Aalto University
School of Science
and Technology

PHYS-E0562 Nuclear Engineering, advanced course
Lecture 7 – Spatial homogenization

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Topics of this lecture

Previous topics revisited:

- Coupled problem: reactivity feedbacks and fuel depletion
- Reactor physics calculation chain

Energy-group condensation:

- General principle of energy-group condensation
- General principle of spectral calculation
- Spatial and resonance self-shielding
- Doppler-broadening of cross sections

Solution of the local heterogeneous problem and spatial homogenization:

- Method of characteristics as an example of a solution method
- Generation of homogenized few-group constants
- Leakage corrections
- Monte Carlo method in spatial homogenization

Coupled problem revisited: reactivity feedbacks

The operation of a nuclear reactor is based on the self-sustaining chain reaction, carried on by fission neutrons. Consequently, a major part of reactor analysis involves the transport and interaction physics of neutrons.

Solution to the neutron transport problem provides sufficient information on neutron-induced reaction rate distributions within the reactor core, which can be used for calculating output, power distribution, depletion and production rates of nuclides, etc.

There are major challenges in the solution of the transport problem:

- High level of heterogeneity, as neutrons are not uniformly distributed in the fuel
- Reaction probabilities (microscopic cross sections) are strongly dependent on neutron energy
- Time-scales of prompt and delayed neutrons differ by several orders of magnitude ([μs] or [ms] vs. [s])

Reactor analysis relies heavily on computational modeling, and any transport method used for solving reactor physics problems needs to be able to cope with these challenges.

Deterministic transport methods rely on the solution of the transport equation, which describes the neutron balance in the six-dimensional phase-space. The Monte Carlo method is based on the simulated random walk of individual neutrons, and stochastic estimation of reaction rate integrals.

Coupled problem revisited: reactivity feedbacks

Even though microscopic cross sections are complicated functions of neutron energy, the transport problem is linear by nature with the following assumptions:

- Neutrons do not interact with each other[1]
- Reaction probabilities are independent of reaction rates

The linearity assumption applies to criticality experiments and very low power research reactors. For commercial power reactors, the reality is unfortunately different, because reaction probabilities depend on:

1) Material temperatures and densities
2) Material compositions

This creates a non-linear problem, in which the neutronics solution is coupled to:

1) Heat transfer and coolant flow (via reactivity feedbacks)
2) Isotopic changes in fuel during the reactor operating cycle (via fuel depletion)

Solving the transport problem alone is not sufficient for the modeling of an operating nuclear reactor – the calculation scheme needs to be able to handle also reactivity feedbacks and fuel depletion

[1] Neutron density in a power reactor is in the order of 10^{10} 1/cm^3, which can be compared to the density of hydrogen atoms in water or uranium atoms in fuel ($\sim 10^{22}$ 1/cm^3).

Coupled problem revisited: reactivity feedbacks

The coupling between neutronics and thermal hydraulics is particularly strong in light water reactors, because the reactor operates on thermal neutrons ($\sim$80% of fissions), and the slowing-down process is sensitive to operating conditions:

- Neutrons are born with a mean energy of 2 MeV, and they require 20 elastic collisions with hydrogen nuclei to reach the thermal region (< 1 eV)
- If the neutron returns to fuel too early, it is more likely to be absorbed in the capture resonances of ^{238}U than cause fission in ^{235}U
- Since coolant serves the purpose of moderator as well, any change in the reactor operating state is immediately reflected in the slowing-down process

There are two primary mechanisms behind reactivity feedbacks:

(i) The probability of the neutron to reach the thermal region is changed, which affects the number of thermalized neutrons (Doppler- and coolant density feedback)

(ii) The position of the thermal distribution on the energy scale is changed, which affects the reaction probabilities of thermalized neutrons (coolant temperature feedback)

Other effects, less significant for LWR's, include changes in leakage rate and thermal expansion.

Thermal reactors are typically very heterogeneous systems, and keeping neutrons away from the fuel before they are completely thermalized is essential for maintaining the chain reaction.

Coupled problem revisited: reactivity feedbacks

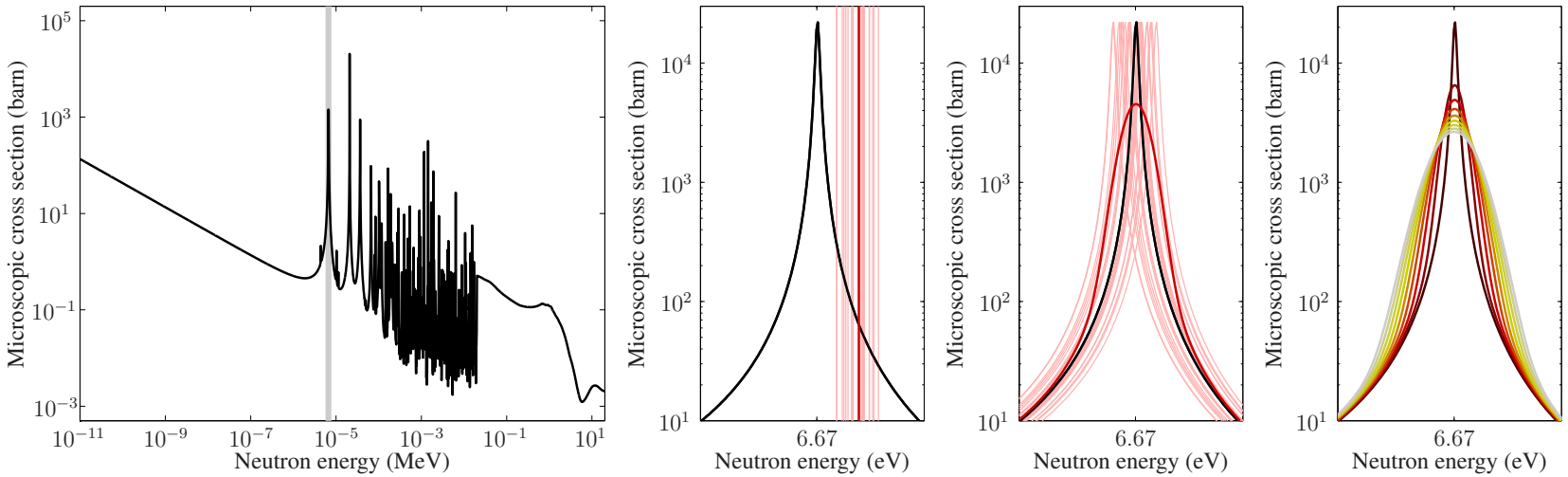


Figure 1 : Doppler-broadening of a ^{238}U resonance peak. The thermal motion of atoms causes a random shift in the relative energy between the neutron and the target nuclide at each collision. The average effect is that narrow resonance peaks appear broader, which increases the overall reaction probability. The effect is most pronounced just above the thermal region, where the predominant reaction mode is parasitic capture by ^{238}U. The result is that increasing fuel temperature leads to reduced reactivity and power (negative feedback).

Coupled problem revisited: reactivity feedbacks

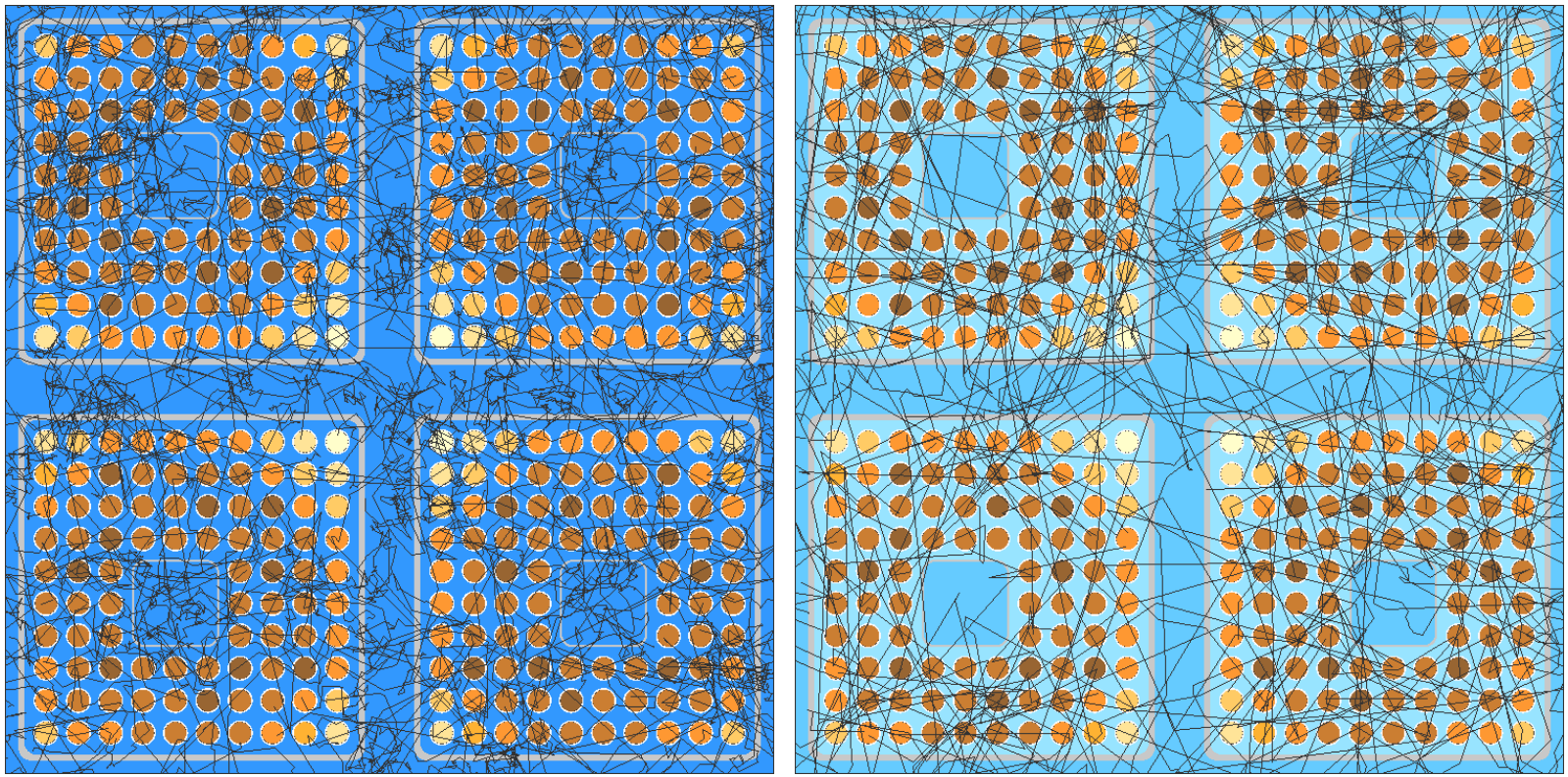


Figure 2 : Neutron tracks in BWR fuel. Left: cold core, high coolant density. Right: hot core, low coolant density. Increase in neutron mean-free-path (average distance between two collisions) increases the probability of the neutron returning to the fuel before thermalization is completed. The predominant reaction mode above thermal region is parasitic capture by ^{238}U, so increase in coolant temperature leads to reduced reactivity and power (negative feedback).

