Differences in the Use of Nuclide χ Vectors Demonstrated with an Analytic k_∞ Problem

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Consider this k_∞ Problem

- Material is plutonium with density 14 g/cm^3

Nuclide	Density [atoms/(b·cm)]	Weight Fraction
Pu-239	0.03385770516	0.96
Pu-240	0.001404851530	0.04

- Geometry is a slab with width 1 cm
- 618-group MENDF71X collapsed to 8 energy groups
- PARTISN (discrete-ordinates) parameters: 0.0005-cm mesh; S_{256}; P_0 scattering expansion
- Nuclide cross sections were put in ACE format using the `simple_ace_mg.pl` utility
- MCNP parameters: 6,400,000 neutrons/cycle, 1000 active cycles (100 inactive)

Results for k_∞

Code	k_∞
PARTISN	2.9445993
MCNP6.2	2.94461 ± 0.00001

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Basically the same k_∞

Results for $S_{k_\infty,\chi^1_{\mathrm{Pu\,240}}}$

Code	$S_{k_\infty,\chi^1_{\mathrm{Pu\,240}}}$
PARTISN	7.442050E-07
MCNP6.2	2.7656E-06 ± 1.50 %

S is 3.7 × different

Analytic Solution for k_∞

- Homogeneous material, isotropic scattering, multigroup transport equation for k_∞:

$$\left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)\overline{\phi} = \frac{1}{k_\infty}\overline{\chi}\,\overline{\nu\Sigma_f}^T\overline{\phi},$$

where

+ $\overline{\nu\Sigma_f}$ is the vector of material $\nu\Sigma_f^g$ cross sections;
+ $\overline{\overline{\Sigma}}_t$ is the diagonal matrix of material Σ_t^g cross sections;
+ $\overline{\overline{\Sigma}}_s$ is the matrix of material group-to-group scattering cross sections;
+ $\overline{\chi}$ is the vector of material fission χ^g elements;
+ superscript T indicates transpose.

- The solution for k_∞ is[a]

$$k_\infty = \overline{\nu\Sigma_f}^T\left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)^{-1}\overline{\chi}$$

[a] A. SOOD, R. A. FORSTER, and D. K. PARSONS, "Analytical Benchmark Test Set for Criticality Code Verification," *Prog. Nucl. Energy*, **42**, *1*, 55–106 (2003); https://doi.org/10.1016/S0149-1970(02)00098-7.

Material Fission χ Vector χ^g

- The material fission $\overline{\chi}$ vector is composed of elements χ^g computed from the isotopic fission vectors $\overline{\chi_i}$ with elements χ_i^g using

$$\chi^g = \frac{\sum_{i=1}^{I} \chi_i^g N_i \sum_{g'=1}^{G} \nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G} \nu\sigma_{f,i}^{g'} f_i^{g'}},$$

where $f_i^{g'}$ is the spectrum weighting function and *I* is the number of fissionable nuclides in the material.

  + The spectrum weighting function is only available through the Nuclear Data Interface (NDI) at LANL.
  + For other cross section libraries, the spectrum weighting function is 1.

- If there is only one fissionable nuclide in the material, $\chi^g = \chi_1^g$, as expected.
- If there is only one energy group, regardless of the number of nuclides, then $\chi^1 = \chi_i^1 = 1$, which is not an interesting case.

- The product $\overline{\chi}\,\overline{\nu\Sigma_f}^T$ is called the *fission transfer matrix*. When isotopic fission χ vectors are used to create a material fission χ vector, the fission transfer matrix is

$$\overline{\chi}\,\overline{\nu\Sigma_f}^T = \begin{bmatrix} \chi^1 \\ \chi^2 \\ \vdots \\ \chi^G \end{bmatrix} \begin{bmatrix} \nu\Sigma_f^1 & \nu\Sigma_f^2 & \cdots & \nu\Sigma_f^G \end{bmatrix}$$

