Some remarks on XS preparation with SERPENT

E. Fridman

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

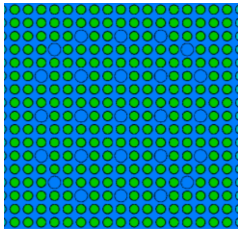
Outline

- Leakage-corrected homogenized XS
- XS preparation for non-multiplying media
- Neutron multiplication due to n,xn reactions

Leakage-corrected homogenized XS

Why to introduce a leakage correction? (1)

- Heter. lattice transport calculations are performed to obtain:
  - Σ_g^r, ϕ_g^r in group $\mathbf{g}$, for every region $\mathbf{r}$ with volume V^r

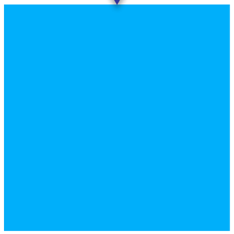


$\Sigma_g^r, \phi_g^r, V^r$

- Σ_g^r, ϕ_g^r are homogenized into a system Σ_g^h, ϕ_g^h
  - Via flux-volume and volume averaging

$$\Sigma_g^h = \frac{\sum \Sigma_g^r \phi_g^r V^r}{\sum \Sigma_g^r V^r}$$

- Homogenized Σ_g^h:
  - Represent the lattice
  - To be collapsed into few-group XSs



Σ_g^h, ϕ_g^h

Why to introduce a leakage correction? (2)

- Lattice calculations are performed with reflective BC
  - Infinite lattice of identical cells
  - $k = k_\infty$
  - ϕ_g^h = infinite-medium flux
- The actual operating conditions are not known
  - But are normally different from the infinite lattice conditions
  - Due to the leakage effects
- What can we do?
  - To assume that the system is a part of a critical configuration
  - To force lattice k_∞=1
  - To estimate the criticality spectrum to be used for XS collapsing
- How?
  - By introducing a leakage model

B_1 equations

- Criticality flux can be obtained by solving B_1 equations
  - Homogeneous, multi-group, dimensionless

$$\begin{cases} \Sigma_{t,g}\varphi_g - \sum_{g'} \Sigma^0_{s,g'\to g}\varphi_{g'} \pm iBJ_g = \chi_g \\ 3a_g\Sigma_{t,g}J_g - 3\sum_{g'} \Sigma^1_{s,g'\to g}J_{g'} = \mp iB\varphi_g \quad \text{where} \quad a_g = f(B, \Sigma_{t,g}) \end{cases}$$

- B_1 equations derived assuming
  - The flux separability in space, and in energy and angle
  - Linear scattering anisotropy

- The solution of B_1 equations yields:
  - Flux and net-current spectra associated with a buckling B^2
  - Diffusion coefficients consistent with linearly anisotropic scattering

- The criticality flux and current spectra are found iteratively
  - By searching B^2 which yields $k_{eff} = 1$

- B1 solver is available in Serpent (version≥1.14)