Coupled problem revisited: reactivity feedbacks

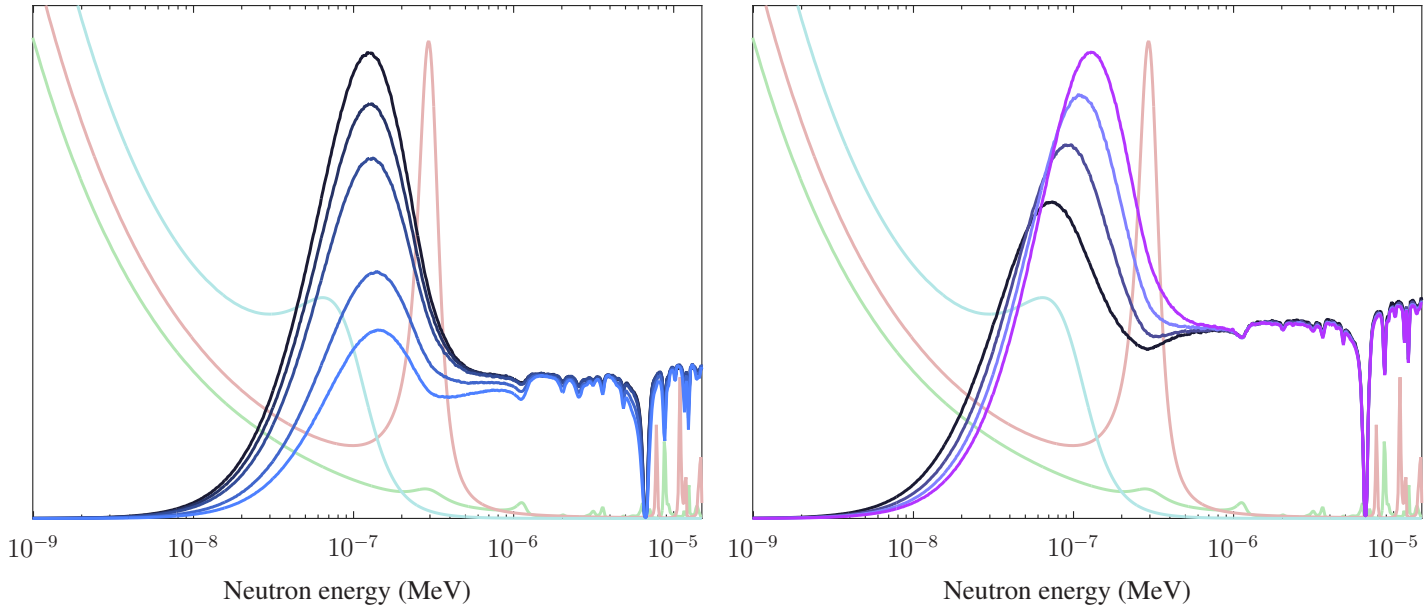


Figure 3 : Effect of coolant density and temperature on the distribution of thermalized neutrons. Shapes of ^{235}U and ^{239}Pu fission cross sections are plotted on the background in green and red, respectively. Left: decrease in density reduces the height of the thermal peak, leading to reduced fission rate and negative feedback. Right: Effect of coolant temperature on the distribution of thermalized neutrons. Shapes of ^{235}U, ^{239}Pu fission and ^{135}Xe capture cross sections are plotted on the background in green, red and cyan, respectively (not to scale). Increasing the temperature moves the thermal peak upwards on the energy scale. This reduces the fission rate of ^{235}U. For ^{239}Pu the impact is opposite, because of the peak located right above the distribution. Also the capture rates of high-absorbing fission products are reduced, which results in a positive rectivity effect. The effect of spectral shift is usually not as strong as the moderator density effect, and the net effect in in LWR's is negative feedback.

Coupled problem revisited: reactivity feedbacks

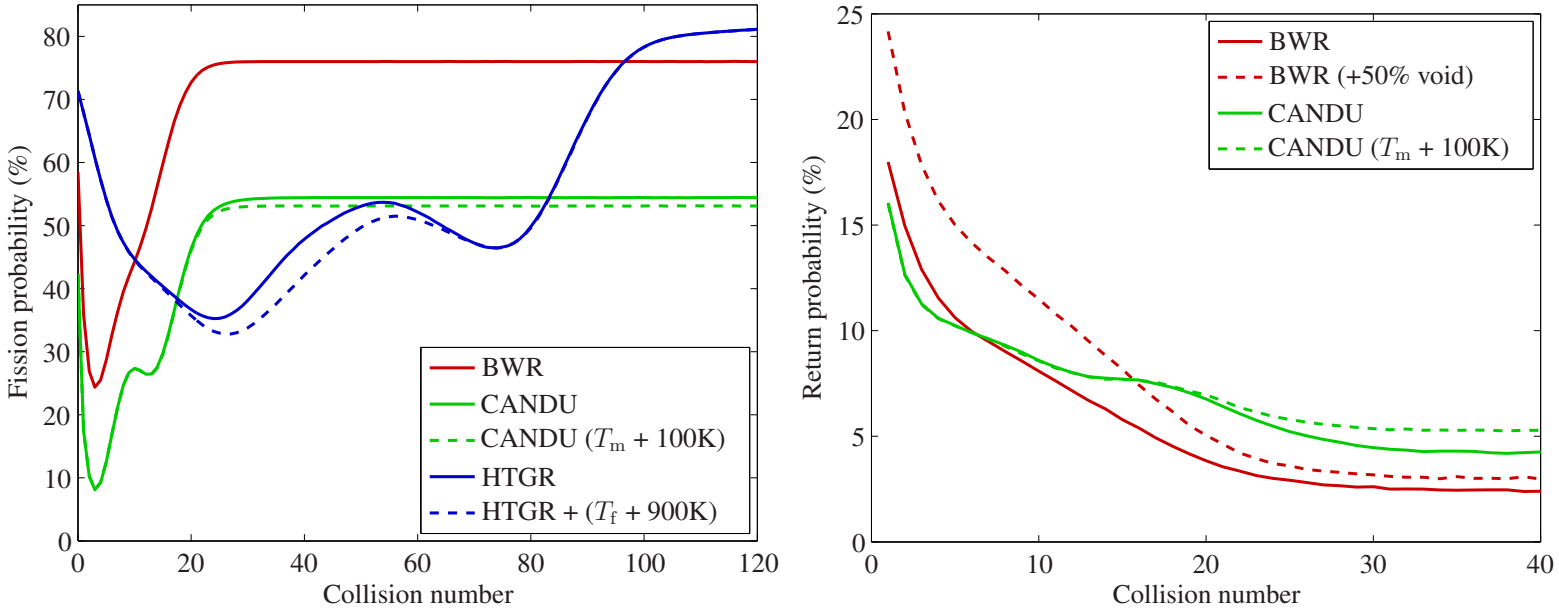


Figure 4 : Fission and return probabilities as function of collision number for different reactor types. Left: Probability of a neutron to undergo fission if its next collision occurs in fuel. The probability drops while passing through the resonances of ^{238}U, which requires different number of collisions for different moderators. The dashed blue line shows the mechanism behind the Doppler-feedback, as the fuel temperature in the HTGR case is increased from 300K to 1200K. Moderator temperature feedback is demonstrated in the CANDU case, with a temperature increase from 500K to 600K (see also Fig. 3). Right: Probability of a neutron colliding in the moderator to undergo its next collision in fuel. The dashed red line demonstrates the effect of increasing neutron mean-free-path (mfp) when the void fraction in the BWR case is increased from 25% to 75% (see also Fig. 2). Similar effect is seen for thermalized neutrons in the CANDU case, as the shift in the thermal peak increases the average mfp.

Coupled problem revisited: fuel depletion

Reactivity feedbacks represent fast, almost immediate coupling between neutronics and reactor operating conditions. In the long time-scale, similar non-linearity is induced by changes in fuel composition by neutron irradiation:

- ^{235}U is depleted and replaced by ^{239}Pu as the primary fissile isotope
- Non-fissile plutonium, minor actinides (Np, Am, Cm) and fission products are accumulated in the fuel, increasing absorption
- Burnable absorber used for passive reactivity control is depleted

Nuclear fuel in light water reactors is loaded in the reactor core for the duration of the entire operating cycle, which is typically 12 or 18 months. After the cycle is completed, 1/3 or 1/4 of the fuel assemblies are removed and replaced with fresh fuel, and the core is shuffled to re-optimize the loading pattern. This means that a single fuel assembly spends 3 to 4 years in the reactor.

