboratory, USA)
- SERPENT (VTT, Finland)

# Basic principles of analog simulation of MC neutron transport



# Principles of analog simulation of MC neutron transport

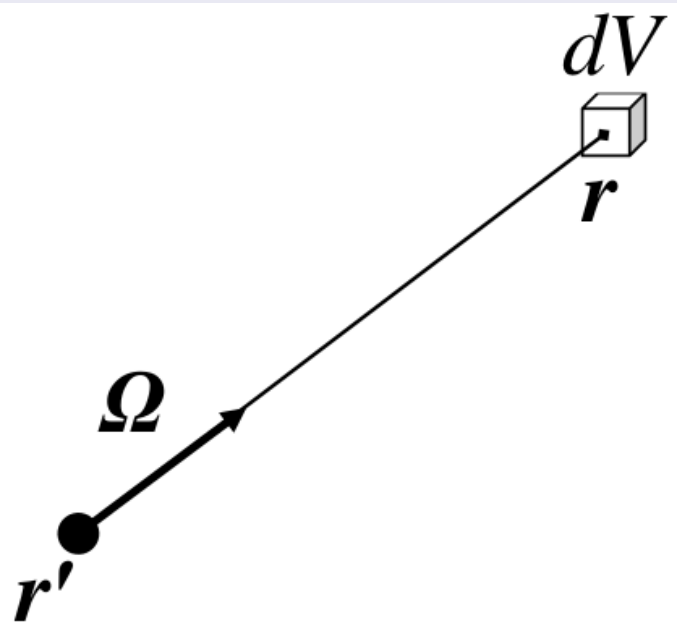
## Analog simulation of MC neutron transport

- In analog Monte Carlo simulation, neutrons are simulated from "birth" (originating from the source) to "death" (absorption or leakage from the system).
- The birth-to-death simulation is called a neutron "history".
- The average behaviour of neutrons is estimated via simulating of a large number of neutron histories.

# Quantities in analog simulation of MC neutron transport

## Transition kernel

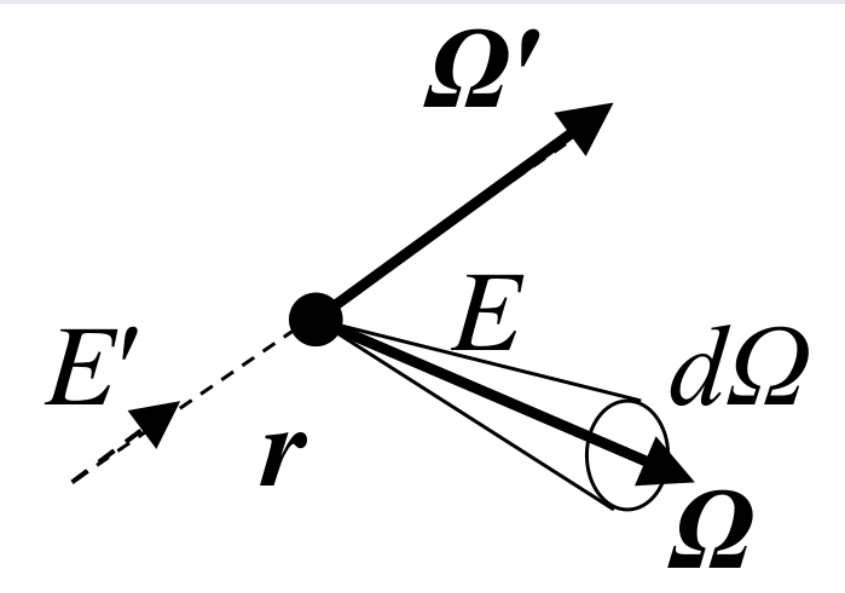
$T(\vec{r}' \rightarrow \vec{r}, E, \vec{\Omega})dV =$ probability for a neutron starting at $\vec{r}'$ with energy $E$ and direction $\vec{\Omega}$ to have its next collision in $dV$ at $r$.