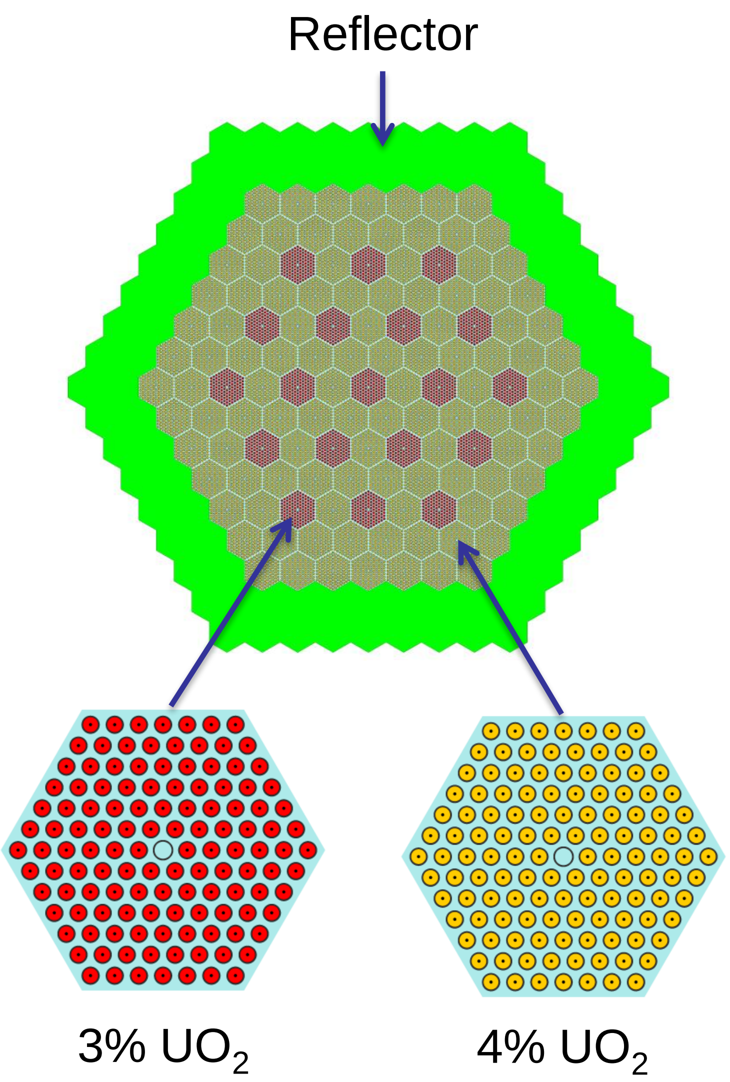
Example case: simplified VVER-440 core

Core data

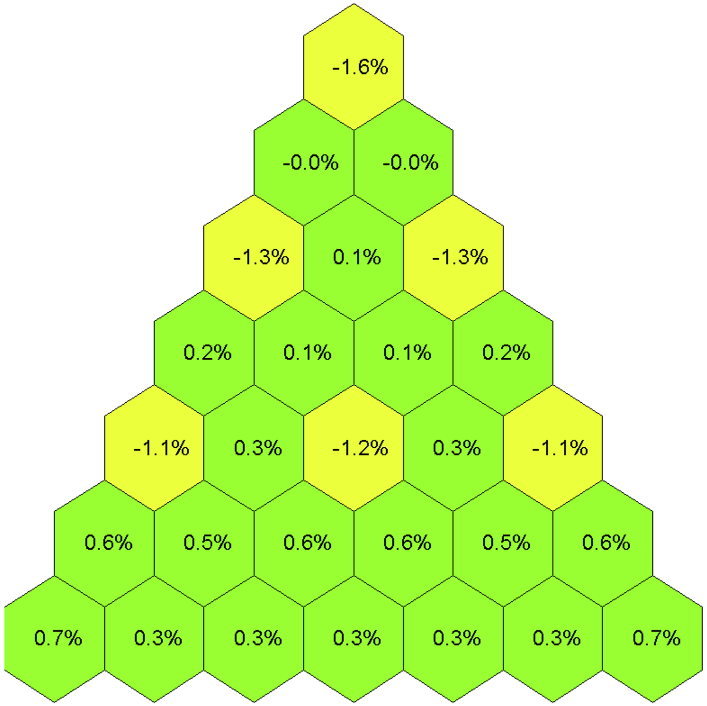
- 2D configuration
- 127 fuel assemblies
- No typical VVER-440 assembly shroud
- 90 reflector positions