The changes in isotopic composition are directly reflected in reactivity and the safety parameters of the reactor core. The accumulation of radioactive fission products also forms the source term for accident analyses and final disposal.

Burnup calculation involves solving the Bateman depletion equations, for example, using the linear chains or matrix exponential methods. Neutron flux and one-group transmutation reactions are obtained from the neutronics solution, and decay constants, branching ratios and fission yields from nuclear data libraries. The calculation proceeds in discrete time-steps, by sequential calls to the transport and depletion solvers.

Coupled problem revisited: fuel depletion

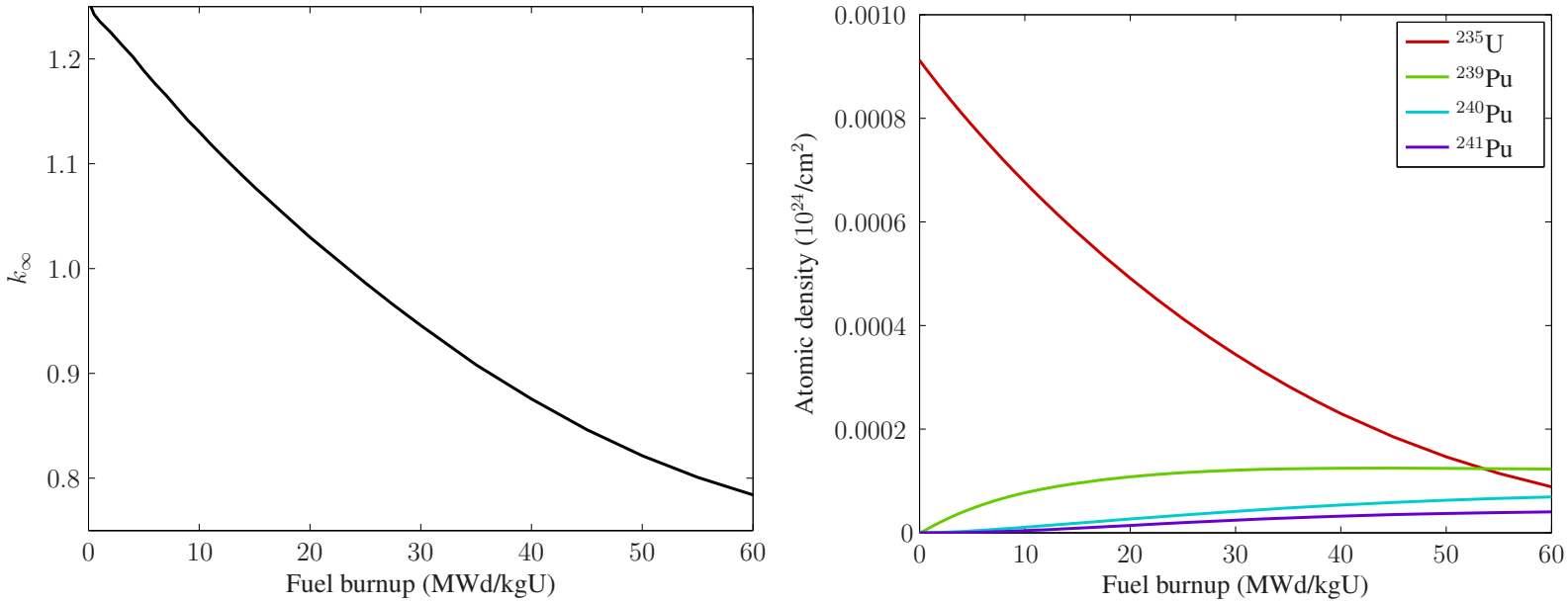


Figure 5 : The composition of nuclear fuel changes along with the reactor operating cycle. The depletion of uranium and build-up of plutonium, minor actinides and fission products changes the neutronics characteristics of the core. Left: Infinite multiplication factor as function of fuel burnup. Right: depletion of ^{235}U and build-up of plutonium isotopes in PWR fuel as function of burnup.

Coupled problem revisited: fuel depletion

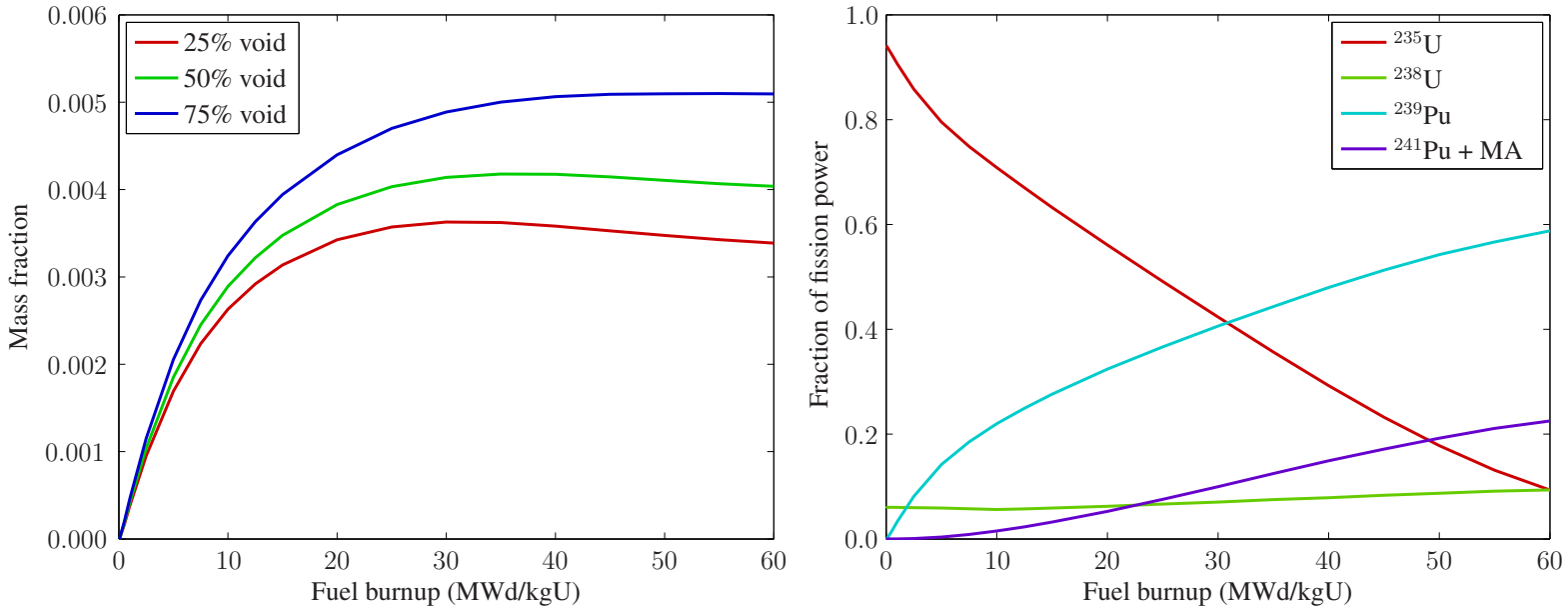


Figure 6 : Left: Plutonium production at different coolant void fractions in a BWR fuel assembly. Right: Contributions of ^{235}U, ^{239}Pu and ^{241}Pu in power production in a BWR assembly (25% void fraction) as function of burnup.

Coupled problem revisited: fuel depletion

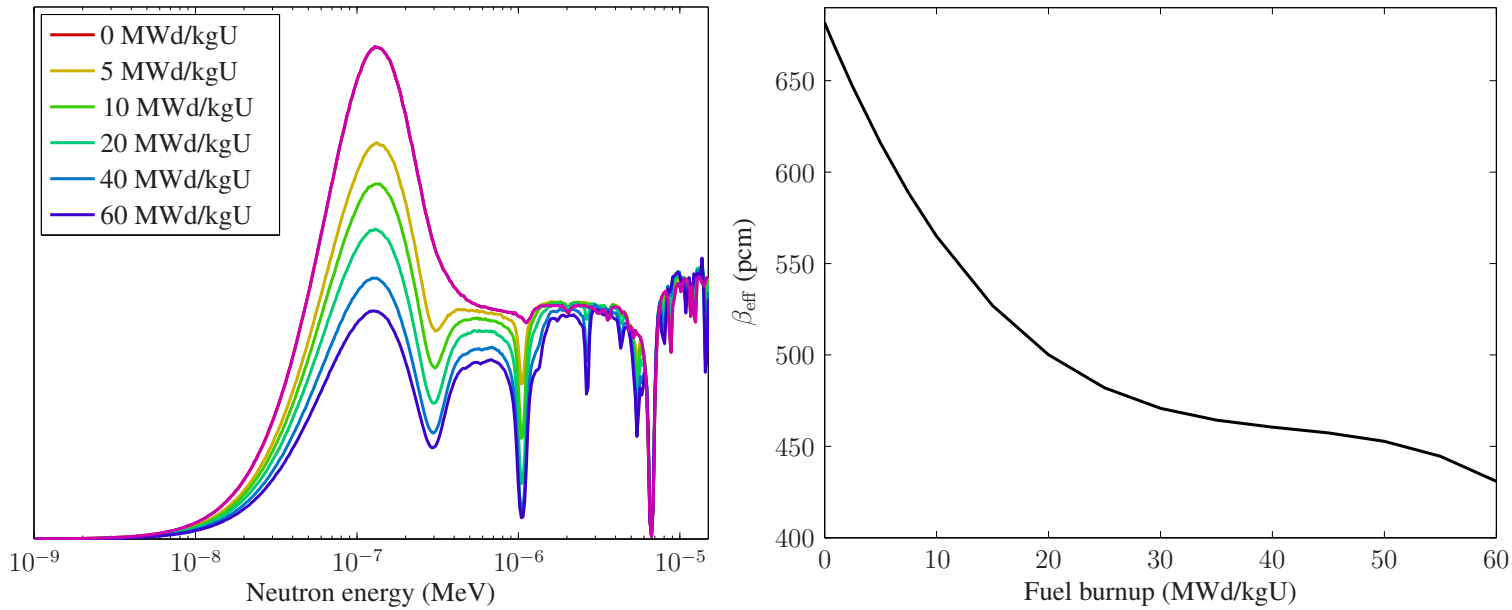


Figure 7 : Left: Effect on increasing burnup on the thermal end of flux spectrum in a BWR fuel pin (40% coolant void fraction). The shape of ^{239}Pu and ^{240}Pu cross sections are clearly reflected in the results. Increasing burnup leads to harder spectrum, which reduces the reactivity worths of absorbers and affects feedback coefficients. Right: Effective delayed neutron fraction in PWR fuel assembly as function of fuel burnup (1 pcm = 0.001%). Large plutonium and minor actinide content leads to lower delayed neutron fraction compared to fresh uranium fuel.