# Quantities in analog simulation of MC neutron transport

## Collision kernel

$C(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega}) dE d\Omega =$ probability for a neutron entering a collision at $\vec{r}$ with energy $E'$ and direction $\vec{\Omega}'$ to exit the collision with energy $E$ in $dE$ and direction $\vec{\Omega}$ in $d\Omega$.



# Sampling neutron histories

## If we can sample

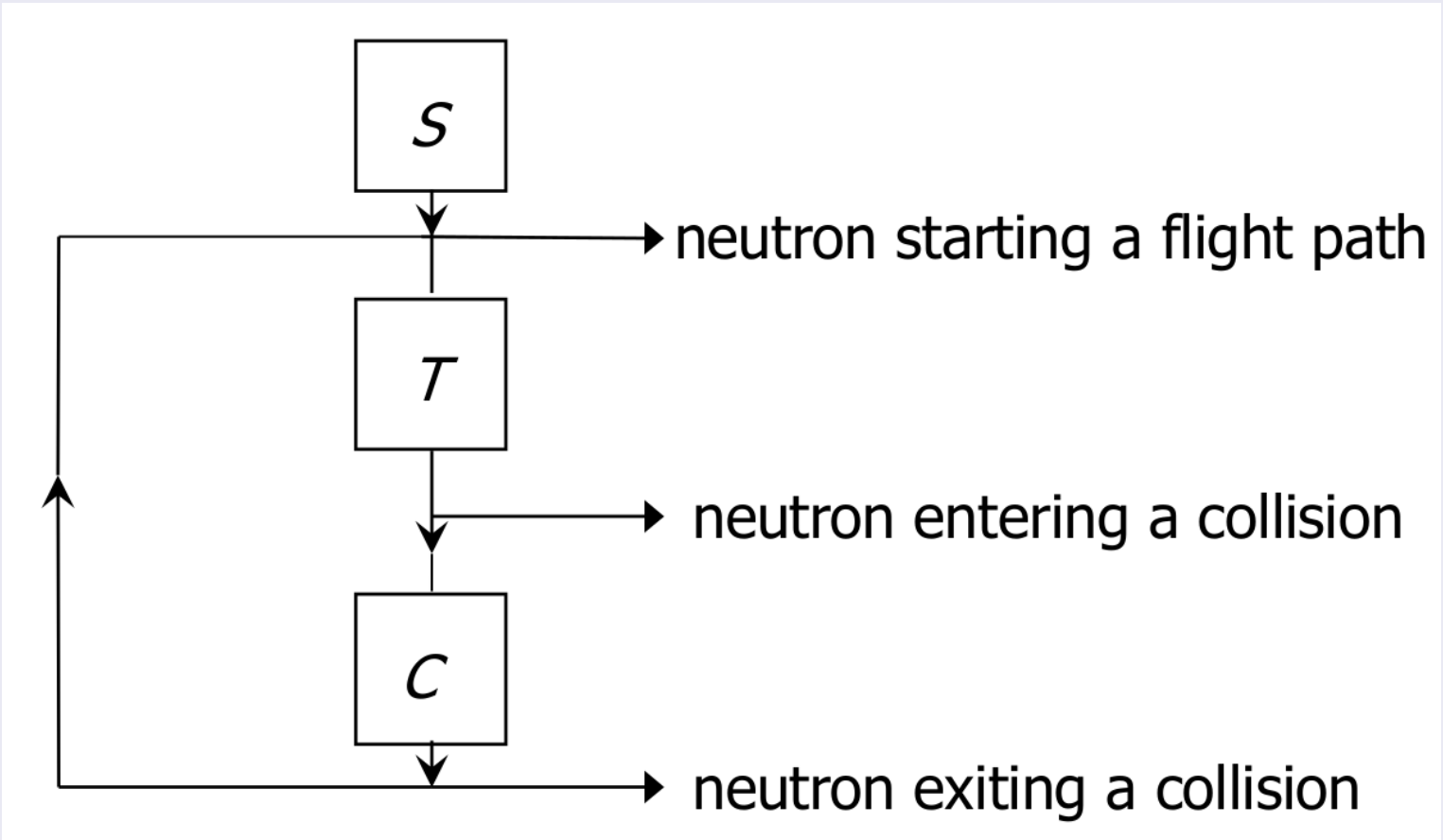
- the source $S$, (i.e. $r, \vec{\Omega}$ and $E$)
- the transition kernel $T$, (i.e. $\vec{r}$, given $\vec{r}'$, $\vec{\Omega}$ and $E$)
- the collision kernel $C$, (i.e. $\vec{\Omega}$ and $E$, given $\vec{r}$, $\vec{\Omega}'$ and $E'$)

## then

we are solving a neutron transport problem without even deriving the transport equation!