Fission Transfer Matrix

$$\overline{\chi}\,\overline{\nu\Sigma_f}^T = \begin{bmatrix} \chi^1 \\ \chi^2 \\ \vdots \\ \chi^G \end{bmatrix} \begin{bmatrix} \nu\Sigma_f^1 & \nu\Sigma_f^2 & \cdots & \nu\Sigma_f^G \end{bmatrix} = \begin{bmatrix} \chi^1\nu\Sigma_f^1 & \chi^1\nu\Sigma_f^2 & \cdots & \chi^1\nu\Sigma_f^G \\ \chi^2\nu\Sigma_f^1 & \chi^2\nu\Sigma_f^2 & \cdots & \chi^2\nu\Sigma_f^G \\ \vdots & \vdots & \ddots & \vdots \\ \chi^G\nu\Sigma_f^1 & \chi^G\nu\Sigma_f^2 & \cdots & \chi^G\nu\Sigma_f^G \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\sum_{i=1}^{I}\chi_i^1 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^1 & \frac{\sum_{i=1}^{I}\chi_i^1 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^2 & \cdots & \frac{\sum_{i=1}^{I}\chi_i^1 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^G \\ \frac{\sum_{i=1}^{I}\chi_i^2 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^1 & \frac{\sum_{i=1}^{I}\chi_i^2 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^2 & \cdots & \frac{\sum_{i=1}^{I}\chi_i^2 N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^G \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sum_{i=1}^{I}\chi_i^G N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^1 & \frac{\sum_{i=1}^{I}\chi_i^G N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^2 & \cdots & \frac{\sum_{i=1}^{I}\chi_i^G N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G}\nu\sigma_{f,i}^{g'} f_i^{g'}}\nu\Sigma_f^G \end{bmatrix}$$

Sensitivities of k_∞

- The vector of partial derivatives of k_∞ with respect to each element of $\overline{\chi}$ is

$$\overline{\partial k_\infty / \partial \chi} = \overline{\nu\Sigma_f}^T \left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)^{-1} .$$

- The derivative of χ^g with respect to χ_i^g for a particular nuclide is

$$\frac{\partial \chi^g}{\partial \chi_i^g} = \frac{N_i \sum_{g'=1}^{G} \nu\sigma_{f,i}^{g'} f_i^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G} \nu\sigma_{f,i}^{g'} f_i^{g'}} .$$

- The unconstrained relative sensitivity of k_∞ to χ_i^g is

$$S_{k_\infty,\chi_i^g} \equiv \frac{\chi_i^g}{k_\infty} \frac{\partial k_\infty}{\partial \chi_i^g} = \frac{\chi_i^g}{k_\infty} \frac{\partial k_\infty}{\partial \chi^g} \frac{\partial \chi^g}{\partial \chi_i^g} .$$

- The constrained relative sensitivity of k_∞ to χ_i^g, which accounts for the fact that changing one entry requires the others to change to preserve the normalization, is

$$S_{k_\infty,\chi_i^g}^{FN} = S_{k_\infty,\chi_i^g} - \chi_i^g \sum_{g=1}^{G} S_{k_\infty,\chi_i^g} ,$$

where *FN* indicates full normalization.[b]

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[b] J. A. FAVORITE, Z. PERKÓ, B. C. KIEDROWSKI, and C. M. PERFETTI, "Adjoint-Based Sensitivity and Uncertainty Analysis for Density and Composition: A User's Guide," *Nucl. Sci. Eng.*, **185**, *3*, 384–405 (2017); https://doi.org/10.1080/00295639.2016.1272990

k_∞ Using χ Matrix

- When the full matrix fission $\overline{\overline{\chi}}$ is used, there is not a closed-form solution for k_∞. The multigroup transport equation for k_∞ becomes

$$\left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)\overline{\phi} = \frac{1}{k_\infty}\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma}}_f\overline{\phi},$$

where $\overline{\overline{\nu\Sigma}}_f$ is the diagonal matrix of material $\nu\Sigma_f^g$ cross sections.

- The equation is solved iteratively, starting with initial guesses for $\overline{\phi}$ and k_∞:

$$\overline{\phi}^{k+1} = \frac{1}{k_\infty^k}\left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)^{-1}\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma}}_f\overline{\phi}^k,$$

(superscript k is the iteration index).