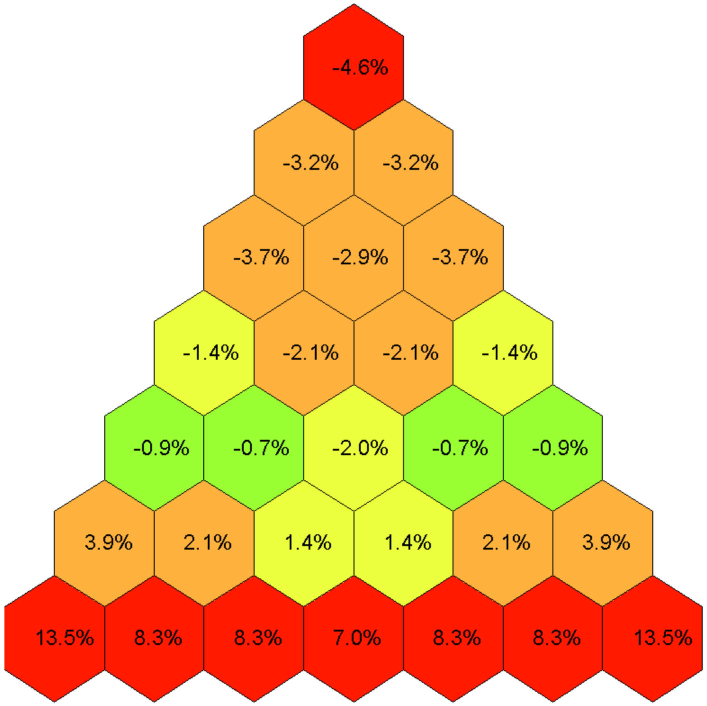
In this example

- Serpent was used
    - To provide a reference solution
    - To generate two XS sets: Inf and B1
- Diffusion calculations are done by DYN3D
    - Nodal diffusion code
    - Using two XS sets
- To compare
    - K-eff
    - Radial power distribution



Example result: Serpent vs. DYN3D





B_1 XS

Difference in radial power:
Max.=**1.6%** RMS=**0.5%**

Difference in k_{eff}:
$\Delta k/k$ = **-0.20%**

Inf XS

Difference in radial power:
Max.=**13.5%** RMS=**6.1%**

Difference in k_{eff}:
$\Delta k/k$ = **0.74%**

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P1 vs. B1 diffusion coefficients

	g1	g2
P1	1.208	0.364
B1	1.473	0.457
Rel. diff	**-21.9%**	**-25.6%**

Reflector modeling

Generation of reflector XS for nodal codes
Some background

- To get a "good" nodal solution one should preserve:
  - Node-averaged reactions rates (RR)
  - Surface-averaged net leakage rates (LR)
- This is done via the use of:
  - Flux-volume weighted (FVW) XS
  - Discontinuity factors (DF):

$$\boldsymbol{DF = \frac{\phi_s^{het}}{\phi_s^{hom}}}$$

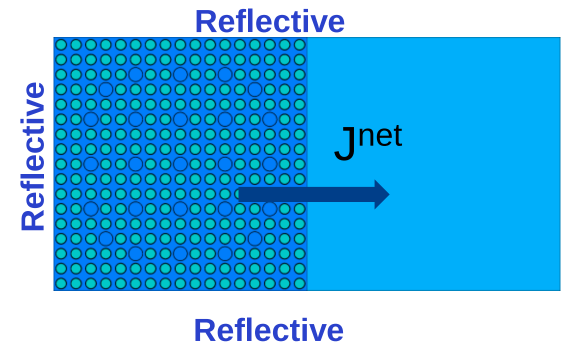
$\boldsymbol{\phi_s^{het}}$ – surface flux from heter. transport solution

$\boldsymbol{\phi_s^{hom}}$ – surface flux from homog. diffusion solution obtained with FVW XS

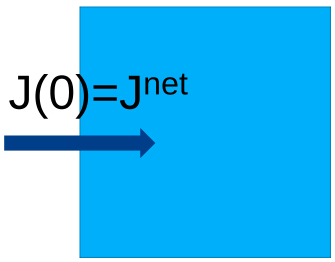
- For a single reflected fuel assembly:
  - ϕ_s^{hom} can be replaced by averaged ϕ^{het} (K. Smith)
  - This is the way how DF are calculated in Serpent
  - **Not valid for reflector regions**