# Schematic representation

## Schematic representation



# Sampling the source $S(\vec{r}, E, \vec{\Omega})$

## Sampling $S(\vec{r}, E, \vec{\Omega})$

- sample position $\vec{r}$ (known for fixed source problems)
- sample direction $\vec{\Omega}$ (often isotropic)
- sample energy $E$
  (e.g. Watt fission spectrum $f_S(E) = Ce^{-aE}\sinh(\sqrt{bE})$)

# Sampling the transition kernel

## Transition kernel

$$T(\vec{r}' \rightarrow \vec{r}, E, \vec{\Omega})dV = \Sigma_t(\vec{r}, E)e^{-\Sigma_t s}ds$$

where:

- $s = |\vec{r} - \vec{r}'|$, i.e. $\vec{r} = \vec{r}' + s\vec{\Omega}$
- $\Sigma_t(\vec{r}, E) = \sum_i N_i \sigma_{t,i}(\vec{r}, E)$ is the total macroscopic cross section of a material, where
- $N_i$ is atomic density of $i-$th isotope in the material
- $\sigma_{t,i}$ is the total microscopic cross section of $i-$th isotope

# Sampling the transition kernel

## Sampling the transition kernel

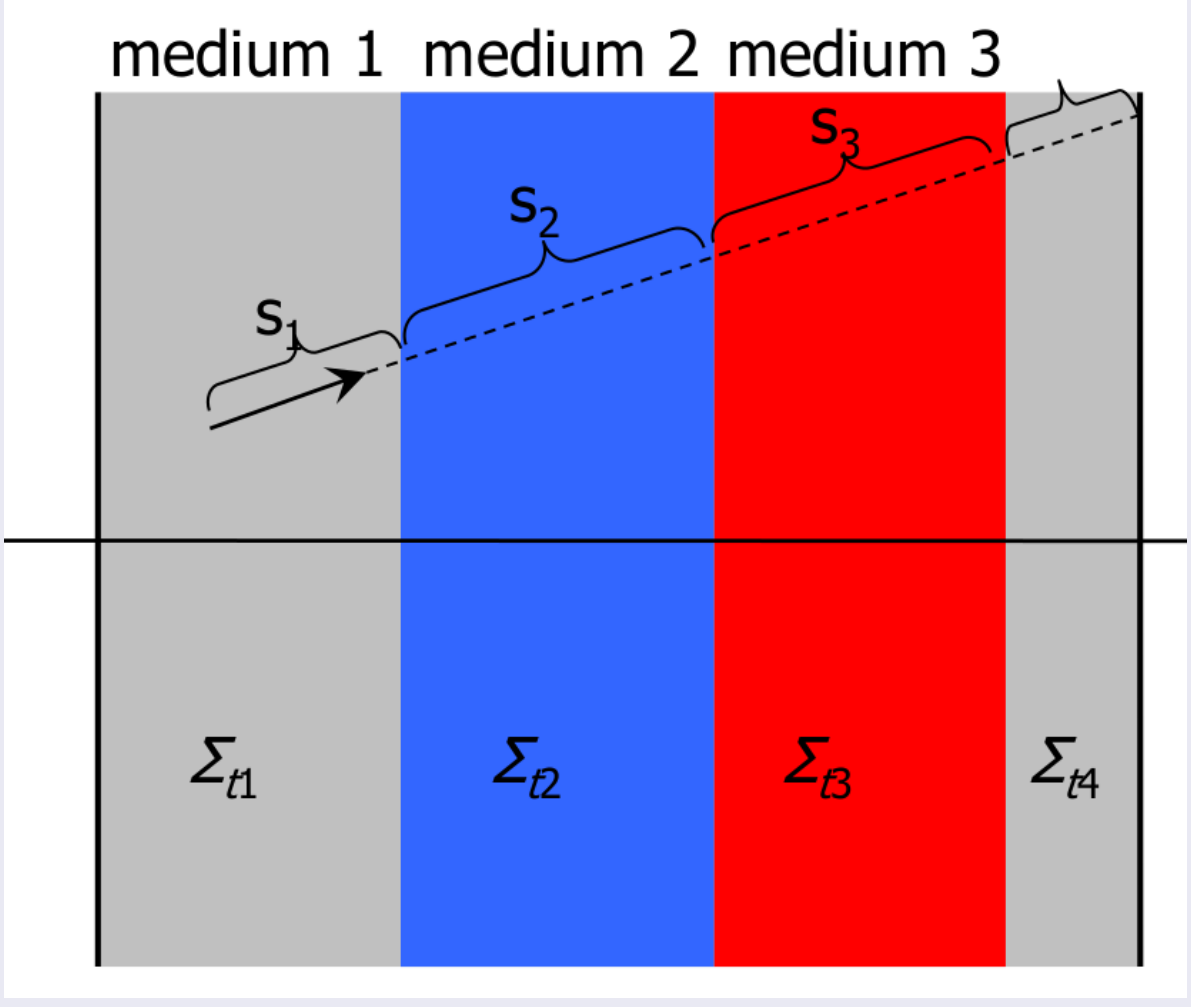
- The transition kernel $T$ is the pdf $f_s$ for the distance $s$.
- We can sample $s$ by the inverse method if we know the cdf function $F_s$.
- $F_s = \int_0^s \Sigma_t(\vec{r}, E) e^{-\Sigma_t s'} ds' = 1 - e^{-\Sigma_t s}$