- At each iteration, the updated k_∞^{k+1} is computed using

$$k_\infty = \left[\overline{I}^T\left(\overline{\overline{\Sigma}}_t - \overline{\overline{\Sigma}}_s\right)\overline{\phi}\right]^{-1}\left[\overline{I}^T\overline{\overline{\chi}}\,\overline{\overline{\nu\Sigma}}_f\overline{\phi}\right],$$

where $\overline{I}$ is a vector whose elements are all unity.

Material Fission χ Matrix $\chi^{g'\to g}$

- The material $\chi^{g'\to g}$ is computed from the isotopic $\chi_i^{g'\to g}$ values using

$$\chi^{g'\to g} = \frac{\sum_{i=1}^{I} \chi_i^{g'\to g} N_i \nu \sigma_{f,i}^{g'}}{\sum_{i=1}^{I} N_i \nu \sigma_{f,i}^{g'}} = \frac{\sum_{i=1}^{I} \chi_i^{g'\to g} N_i \nu \sigma_{f,i}^{g'}}{\nu \Sigma_f^{g'}}.$$

(Note that this does not have the spectrum weighting function $f_i^{g'}$.)

- If there is only one fissionable nuclide in the material, $\chi^{g'\to g} = \chi_1^{g'\to g}$, as expected.
- If there is only one energy group, regardless of the number of nuclides, then $\chi^{1\to 1} = \chi_i^{1\to 1} = 1$, again not an interesting case.

- When isotopic fission χ matrices are used to create a material fission χ matrix, the fission transfer matrix is

$$\overline{\overline{\chi \nu \Sigma_f}} = \begin{bmatrix} \chi^{1\to 1} & \chi^{2\to 1} & \cdots & \chi^{G\to 1} \\ \chi^{1\to 2} & \chi^{2\to 2} & \cdots & \chi^{G\to 2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi^{1\to G} & \chi^{2\to G} & \cdots & \chi^{G\to G} \end{bmatrix} \begin{bmatrix} \nu\Sigma_f^1 & 0 & \cdots & 0 \\ 0 & \nu\Sigma_f^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \nu\Sigma_f^G \end{bmatrix}$$

Fission Transfer Matrix

$$\overline{\overline{\chi \nu \Sigma_f}} = \begin{bmatrix} \chi^{1\to1} & \chi^{2\to1} & \cdots & \chi^{G\to1} \\ \chi^{1\to2} & \chi^{2\to2} & \cdots & \chi^{G\to2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi^{1\to G} & \chi^{2\to G} & \cdots & \chi^{G\to G} \end{bmatrix} \begin{bmatrix} \nu\Sigma_f^1 & 0 & \cdots & 0 \\ 0 & \nu\Sigma_f^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \nu\Sigma_f^G \end{bmatrix}$$

$$= \begin{bmatrix} \chi^{1\to1}\nu\Sigma_f^1 & \chi^{2\to1}\nu\Sigma_f^2 & \cdots & \chi^{G\to1}\nu\Sigma_f^G \\ \chi^{1\to2}\nu\Sigma_f^1 & \chi^{2\to2}\nu\Sigma_f^2 & \cdots & \chi^{G\to2}\nu\Sigma_f^G \\ \vdots & \vdots & \ddots & \vdots \\ \chi^{1\to G}\nu\Sigma_f^1 & \chi^{2\to G}\nu\Sigma_f^2 & \cdots & \chi^{G\to G}\nu\Sigma_f^G \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{i=1}^{I} \chi_i^{1\to1} N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^{2\to1} N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^{G\to1} N_i \nu\sigma_{f,i}^G \\ \sum_{i=1}^{I} \chi_i^{1\to2} N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^{2\to2} N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^{G\to2} N_i \nu\sigma_{f,i}^G \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{I} \chi_i^{1\to G} N_i \nu\sigma_{f,i}^1 & \sum_{i=1}^{I} \chi_i^{2\to G} N_i \nu\sigma_{f,i}^2 & \cdots & \sum_{i=1}^{I} \chi_i^{G\to G} N_i \nu\sigma_{f,i}^G \end{bmatrix}$$