Generation of reflector XS for nodal codes
How it's done with deterministic transport lattice codes

- Solve 1D heter. fuel-reflector (F/R) problem
  - To obtain homogenized XS,
    F/R interface fluxes and currents



- Solve 1D homo. diffusion equation with a fixed source
  - Separately for the fuel and reflector regions
  - Using homogenized XS
  - Using net currents as a boundary condition
  - To obtain diffusion surface flux



- Calculate DF
  - as a ratio between transport and diffusion surface fluxes

Generation of reflector XS for nodal codes
Estimation of the leakage rates in Serpent

- Homogenized XS are directly available

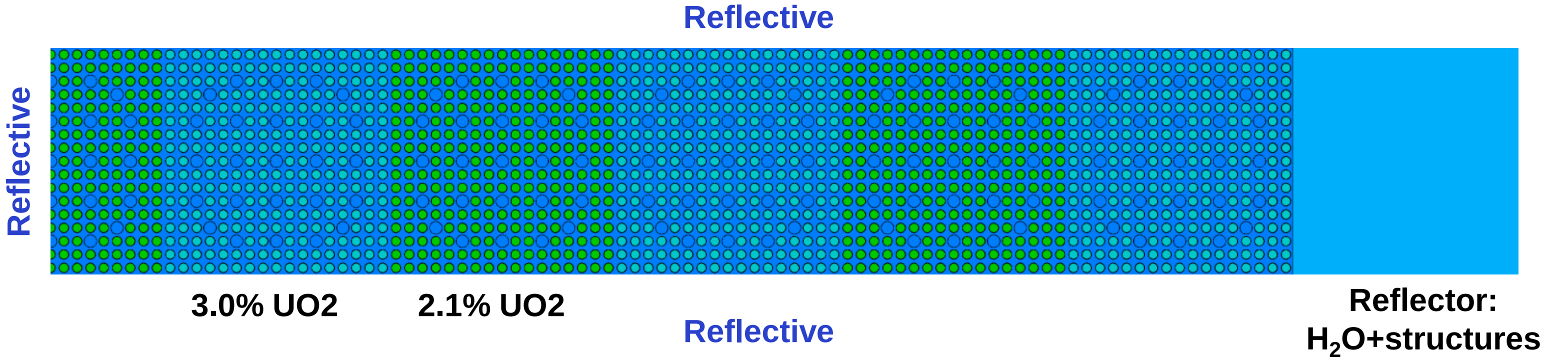
- Interface currents are not
  - In Serpent there is no MCNP F1-like surface current tally

- How to estimate the leakage?
  - Via the use of MCNP – not "sustainable" solution
  - Via the nodal neutron balance
    - "Elegant" solution - requires minor additional effort
    - Proposed by Bryan Herman of MIT