## Sampling the distance $s$

- Generate random number $u$ from (0,1)
- Solve $u = 1 - e^{-\Sigma_t s}$ for $s$.
- $\Rightarrow s = -\frac{1}{\Sigma_t} \ln(1-u)$
- You can also use $s = -\frac{1}{\Sigma_t} \ln(u)$

# Sampling the transition kernel

## How to sample $s$ in inhomogeneous media?



# Sampling the transition kernel

## How to sample $s$ in inhomogeneous media?

Neutron has no memory, so once a neutron has reached an interface, start a new flight path.

## Algorithm

Select $s$ as $s = -\frac{1}{\Sigma_{t1}} \ln(u_1)$

- if $s < s_1$ then the collision point was found
- if $s \geq s_1$ then position neutron at interface boundary and select a new flight path as $s = -\frac{1}{\Sigma_{t2}} \ln(u_2)$

## Note

Tracking the distances to the boundaries may be difficult in complex geometries...

# Sampling the collision kernel

## Collision kernel

$$C(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega}) = \sum_i \sum_j \frac{\Sigma_{ji}(\vec{r}, E')}{\Sigma_t(\vec{r}, E')} p_{i,j}(E' \to E, \vec{\Omega}' \to \vec{\Omega})$$

where:

- $i$ sums over the isotopes
- $j$ sums over the reaction types (elastic, inelastic, (n,2n), ...)
- $p_{i,j}$ conditional probability for changing $\vec{\Omega}$ and $E$ knowing $j$-th reaction occurred on $i$-th isotope

# Sampling the collision kernel

## Sampling procedure

- select $i$-th nuclide with probability $p(i) = \frac{\Sigma_{ti}(\vec{r},E')}{\Sigma_t(\vec{r},E')}$
- select reaction type $j$ with probability $p(j|i) = \frac{\Sigma_{j,i}(\vec{r},E')}{\Sigma_{t,i}(\vec{r},E')}$
- select energy $E$ and direction from $p_{i,j}(E' \to E, \vec{\Omega}' \to \vec{\Omega})$
- then we have selected from the pdf given by the collision kernel.