Coupled problem revisited: fuel depletion

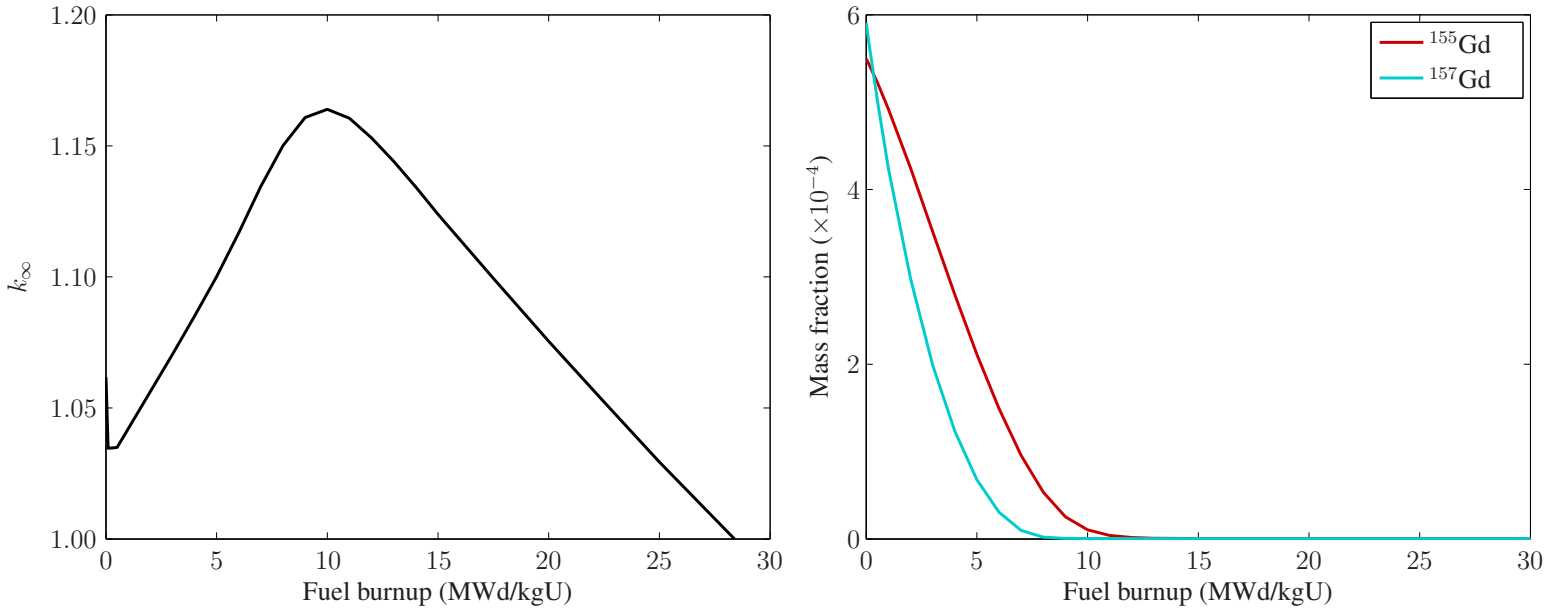


Figure 8 : Depletion of a gadolinium oxide burnable absorber in a BWR fuel assembly calculation. Left: Infinite multiplication factor, Right: Absorber concentrations. The absorber is natural gadolinium (0.2% ^{152}Gd, 2.1% ^{154}Gd, 14.8% ^{155}Gd, 20.6% ^{156}Gd, 15.7% ^{157}Gd, 24.8% ^{158}Gd, 21.8% ^{160}Gd), but only the two high-absorbing isotopes are depleted.

Coupled problem revisited

In practice, the real challenge in reactor modeling is to obtain the solution to the coupled problem by assuming that the problem can be linearized over some time interval and performing iterations between the different solvers (see examples on burnup algorithms in Lecture 5).

Obtaining high-fidelity solutions to neutronics, heat transfer, coolant flow and fuel depletion becomes a tremendous task:

- Typical LWR core contains 50,000 - 100,000 fuel rods, number of fuel pellets is counted in millions
- Fuel temperature varies by hundreds of degrees, depending on local power[2]
- Significant variation in coolant density, especially in BWR's
- Accurate simulation of fuel burnup would require tracking the concentrations of hundreds of isotopes in millions of depletion zones

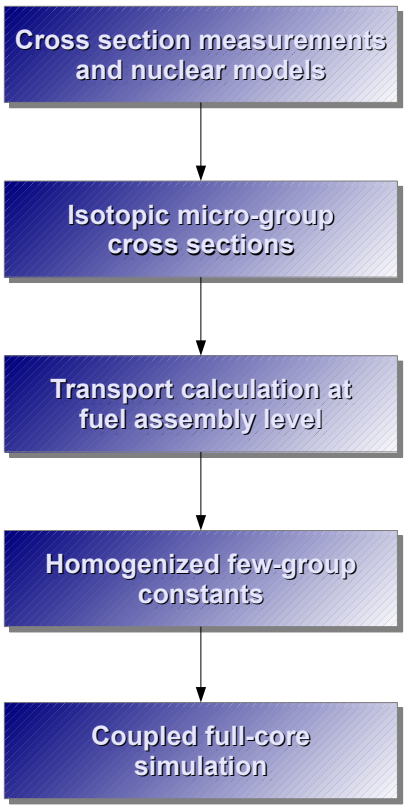
Calculations involving a single state-point without burnup are barely within the capabilities of modern super-computers.

Reactor design and safety analyses require covering various operating states, time-dependent simulations, modeling of core depletion over multiple cycles, modeling of reactivity control, etc., which renders the direct approach unfeasible in practice.

[2] Even the difference between surface and center-line temperature in a fuel pellet can exceed 400 K during normal operation.

Reactor physics calculation chain revisited

Instead, the traditional approach to coupled problems is to divide the neutronics solution in parts:



- The scale of the modeled system is gradually increased, while simultaneously moving towards more simplified description of physics
- Spatial resolution: nuclide-level $\rightarrow$ homogeneous medium $\rightarrow$ pin-level $\rightarrow$ assembly-level $\rightarrow$ core-level
- Energy resolution: continuous-energy $\rightarrow$ thousands of groups $\rightarrow$ tens/hundreds of groups $\rightarrow$ few-group structure
- Transition from one stage to the next is carried out in such way that local reaction rate balance is preserved
- The details of the calculation chain depend on the modeled system and the methods used

The final stage involves a simplified description of the full-scale system, which can be coupled to the solution of heat transfer and coolant flow.

Reactor physics calculation chain revisited

From an engineering point of view, the typical LWR calculation chain can be divided into three computational tasks:

(i) Production of nuclide-wise microscopic interaction data for neutron transport codes from evaluated nuclear data (spectral calculation)

(ii) Solution of the local heterogeneous transport problem at fuel assembly level using higher-order transport methods

(iii) Solution of the global homogeneous transport problem using diffusion theory[3]

The second step is referred to as spatial homogenization, and it provides the sufficient building blocks for the full-scale simulation:

- Traditionally carried out using deterministic 2D lattice transport codes
- Input: isotopic multi-group reaction cross sections (tens or hundreds of groups), detailed description of the geometry at fuel assembly level
- Output: handful of macroscopic few-group constants (typically two energy groups) representing the transport physics

[3] The terms “local” and “global” transport problem are used constantly in this and the following lecture, in reference to fuel assembly and core-level calculations, respectively. Heterogeneous problem refers to detailed geometry and higher-order multi-group solution (or continuous-energy Monte Carlo), and homogeneous problem to few-group diffusion theory applied to homogenized geometry.

Reactor physics calculation chain revisited

Dividing the calculation chain into separate steps enables running coupled full-core simulations at an acceptable computational cost without compromising the accuracy.

The cost of reducing the physical complexity by spatial homogenization is that all information on reactivity feedback effects and dependence of reaction rates on fuel burnup is completely lost. This information is recovered by repeating the procedure over and over again in such way that all reactor operating conditions are covered:

- Assembly types
- Variation in thermal-hydraulic state variables: fuel temperature, coolant temperature and density
- Reactivity control: soluble boron, insertion of control rods
- Fuel depletion

The result is a parametrized library of reactor-specific group constants, from which the data corresponding to local operating conditions can be obtained by interpolation.[4]

Topics of this lecture cover the calculation chain from spectral calculation to spatial homogenization. Full-core calculations are typically carried out using nodal diffusion methods, which is the topic of Lecture 8.

[4] It should be noted that while the coupling of neutronics to heat transfer and coolant flow is handled in the core-level calculation, coupling to fuel depletion is actually carried out within the previous stage, i.e. at the assembly level.