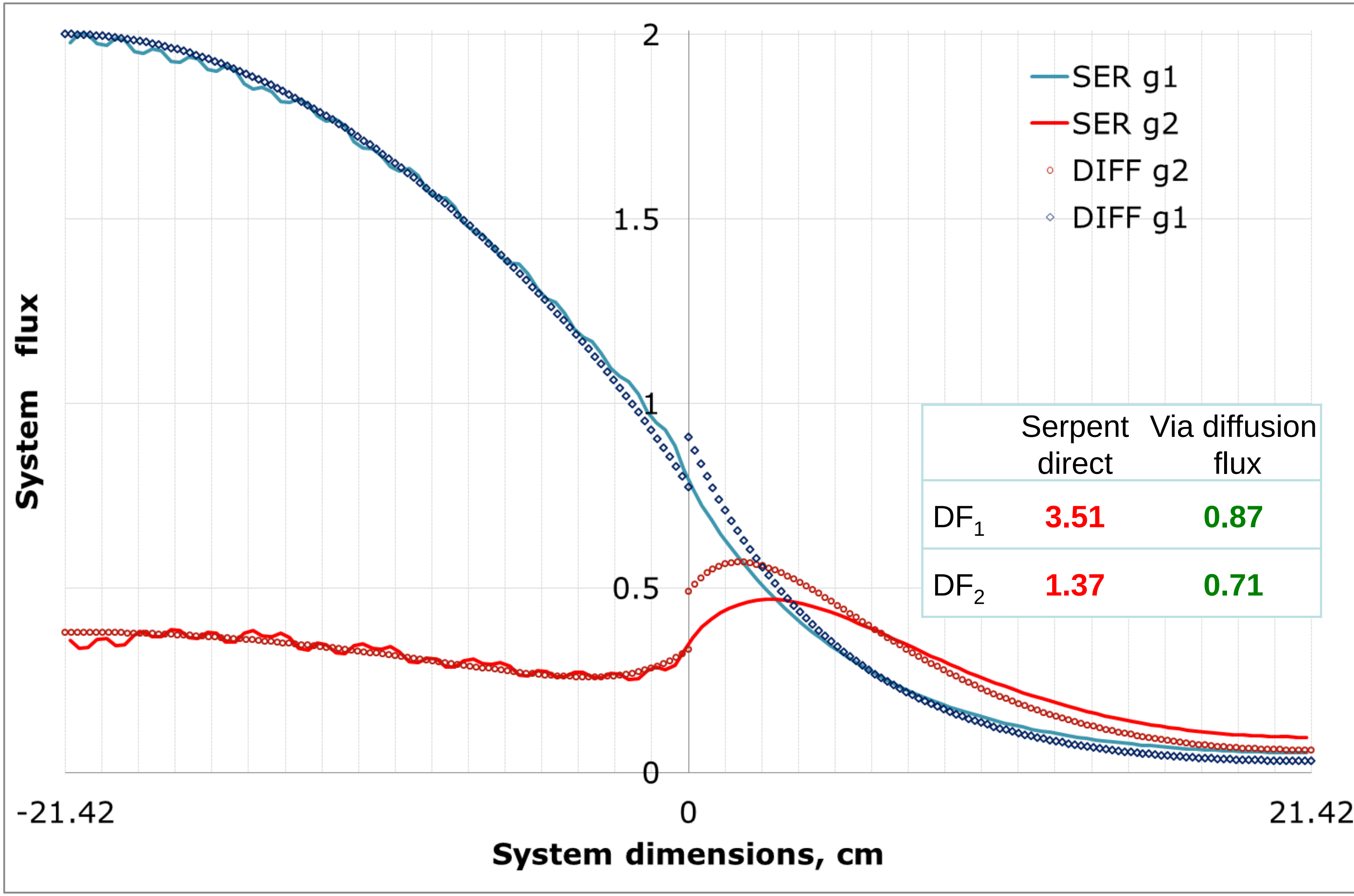
$$LR_g + \Sigma_{t,g}\varphi_g = \sum_{h=1}^{G} \upsilon\Sigma_s^{h\to g}\varphi_h + \frac{\chi_g}{k}\sum_{h=1}^{G} \nu\Sigma_{f,h}\varphi_h$$

Generation of reflector XS for nodal codes
A test problem

- A single raw of PWR fuel assemblies with reflector
- Serpent was used
  - To generate 2-G homogenized XS for the nodal diffusion code DYN3D
  - To provide a reference solution
- The compared parameters:
  - K-eff
  - Nodal power distribution