# Sampling the collision kernel

## Sampling the new angle and energy

- Scattering (often) isotropic in CM-system $\Rightarrow$ select $\mu_C$ as $\mu_C = \cos\theta_C = 1 - 2u$.
- Energy and scattering angle are related, so calculate $E$ from

$$\frac{E}{E'} = \frac{A^2 + 2A\mu_C + 1}{(A+1)^2},$$

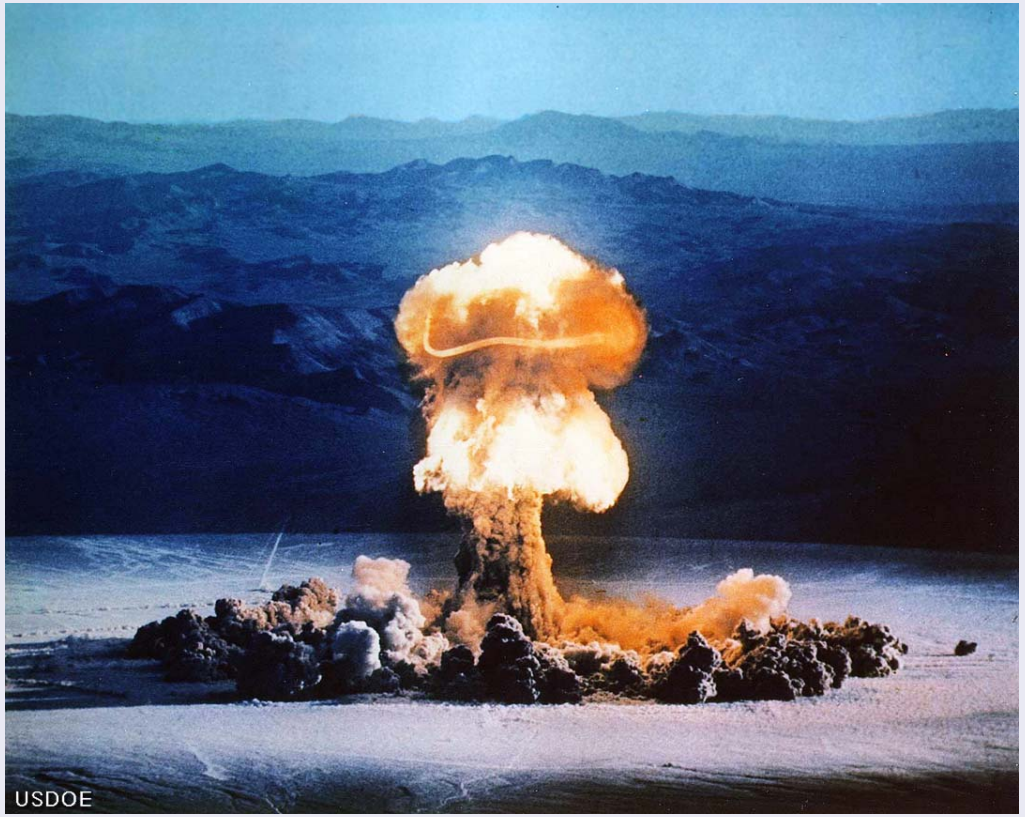
where $A$ is the mass number of the nucleus that the neutron collided with.

# Sampling the collision kernel

## Transformation of angle from CM- to L-system

$$\vec{\Omega} = \frac{1}{\sqrt{A^2 + 2A\mu_C + 1}}(A\vec{\Omega}_C + \vec{\Omega}')$$

## Neutron Transport in Fissile Materials



# Neutron Transport in Fissile Materials

## Problem

The distribution of the fission source is not known in fissile systems.

## Solution

The fission source (together with the fundamental neutron flux and eigenvalue $k_{\text{eff}}$) need to be established over a simulation of a number of successive neutron generations (iterations).

# Criticality/Eigenvalue Calculations

## Active/inactive cycles

- The iterations are called "cycles" in MC terminology.
- Unlike in deterministic calculations, the cycles have to **continue after** the convergence is reached in order to sample well the required result.
- The cycles where the source converges are called **inactive**, and no results are collected during these cycles.
- When the source is converged, **active** cycles can start, and results can start to be collected.
- Active cycles can be stopped when the results are computed to the required precision.