Reactor physics calculation chain revisited

The reason why the solution to the global homogeneous problem can be obtained at an acceptable computational cost is that most of the complicated physics is moved from the core-level calculation to the previous steps in the calculation chain.

Consequently, the amount of physics contained within the cross sections increases as the calculation proceeds. The few-group reaction cross sections and diffusion coefficients used for solving the global problem represent the entire complexity of the transport process averaged over space and energy with a handful of numbers.[5]

The multi-group cross sections used for solving the heterogeneous problem at the fuel assembly level already contain corrections for material temperatures (Doppler-broadening of resonances) and spatial and resonance self-shielding.

In addition to reducing the number of energy groups and homogenizing the geometry at the assembly level, group constant generation destroys the information on detailed isotopic compositions.

Burnup calculation is done for the heterogeneous system, which means that the cross sections used for forming the transport equation are calculated from microscopic cross sections and nuclide densities:

$$\Sigma = N_i \sigma_i + N_{i+1} \sigma_{i+1} + \dots \tag{1}$$

[5] 7 parameters in two-group diffusion theory (9 if time-dependence is included) + discontinuity factors.

Energy-group condensation: general principle

The reactor physics calculation chain starts with the production of multi-group cross section data needed for formulating the heterogeneous transport problem at the fuel assembly level.

Neutron interaction data is stored and distributed in the form of evaluated nuclear data files, as background cross sections, resonance parameters, etc., obtained from experimental measurements and theoretical nuclear models. This data represents the best available knowledge on neutron interactions with matter, but as such is not usable to transport codes.

In order to make use of this data, the cross sections are first condensed into multi-group form. This means that the continuous energy-dependence of flux and cross sections is discretized into G energy groups with boundaries E_{g-1} and E_g, indexed in such way that:

$$E_0 > E_1 > E_2 > \cdots > E_G \tag{2}$$

Indexing the groups in the order of decreasing energy results from the fact that neutrons are born at high energy and scatter towards lower energies during their random walk.

For neutron flux the energy-group condensation means integration over the energy variable:

$$\phi_g(\boldsymbol{r}) = \int_{E_g}^{E_{g-1}} \phi(\boldsymbol{r}, E) dE \tag{3}$$

Similar multi-group condensation can be applied to neutron current density, as was seen in the derivation of diffusion theory in Lecture 4.

Energy-group condensation: general principle

Energy-group condensation of cross sections is carried out by preserving the local reaction rate balance, which means that the volume-integral of the product of multi-group flux and cross section must be equal to the corresponding integral reaction rate.

Energy-group condensation was performed in Lecture 4 for macroscopic cross sections, but the same principle applies to microscopic cross sections:[6]

$$\int_V \sigma_g \phi_g(\boldsymbol{r}) dV = \int_V \int_{E_g}^{E_{g-1}} \sigma(E) \phi(\boldsymbol{r}, E) dV dE \tag{4}$$

Which combined with Eq. (3) gives the formal definition of the group wise-cross section:

$$\sigma_g = \frac{\int_V \int_{E_g}^{E_{g-1}} \sigma(E) \phi(\boldsymbol{r}, E) dV dE}{\int_V \int_{E_g}^{E_{g-1}} \phi(\boldsymbol{r}, E) dV dE} \tag{5}$$

In other words, σ_g is calculated as the flux-volume-weighted average of the energy-dependent microscopic cross section.

[6] The same principle was also applied in Lecture 5 for calculating the one-group transmutation cross sections for the Bateman depletion equations.

Energy-group condensation: general principle

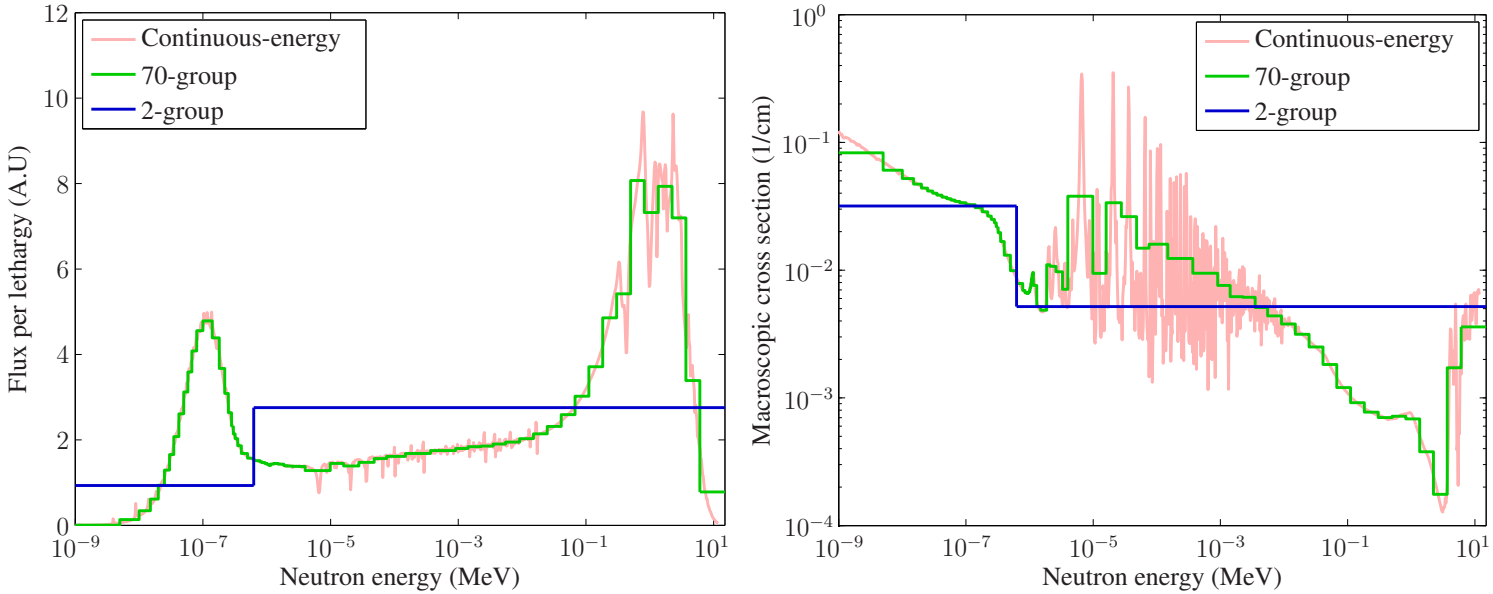


Figure 9 : Illustration of energy group condensation for flux (left) and total absorption cross section (right) in a typical LWR fuel. Condensation of flux is performed by integration over energy groups as in Eq. (3). Condensation of cross sections is carried out by calculating flux-volume-weighted averages that preserve the reaction rate balance as in Eq. (5). The macroscopic cross sections are obtained by summation over the microscopic cross sections of the constituent nuclides.

Energy-group condensation: general principle

The calculation of flux-volume-weighted cross sections in (5) reveals a fundamental paradox in multi-group transport calculation:

- Solution to the transport problem (neutron flux) is needed for the calculation of flux-volume-weighted cross sections
- Flux-volume-weighted cross sections are needed for the solution of the transport problem

In practice, the procedure starts with a simplified geometry description (infinite medium or 1D) and high energy resolution (point-wise or thousands of groups). This allows using a simplified analytical form as the starting point for the intra-group flux shape.

The solution of the transport equation provides the flux spectrum, which can be used for collapsing the energy group structure. For example, when the flux spectrum is obtained in multi-group form with H groups in a homogeneous material region, collapsing into G groups ($G < H$) means approximating the integrals in (5) with sums:

$$\sigma_g = \frac{\sum_{h \in g} \sigma_h \phi_h}{\sum_{h \in g} \phi_h} \tag{6}$$

The resulting multi-group data can then be used for re-formulating the transport problem, while moving towards larger scale (2D pin-cell, etc.), i.e. taking into account an increasing number of spatial effects.

Energy-group condensation: general principle

The exact procedures carried out by spectral codes (for example, CENTRM/PMC in SCALE) are complex and case/code-dependent, and the details are not discussed here. The important points about energy-group condensation are:

- The physics of energy dependence is preserved by preserving the reaction rate balance. In practice this means averaging with the flux spectrum.
- Performing the spectral calculations for simplified sub-problems introduces approximations in the calculation chain.
- As the calculation proceeds, the resulting cross sections become increasingly case-dependent.[7]

The overall result is that the multi-group cross sections used in 2D lattice calculations, for example, already contain a lot of physics even before the local heterogeneous problem is solved. Two important factors are discussed in the following:

- Spatial and resonance self-shielding
- Doppler-broadening of cross sections

[7] The larger the scale of the solved sub-problem, the more assumptions have to be made on the application in which the cross sections are to be used.

Spatial and resonance self-shielding

When cross sections are averaged over the neutron spectrum, they become dependent on the flux solution. This dependence becomes increasingly important as the number of energy groups is reduced and the spatial scale increased.

For the energy dependence this means that:

- The flux is depressed at and near the locations of high resonance peaks (see Fig. 10)
- The depression of flux compensates for the high reaction probability, which is reflected in the integral reaction rate

This effect is called resonance self-shielding.

Similar flux depression occurs spatially:

- Low-energy neutrons are effectively absorbed in the surface layer of fuel pins and strong absorbers
- The fact that the reaction rate is low inside is reflected in the volume-averaged cross sections

Spatial and resonance self-shielding

It is important to note that individual neutrons are completely unaware of what the other neutrons in the population are doing, and therefore do not experience any self-shielding effects either.[8]

Self-shielding is instead an artifact of averaging reaction rates over space and energy, and that the weighting function (flux) that preserves the local reaction rate balance depends on these reaction rates.