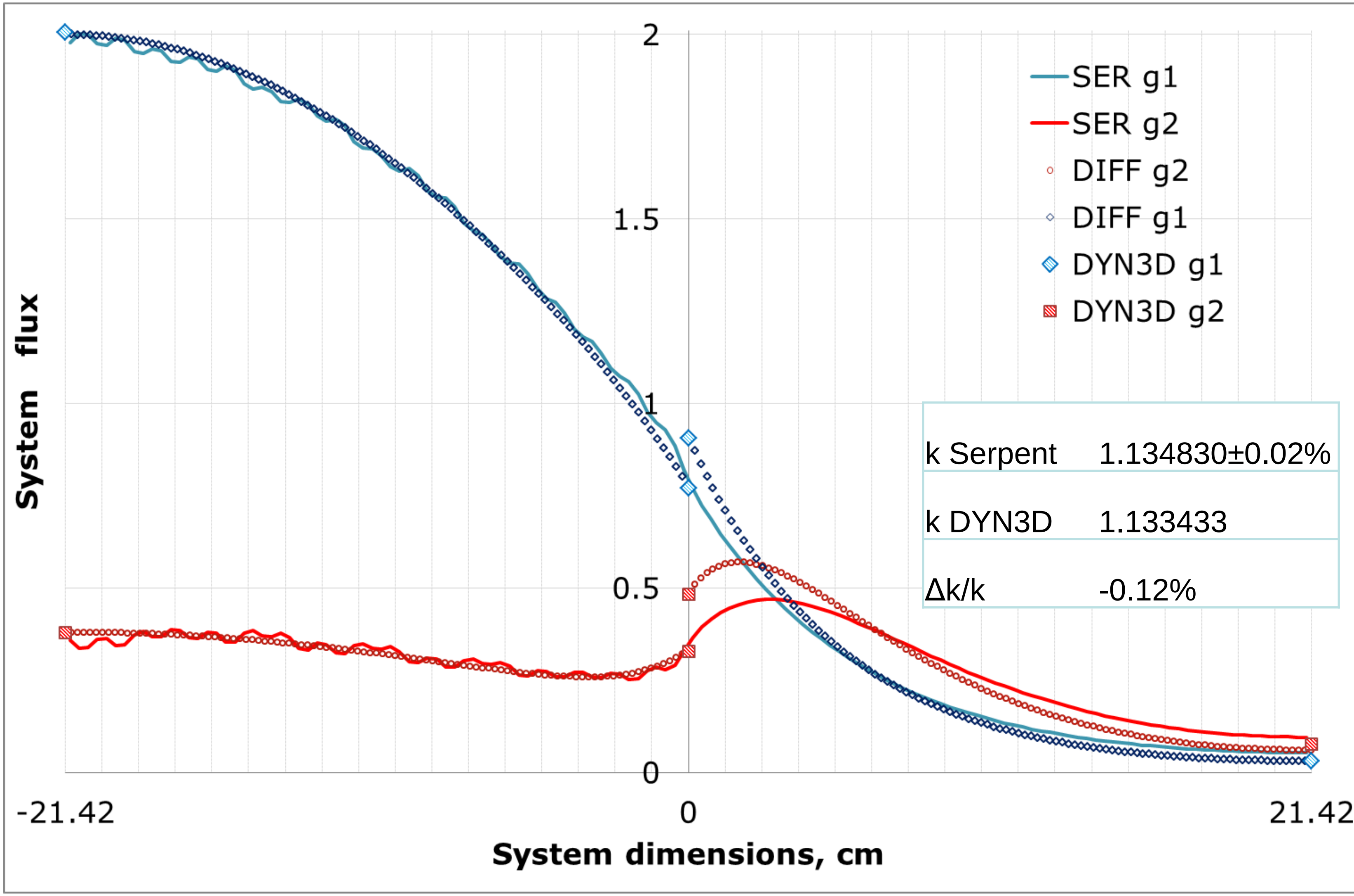


Flux in the F/R region



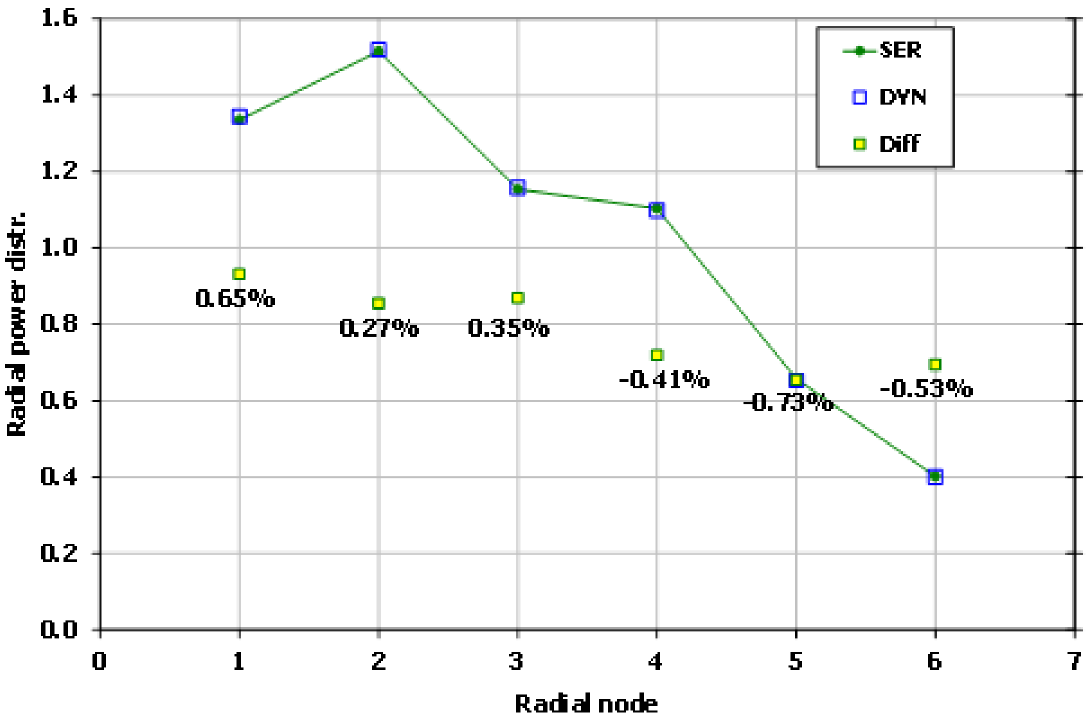
	Serpent direct	Via diffusion flux
DF_1	3.51	0.87
DF_2	1.37	0.71

Flux in the F/R region



Generation of reflector XS for nodal codes
Results of the test case

	k-eff	Δk/k
SERPENT	1.28148	
DYN3D	1.27990	0.12%
$\sigma_{k\text{-eff}}$=0.005%		



Neutron multiplication due to n,xn reactions

Neutron multiplication due to n,xn reactions

Neutron balance for group **g**, leakage excluded:

$$\overbrace{\Sigma_{a,g}\phi_g + \Sigma_{n1n,g}\phi_g + \Sigma_{n2n,g}\phi_g + \Sigma_{n3n,g}\phi_g \ldots}^{\Sigma_{t,g}}$$

$$= \overbrace{\sum_{h=1}^{G}\Sigma_{n1n}^{h\to g}\phi_h + 2\sum_{h=1}^{G}\Sigma_{n2n}^{h\to g}\phi_h + 3\sum_{h=1}^{G}\Sigma_{n3n}^{h\to g}\phi_h \ldots}^{\text{Full in-group scattering source}} + \frac{1}{k}\chi_g \overbrace{\sum_{h=1}^{G}\nu\Sigma_{f,h}\phi_h}^{\text{Fission source}}$$

In previous Serpent versions (before ver. 1.15):

- Only GTRANSFXS (group transfer XS matrix) was available
- GTRANSFXS = $\Sigma_{n1n}^{h\to g}$

Neutron multiplication due to n,xn reactions

The direct use of GTRANSFXS effectively means:

$$\overbrace{\Sigma_{a,g}\phi_g + \Sigma_{n1n,g}\phi_g + \cancel{\Sigma_{n2n,g}\phi_g} + \cancel{\Sigma_{n3n,g}\phi_g}\ldots}^{\Sigma_{t,g}} =$$

$$= \overbrace{\sum_{h=1}^{G}\Sigma_{n,1n}^{h\to g}\phi_h + 2\cancel{\sum_{h=1}^{G}\Sigma_{n,2n}^{h\to g}\phi_h} + 3\cancel{\sum_{h=1}^{G}\Sigma_{n,3n}^{h\to g}\phi_h}\ldots}^{\text{Full in-group scattering source}} + \frac{1}{k}\chi_g\overbrace{\sum_{h=1}^{G}\nu\Sigma_{f,h}\phi_h}^{\text{Fission source}}$$

The question: how to account for n,xn reactions (x>1) correctly?