The result of spatial and resonance self-shielding is that the flux-volume-averaged cross sections become dependent on:

- Concentrations of strong (resonance) absorbers
- Geometry configuration (dimensions vs. neutron mfp)

The generation of multi-group cross sections is complicated by the fact that material compositions change as function of burnup, and nuclides also shield each other.[9]

The calculation of self-shielded cross sections requires special techniques in the unresolved resonance range, where the positions of individual peaks are not known, but rather represented by probabilistic resonance parameters.

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[8] This is also the case for continuous-energy Monte Carlo simulation.

[9] The result is that burnup calculation requires cross sections pre-generated for different fuel types and several burnups, or that the spectral calculation is repeated from the start after every burnup step.

Spatial and resonance self-shielding

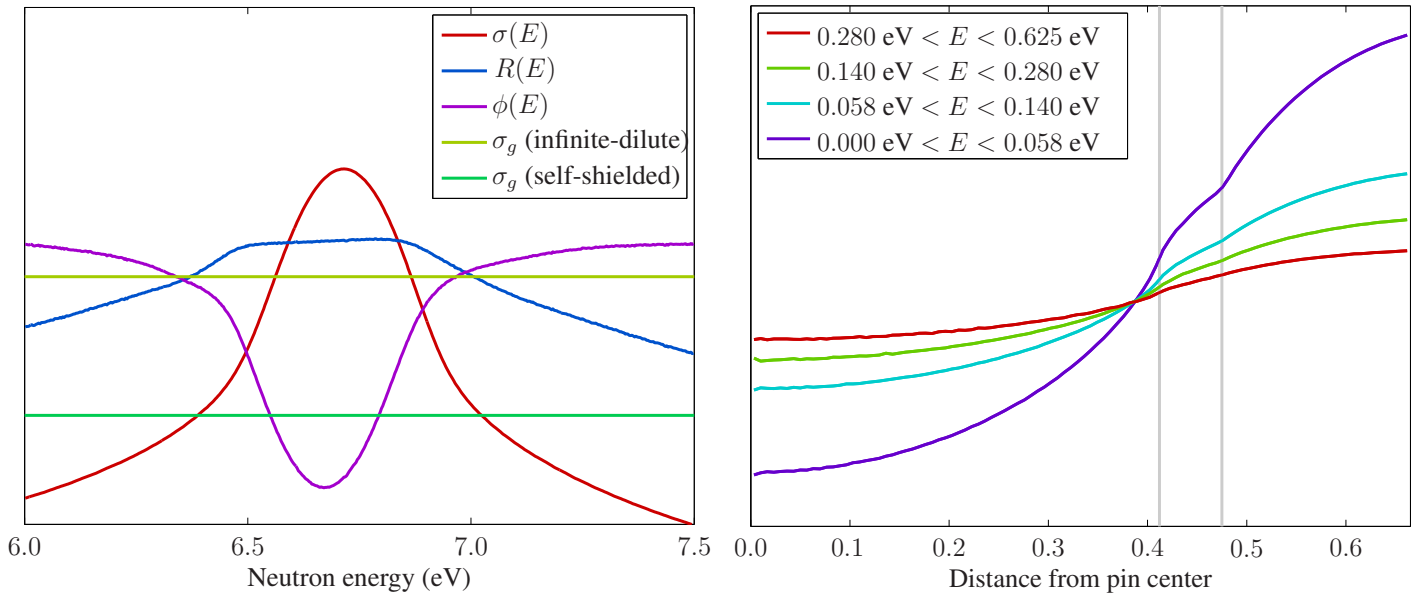


Figure 10 : Left: effect of resonance self-shielding on the capture cross section of ^{238}U. Flux (ϕ) is depressed near the resonance, which means that the shape of the reaction rate (R) differs considerably from the shape of the cross section (σ). Flux-weighted "self-shielded" average results in a much lower value compared to direct "infinite-dilute" average, which ignores the effect of cross section on flux. Right: spatial depression of low-energy components of flux in a PWR fuel pin. The vertical lines mark the inner and outer diameter of cladding.

Doppler-broadening of cross sections

Deterministic transport methods cannot explicitly account for the thermal motion of atoms in the medium, the corresponding shift in the relative neutron energy, or the resulting change in interaction probability (see Fig. 1).[10]

Temperature effects on reaction probabilities are instead handled by a temperature correction known as Doppler-broadening, which essentially implies averaging the cross sections at each energy point over thermal motion.

The procedure is based on the Maxwell-Boltzmann distribution of atoms in free gas. The kinetic energy distribution at temperature T is given by:

$$P_{\mathrm{MB}}(E,T) = 2\sqrt{\frac{E}{\pi}}\left(\frac{1}{kT}\right)^{3/2}\exp\left(\frac{-E}{kT}\right) \tag{7}$$

where k = 1.38065·10^{-23} m^{2}kg s^{-2}K^{-1} is the Boltzmann constant.

This approximation applies reasonably well to crystalline solids and liquids as well, although molecular and lattice binding effects require more elaborate models to account for low energy scattering (see Lecture 3). Doppler-broadening is most important for fuel isotopes, for which the Maxwellian based model is considered sufficient.

[10] Thermal motion can be handled explicitly in continuous-energy Monte Carlo simulation, but the conventional approach is to use temperature-corrected cross sections similar to deterministic calculations.

Doppler-broadening of cross sections

The temperature correction can be written by requiring that the effective temperature-corrected cross section preserves the local reaction rate balance. By replacing the energy variable with speed, this condition can be written as:[11]

$$\phi(v)\Sigma_{\mathrm{eff}}(v,T) = \int \phi(v,v')\Sigma(v')P_{\mathrm{MB}}(V,T,M)d\mathbf{v}' \tag{8}$$

where v is the neutron speed, V is the target speed, M is the target mass and P_{MB} is the thermal distribution function written for target velocity. The velocities are related by:

$$\mathbf{v}' = \mathbf{v} - \mathbf{V} \tag{9}$$

i.e. the integration in (8) is carried over the relative velocity between the neutron and the target.

When flux is written using neutron density and speed, and macroscopic cross section using microscopic cross section and nuclide density, Eq. (8) can be simplified into:

$$\begin{aligned} vn(v)N\sigma_{\mathrm{eff}}(v,T) &= \int v'n(v)N\sigma(v')P_{\mathrm{MB}}(V,T,M)d\mathbf{v}' \\ \sigma_{\mathrm{eff}}(v,T) &= \frac{1}{v}\int v'\sigma(v')P_{\mathrm{MB}}(V,T,M)d\mathbf{v}' \end{aligned} \tag{10}$$

It is important to note here that the neutron density is really a function of v, not v'.

[11] Notice the difference between scalar (*italic*) and vector (**boldface**) quantities, $v = |\mathbf{v}|$, etc.

Doppler-broadening of cross sections

The Maxwell-Boltzmann distribution for velocity is written as:

$$P_{\mathrm{MB}}(V,T,M) = \left(\frac{\gamma}{\sqrt{\pi}}\right)^3 e^{-\gamma^2 V^2} \tag{11}$$

where:

$$\gamma = \sqrt{\frac{M}{2kT}} \tag{12}$$

The target velocity can be written as:

$$\mathbf{V} = \mathbf{v} - \mathbf{v}' \tag{13}$$

which gives for the square speed

$$V^2 = v^2 + v'^2 - 2vv' \cos\beta \tag{14}$$

where β is the angle between $\mathbf{v}$ and $\mathbf{v}'$. By substituting(14) and (11) into (10), the integration can be written in spherical coordinates as:

$$\sigma_{\mathrm{eff}}(v,T) = \frac{1}{v}\left(\frac{\gamma}{\sqrt{\pi}}\right)^3 \int_0^\infty \int_0^\pi \int_0^{2\pi} v'\sigma(v') e^{-\gamma^2\left(v^2+v'^2-2vv'\cos\beta\right)} v'^2 \sin\beta dv' d\beta d\theta \tag{15}$$

where θ is the azimuthal angle.

Doppler-broadening of cross sections

By skipping a few intermediate steps, integration over the two angles yields:

$$\sigma_{\mathrm{eff}}(v,T) = \frac{\gamma}{v^2\sqrt{\pi}} \int_0^\infty v'^2 \sigma(v') \left[e^{-\gamma^2 (v-v')^2} - e^{-\gamma^2 (v+v')^2} \right] dv' \tag{16}$$

which is known as the Solbrig's kernel broadening equation. This integration is relatively easy to perform for analytical resonance functions or point-wise data, and the result is the temperature-corrected cross section at temperature T, that preserves the reaction rate.[12]

The most significant consequence is that resonance peaks become lower and wider (see Fig. 1). As discussed in Lecture 1, the result is that neutrons traveling in the medium with energy close to the resonance peak are more likely to collide with the nuclide. In deterministic transport theory the increase in reaction rate can also be understood via reduced resonance self-shielding.

In the case of a $1/v$-cross section (background shape of compound nucleus reactions) it can be shown that the integral preserves the shape:

$$\sigma(v) = \frac{C}{v} \Longrightarrow \sigma_{\mathrm{eff}}(v,T) = \frac{C}{v} \tag{17}$$

This can be intuitively understood by considering the fact that the weighting function is symmetrical on logarithmic scale and $1/v$ forms a straight line.

[12] The infinite integration interval results from the infinite tail of the Maxwell-Boltzmann distribution. In practice, this interval can be approximated by finite bounds based on physical considerations.

Doppler-broadening of cross sections

In the case of a constant cross section, Eq. (16) is reduced to:[13]

$$\sigma(v) = C \Longrightarrow \sigma_{\text{eff}}(v,T) = C\left[\left(1+\frac{1}{2\gamma^2 v^2}\right)\text{erf}(\gamma v) + \frac{e^{-\gamma^2 v^2}}{\sqrt{\pi}\gamma v}\right] \tag{18}$$

When $v \gg 0$, the exponential and $1/v$ terms approach zero, and the cross section is reduced to constant C, which is expected as the averaging is performed for a constant value.

When $v \to 0$, the error function is reduced to zero and the exponential term approaches unity, leaving:

$$\sigma_{\text{eff}}(v,T) = \frac{C}{\sqrt{\pi}\gamma v} \tag{19}$$

In other words, constant cross sections assume a $1/v$ shape at low energy. This was already noted for elastic scattering cross sections in Lecture 1, and the phenomenon is understood intuitively by considering the reaction rate per traveled path length in a medium where the target nuclides are moving faster than the neutron.

In addition to Doppler-broadening of cross sections, the same temperature correction can be applied to scattering kernels, as thermal motion also affects the energy and angular distributions of scattered neutrons. This topic is left outside the scope of this course.

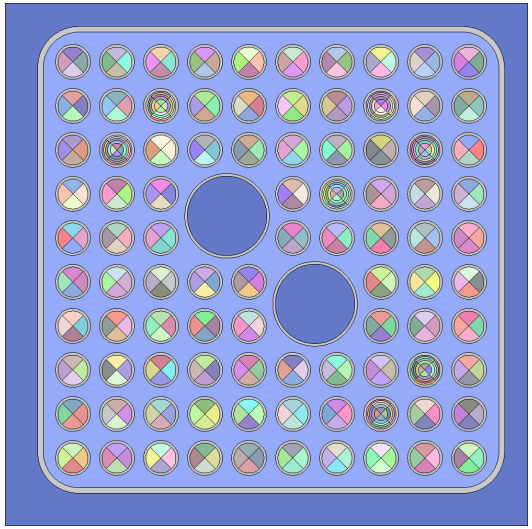
[13] $\text{erf}(0) = 0;\ \lim_{x\to\infty}\text{erf}(x) = 1$

Solution of the local heterogeneous problem

The production of homogenized croup constants for nodal diffusion calculations requires solving the heterogeneous transport problem at the fuel assembly level.

The problem is formulated using:

- Heterogeneous description of the local geometry, most typically a 2D model of a single fuel assembly, surrounded by reflective boundary conditions
- Microscopic Doppler-broadened and self-shielded multi-group cross sections (typically tens or hundreds of groups) from the spectral calculation



In other words, the fuel assembly is removed from its actual surroundings and placed in an infinite lattice of identical assemblies. The use of reflective boundary conditions reduces the net current over each outer boundary surface to zero.

The calculation is traditionally based on higher-order deterministic transport methods, and the procedure also involves tracking the changes in isotopic compositions over the reactor operating cycle (assembly burnup calculation).

The method of characteristics (MOC) is introduced in the following, but the general procedure is very similar regardless of the transport method used for solving the heterogeneous flux.

Solution of the local heterogeneous problem: MOC

The multi-group k-eigenvalue form of the transport equation is written for the angular flux as:

$$\hat{\boldsymbol{\Omega}} \cdot \nabla \psi_g(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}) + \Sigma_g \psi_g(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}) = Q_g(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}) \tag{20}$$

where the source term consists of fission and scattering source:

$$Q_g(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}) = \sum_{g'} \Sigma_{\mathrm{s},g'g}(\hat{\boldsymbol{\Omega}}' \rightarrow \hat{\boldsymbol{\Omega}}) \psi_{g'}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}) + \frac{1}{k} \frac{\chi_g}{4\pi} \sum_{g'} \nu \Sigma_{\mathrm{f},g'} \phi_{g'}(\boldsymbol{r}) \tag{21}$$

The idea in the method of characteristics is to look at the neutron balance within a number of evenly-spaced lines, or characteristics, spanning over the geometry in multiple directions. The transport equation for direction m is written as:

$$\hat{\boldsymbol{\Omega}}_m \cdot \nabla \psi_g(\mathbf{r}, \hat{\boldsymbol{\Omega}}_m) + \Sigma_g \psi_g(\mathbf{r}, \hat{\boldsymbol{\Omega}}_m) = Q_g(\mathbf{r}, \hat{\boldsymbol{\Omega}}_m) \tag{22}$$

where the source term includes all neutrons emitted in direction m in fission and scattering events.

The transport equation is first written in one-dimensional form, by relating the position vector to a segment starting from $\mathbf{r}_0$ and extending distance s in direction $\hat{\boldsymbol{\Omega}}_m$:

$$\mathbf{r} = \mathbf{r}_0 + s\hat{\boldsymbol{\Omega}}_m \tag{23}$$

These segments are formed when the characteristics intersect with the boundary surfaces in the geometry.

Solution of the local heterogeneous problem: MOC

Since:

$$\partial \mathbf{r} \cdot \nabla \psi(\mathbf{r}, \hat{\mathbf{\Omega}}_m) = \partial \psi(\mathbf{r}, \hat{\mathbf{\Omega}}_m) \tag{24}$$

and the differentiation of (23) yields:

$$\partial \mathbf{r} = \hat{\mathbf{\Omega}}_m \partial s \tag{25}$$

the streaming term in (22) can be written as:

$$\hat{\mathbf{\Omega}}_m \cdot \nabla \psi_g(\mathbf{r}, \hat{\mathbf{\Omega}}_m) = \frac{\partial}{\partial s} \psi(\mathbf{r}, \hat{\mathbf{\Omega}}_m) \tag{26}$$

The one-dimensional transport equation in direction m can then be written using the scalar variable s as:

$$\frac{\partial}{\partial s} \psi_g(s, \hat{\mathbf{\Omega}}_m) + \Sigma_g \psi_g(s, \hat{\mathbf{\Omega}}_m) = Q_g(s, \hat{\mathbf{\Omega}}_m) \tag{27}$$

The usual approach for handling the source term in the method of characteristics is to sub-divide the geometry into small flat-source regions, inside which the source is independent of position s. With this approximation the solution inside flat-source region i takes the form:

$$\psi_{i,g}(s, \hat{\mathbf{\Omega}}_m) = \psi_{i,g}(0, \hat{\mathbf{\Omega}}_m) e^{-\Sigma_{i,g} s} + \frac{Q_{i,g}(\hat{\mathbf{\Omega}}_m)}{\Sigma_{i,g}} \left(1 - e^{-\Sigma_{i,g} s}\right) \tag{28}$$

where distance s is measured from the point where the characteristic enters the flat-source region.

Solution of the local heterogeneous problem: MOC

It is easy to show that the average flux over a segment with length l crossing flat-source region i in direction m is given by:

$$\psi_{i,g}(\hat{\mathbf{\Omega}}_m) = \frac{Q_{i,g}(\hat{\mathbf{\Omega}}_m)}{\Sigma_{i,g}} + \frac{\psi_{i,g}(0,\hat{\mathbf{\Omega}}_m) - \psi_{i,g}(l,\hat{\mathbf{\Omega}}_m)}{\Sigma_{i,g} l} \tag{29}$$

This can be used for calculating the source term:

$$Q_{i,g}(\hat{\mathbf{\Omega}}_m) = \sum_n \left[\sum_{g'} \int_{4\pi} \Sigma_{\mathrm{s},i,g'g}(\hat{\mathbf{\Omega}}' \to \hat{\mathbf{\Omega}}_m)\psi_{n,g'}(\hat{\mathbf{\Omega}}')d\hat{\mathbf{\Omega}}' + \frac{1}{k}\frac{\chi_g}{4\pi}\sum_{g'}\nu\Sigma_{\mathrm{f},g'}\phi_{n,g'} \right] \tag{30}$$

where the outermost summation is carried over all characteristics n passing through flat source region i, and the scalar flux is written as:

$$\phi_{i,g} = \int_{4\pi} \psi_{i,g}(\hat{\mathbf{\Omega}})d\hat{\mathbf{\Omega}} \tag{31}$$

Since the number of directions is finite, the integrals over full solid angle can be replaced by summations over all directions.[14]

[14] It was assumed here that the method of characteristics was applied in a two-dimensional geometry, in which case axial streaming can be accounted for by scalar multipliers in the source term. Effectively this means that the characteristics are projections in the 2D plane.

Solution of the local heterogeneous problem: MOC

The number of parallel characteristics used for covering the geometry in 2D assembly calculations ranges from 150 to 200 per energy group. The number of directions is between 10 and 200, depending on the energy group.

The solution proceeds by iteration:

1) The intersection points between the characteristics and the flat-source regions are determined (a ray-tracing problem). Each characteristic is sub-divided into segments, in which the total cross section and source term is assumed constant.
2) The flux solution is written as (28), which can be used to calculate the average (29) and end-point flux for each segment.
3) The end-point flux gives the boundary condition for the next segment, and the average flux is used for obtaining the source terms (30) for the next iteration.[15]

The procedure is repeated for all characteristics in all directions. The iteration starts with an initial guess, and each cycle updates the flux solution and source distribution.

The method of characteristics is an efficient way to solve the heterogeneous transport problem in 2D fuel assembly geometries. The accuracy is good, provided that the number of energy groups, characteristics and directions is sufficient.

[15] Reflective boundary conditions are handled by reflecting the characteristic back into the geometry, where it eventually coincides with itself.

Spatial homogenization

Once the space-dependent flux has been obtained from the heterogeneous transport calculation, it can be used for homogenizing the geometry. Formally this is carried out similar to (5):

$$\Sigma_g = \frac{\int_V \int_{E_g}^{E_{g-1}} \Sigma(\boldsymbol{r}, E)\phi(\boldsymbol{r}, E) dV dE}{\int_V \int_{E_g}^{E_{g-1}} \phi(\boldsymbol{r}, E) dV dE} \tag{32}$$

but since the flux solution is obtained in multi-group space-discretized form, the procedure is written as:

$$\Sigma_g = \frac{\sum_{h \in g} \sum_i V_i \Sigma_{i,h} \Phi_{i,h}}{\sum_{h \in g} \sum_i V_i \Phi_{i,h}} \tag{33}$$

where h refers to the multi-group division used in the heterogeneous solution and g to the final few-group division. Index i refers to spatial sub-division, such as the flat-source regions in MOC.