Neutron multiplication due to n,xn reactions

Typical few-group XS libraries used by nodal codes:

- Can contain only a single group transfer XS matrix
- Some re-arrangement of neutron balance equation is required

1. Lump all n,xn XS into the one ***production*** scattering XS:

$$\upsilon\Sigma_s = \Sigma_{n1n} + 2\Sigma_{n2n} + 3\Sigma_{n3n} + \ldots$$

2. Re-write $\mathbf{\Sigma_t}$ in terms of $\mathbf{\upsilon\Sigma_s}$ and $\mathbf{\Sigma_{n,xn}}$

$$\Sigma_t = \Sigma_a + \upsilon\Sigma_s - (\Sigma_{n2n} + 2\Sigma_{n3n} + \ldots)$$

3. Define a modified $\mathbf{\Sigma_a}$

$$\Sigma_a^{mod} = \Sigma_a - (\Sigma_{n2n} + 2\Sigma_{n3n} + \ldots)$$

4. Re-write the balance equation in terms of $\mathbf{\upsilon\Sigma_s}$ and modified $\mathbf{\Sigma_a}$

$$\Sigma_{a,g}^{mod}\phi_g + \upsilon\Sigma_{s,g}\phi_g = \sum_{h=1}^{G}\upsilon\Sigma_s^{h\to g}\phi_h + \frac{1}{k}\chi_g\sum_{h=1}^{G}\nu\Sigma_{f,h}\phi_h$$

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Neutron multiplication due to n,xn reactions
Relevant modifications in few-group XS in Serpent 1.15

- Modifications
  - GTRANSFXS now includes **all** n,xn reactions
- New XS types
  - SCATTPRODXS = ***production*** scattering XS ($\upsilon\Sigma_s$)
  - GPRODXS = ***production*** group transfer XS matrix ($\upsilon\Sigma_s^{h\rightarrow g}$)
  - RABSXS = ***modified*** absorption XS (Σ_a^{mod})

Neutron multiplication due to n,xn reactions
Numerical example

Test case: typical PWR fuel assembly

	k-inf	Diff, pcm
SERPENT MC	1.33419 ± 7pcm	-
Neutron balance in 2g using **ABSXS + GTRANSFXS**	1.33204	**-121**
Neutron balance in 2g using **RABSXS + GPRODXS**	1.33407	**-8**

In deterministic codes…

From Helios methods:

II. 5.3 Cross-section adjustments for (n,2n) and (n,3n)

II. 5.3.1 Reactivity effects

To avoid the use of (n,2n) and (n,3n) cross-sections in the transport calculations, their effect is included in the definitions of the absorption cross-sections and scattering matrices in the library. This is done as follows:

$$\left.\begin{aligned} \sigma_a &\rightarrow \sigma_a^{\prime} = \sigma_a - \sigma_{n2n} - 2\sigma_{n3n} \\ \sigma_s &\rightarrow \sigma_s^{\prime} = \sigma_s + 2\sigma_{n2n} + 3\sigma_{n3n} \end{aligned}\right\} . \tag{40}$$

Summary

- In this presentation you saw
  - Some issues associated with few-group XS generation
  - As well as possible solutions
  - Supported by numerical examples

- Serpent can be used for few-group XS generation
  - For both multiplying and non-multiplying media

- Future work
  - Automatic scripts for branching calculations and data management
  - Generation of the data for transient nodal calculations
  - Verification via existing numerical benchmarks
    - RIA, boron dilution, etc

Thank you!