In addition to reaction cross sections, spatial homogenization includes calculation of discontinuity factors (topic of Lecture 8) and performing leakage-correction on the flux spectrum.

As mentioned above, the information on isotopic compositions is lost in the process of homogenization, which means that burnup calculation has to be performed before proceeding to the next stage in the calculation chain. This is typically carried out using the same code that produces the homogenized group constants, and the calculation of one-group transmutation cross sections used for forming the Bateman depletion equations in carried out similar to (33).

Spatial homogenization

Diffusion coefficient differs from the homogenized reaction cross sections in several respects:

- No direct connection to a physical, continuous-energy reaction rate
- Based on an approximation (Fick's law) that connects flux gradient to current density
- Determines the neutron streaming term in the diffusion equation

In Lecture 4 it was noted that the diffusion coefficient can be related to the inverse of the transport cross section, written here in multi-group form as:

$$D_h = \frac{1}{3\Sigma_{\mathrm{tr},h}} , \tag{34}$$

where:

$$\Sigma_{\mathrm{tr},h} = \Sigma_h - \frac{\sum_{h'} \overline{\mu}\, \Sigma_{\mathrm{s},h'h} J_{h'}(x)}{J_h(x)} . \tag{35}$$

This in-scattering form can be further simplified by applying the out-scattering approximation:[16]

$$\Sigma_{\mathrm{tr},h} \approx \Sigma_h - \overline{\mu}\, \Sigma_{\mathrm{s},h} , \tag{36}$$

where $\Sigma_{\mathrm{s},h}$ is the total scattering cross section and $\overline{\mu}$ is the average scattering cosine.

[16] It should be noted that the out-scattering approximation is indeed an approximation that leads to certain inconsistencies in the streaming of high-energy neutrons in hydrogeneous media.

Spatial homogenization

Deriving (36) from transport theory is a non-trivial procedure and subject to several approximations. There are two additional important observations related to obtaining the few-group diffusion coefficient.

First, it should be noted that it is the inverse of the transport cross section that should be condensed into the final few-group form.[17]

Second, Fick's law:

$$\mathbf{J}_h(\boldsymbol{r}) = -D_h \nabla \phi_h(\boldsymbol{r}) \tag{37}$$

implies that the inverse of the transport cross section should be weighted by the flux gradient spectrum rather than the flux spectrum.

However, it is often assumed that the spatial and spectral components of the flux are separable within every broad energy group g, i.e. assuming identical shape for all ϕ_h with $h \in g$. Canceling out the space-dependent gradient terms allows writing the condensation with flux spectrum instead. With multi-group space-discretized flux this procedure is written as:

$$D_g = \frac{\sum_{h \in g} \sum_i \frac{\Phi_{i,h}}{3\Sigma_{\mathrm{tr},i,h}}}{\sum_{h \in g} \sum_i V_i \Phi_{i,h}} \,. \tag{38}$$

[17] This may seem trivial, but in some literature sources the condensation is performed for the transport cross section as if it was simply one of the reaction cross sections. This produces inconsistent results, as it is the diffusion coefficient (proportional to $1/\Sigma_{\mathrm{tr},h}$), not the transport cross section itself, that is the quantity of interest.

Leakage corrections

Lattice physics calculations are typically based on methods derived from the k-eigenvalue form of the transport equation:

$$\hat{\boldsymbol{\Omega}} \cdot \nabla \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) + \Sigma \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) = \frac{1}{k} F(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) + S(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \tag{39}$$

As noted in Lecture 2, this implies that the solution obtained for this equation is not the solution to the actual transport problem, but to a modified problem in which the fission source term is divided by k.

In other words: the time-dependence of flux is dropped, and balance between source and loss rates is obtained by modifying the average number of emitted fission neutrons.

The first eigenvalue, denoted as k_{eff}, corresponds to the fundamental mode flux solution, and it is interpreted as the effective multiplication factor of the system.

Similar approximation is applied in the Monte Carlo method, when the simulation is run in the k-eigenvalue criticality source mode: the number of emitted fission neutrons is adjusted to maintain constant source population from cycle to cycle (see Lecture 3).

Leakage corrections

Performing spatial homogenization as an infinite-lattice calculation ignores the fact that neutrons are moving between assemblies, and that the inward or outward current contributes to local neutron balance. When the net current is forced to zero by reflective boundary conditions, there is, in general, an imbalance between the source and loss terms and $k_{\text{eff}} \neq 1$.

When the fission source term is scaled up ($k_{\text{eff}} < 1$) or down ($k_{\text{eff}} > 1$), the contribution of fission neutrons is correspondingly over- ($k_{\text{eff}} > 1$) or under-estimated ($k_{\text{eff}} < 1$). This distorts the flux spectrum, but also the spatial distribution of flux.

Since spatial homogenization is performed by calculating flux-volume weighted averages of cross sections, the resulting group constants are also affected.

It should be noted that the root cause of this issue is not in the way the transport problem is solved, but rather in its formulation: a time-dependent system is forced to steady-state condition by adjusting one of the source terms.

As long as the homogenized assembly is removed from its actual surroundings and modeled as an infinite lattice of identical copies, there is no physical solution to this problem.

Leakage corrections

However, since the purpose of homogenization is not to simulate physical reality, but rather to produce input parameters for the next stage in the calculation chain, the flux solution can be artificially improved by leakage corrections.

The general idea is to introduce an additional source or loss term, representing the transfer of neutrons across the boundaries in such way that the local neutron balance is restored.

One of the simplest corrections is based on the B_1 method, in which the geometry is homogenized and the spatial dependence of the leakage term is assumed separable (uniform leakage throughout the geometry).

The procedure involves the solution of yet another transport problem:[18]

- Performed in homogenized geometry, but using the original micro-group structure, or some multi-group subset of it
- The B_1 equations are solved by performing critical buckling iteration in such way that $k_{\text{eff}} = 1$ when the leakage term is included in the balance
- The result is the leakage-corrected flux spectrum, which can be used to collapse cross sections into the final multi-group form
- Diffusion coefficients are obtained directly from the leakage term

[18] For details, see: R. Stamm'ler and M. Abbate, "Methods of Steady-State Reactor Physics in Nuclear Design." Academic Press Inc. 1983.

Monte Carlo method in spatial homogenization

In Lecture 3 it was noted that the continuous-energy Monte Carlo simulation has several advantages over deterministic transport methods:

- Transport simulation is inherently three-dimensional
- Capable of handling complex geometries, scalable to arbitrary resolution and level of spatial detail
- Capable of using the best available knowledge on neutron interactions without major approximations
- No application-specific limitations – same code and cross section data can be used for modeling any fuel or reactor type

Many of these advantages also apply to spatial homogenization. What is particularly important is the fact the continuous-energy simulation is not subject to limitations resulting from self-shielding effects.

In practice this means that the generation of few-group constants can be performed without intermediate steps involving spectral calculation, which makes the entire calculation chain shorter, more transparent to the user, and less prone to errors resulting from modeling approximations.

In Lecture 8 it will also be noted that Monte Carlo codes are capable of providing the ideal reference solution for validating the calculation chain, since the same code and cross section data can be used for both homogenization and heterogeneous 3D calculation (albeit with a high computational cost).

Monte Carlo method in spatial homogenization

Even so, Monte Carlo codes are not used for spatial homogenization in a routinely manner, mainly because the computational cost is high and the methodology is not fully developed:

- Running a single infinite-lattice calculation is relatively cheap, but when the procedure needs to cover thousands of burnup and state points, the total cost adds to several months of CPU time.
- Calculation of certain parameters (e.g. diffusion coefficients) requires special tricks that are beyond the standard tally capabilities of general purpose Monte Carlo codes.
- Managing the calculation sequence with branch and history calculations (topics of Lecture 8) is a non-trivial task.

The development in calculation codes, computer capacity and especially parallel computing makes the Monte Carlo method an increasingly attractive option for spatial homogenization.

The Serpent code developed at VTT since 2004 was originally started as a lattice physics code for the purpose of spatial homogenization, and it is one of the first Monte Carlo codes specifically dedicated for this task.

Summary of main topics

Modeling of an operating nuclear reactor requires solving the coupled problem between neutronics, heat transfer, coolant flow and fuel depletion. Obtaining a full-scale heterogeneous solution to this problem is beyond the currently-available computer resources.

Instead, the problem is divided into a calculation chain, in which the physical complexity of the transport problem is gradually reduced, while simultaneously moving towards larger spatial scale. The final stage in the chain involves coupled full-scale simulation with a homogenized model, using simplified transport methods, typically based on diffusion theory.

The reason why the solution to the full-scale homogeneous problem can be obtained with a relatively low computational cost without compromising the accuracy is that much of the physics is handled in the previous steps, while preparing the homogenized few-group constants.

Spatial homogenization involves solving the heterogeneous multi-group transport problem at the fuel assembly level, using higher-order transport methods, such as the method of characteristics. The preparation of multi-group cross sections for this calculation from the evaluated nuclear data involves Doppler-broadening of cross sections and spectral calculation, which takes into account the resonance and spatial self-shielding effects.

Topics of next lecture

The next lecture continues the reactor physics calculation chain from spatial homogenization to full-core calculations using nodal diffusion methods.

Specific topics include:

- Diffusion theory revisited
- Equivalence theory and discontinuity factors
- Basics of nodal diffusion calculation
- Covering all reactor operating conditions in group constant generation
- Parametrization of group constant data