If Only the Vector χ Is Available for Each Nuclide

- The elements of each isotopic fission χ matrix $\overline{\overline{\chi_i}}$ are

$$\overline{\overline{\chi_i}} = \begin{bmatrix} \chi_i^{1\to1} & \chi_i^{2\to1} & \cdots & \chi_i^{G\to1} \\ \chi_i^{1\to2} & \chi_i^{2\to2} & \cdots & \chi_i^{G\to2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_i^{1\to G} & \chi_i^{2\to G} & \cdots & \chi_i^{G\to G} \end{bmatrix}.$$

- However, if only the vector $\overline{\chi_i}$ is available for each nuclide, then every group g' has the same contribution to group g.

- The elements of $\overline{\overline{\chi_i}}$ become

$$\overline{\overline{\chi_i}} = \begin{bmatrix} \chi_i^{1\to1} & \chi_i^{1\to1} & \cdots & \chi_i^{1\to1} \\ \chi_i^{2\to2} & \chi_i^{2\to2} & \cdots & \chi_i^{2\to2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_i^{G\to G} & \chi_i^{G\to G} & \cdots & \chi_i^{G\to G} \end{bmatrix} = \begin{bmatrix} \chi_i^{1} & \chi_i^{1} & \cdots & \chi_i^{1} \\ \chi_i^{2} & \chi_i^{2} & \cdots & \chi_i^{2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_i^{G} & \chi_i^{G} & \cdots & \chi_i^{G} \end{bmatrix}.$$

If Only the Vector χ Is Available for Each Nuclide (cont.)

- Using $\chi^{g'\to g} = \dfrac{\sum_{i=1}^{I} \chi_i^{g'\to g} N_i \nu\sigma_{f,i}^{g'}}{\nu\Sigma_f^{g'}}$, the material χ matrix is

$$\overline{\overline{\chi}} = \begin{bmatrix} \dfrac{\sum_{i=1}^{I}\chi_i^1 N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \dfrac{\sum_{i=1}^{I}\chi_i^1 N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \dfrac{\sum_{i=1}^{I}\chi_i^1 N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \\ \dfrac{\sum_{i=1}^{I}\chi_i^2 N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \dfrac{\sum_{i=1}^{I}\chi_i^2 N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \dfrac{\sum_{i=1}^{I}\chi_i^2 N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\sum_{i=1}^{I}\chi_i^G N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \dfrac{\sum_{i=1}^{I}\chi_i^G N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \dfrac{\sum_{i=1}^{I}\chi_i^G N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \end{bmatrix}$$

- In general, the columns of $\overline{\overline{\chi}}$ are not the same, unlike the columns of $\overline{\overline{\chi_i}}$.

- Thus, even though only χ vectors for isotopes may be given, a material χ matrix may result, depending on assumptions or conventions.

Sensitivities of k_∞

- There is no convenient expression for $\dfrac{\partial k_\infty}{\partial \chi^{g' \to g}}$.

- Sensitivities are calculated using direct perturbations in a central difference.

  + Perturb χ_i^g to $\chi_i^g + \Delta\chi_i^g$; then, normalize every element of the perturbed $\overline{\chi_i}$.
  Solve for $k_{\infty,+}$ with the perturbed, renormalized $\overline{\chi_i}$.
  + Do the same with the opposite perturbation $-\Delta\chi_i^g$ to compute $k_{\infty,-}$.
  + The relative sensitivity is approximately

$$S_{k_\infty,\chi_i^g}^{FN} \approx \frac{\chi_i^g}{k_\infty} \frac{k_{\infty,+} - k_{\infty,-}}{2\Delta\chi_i^g}.$$

  + The accuracy depends on the linearity of the three points $(-\Delta\chi_i^g, k_{\infty,-})$, $(0, k_\infty)$, and $(\Delta\chi_i^g, k_{\infty,+})$.
  + Note that the central difference uses the input $\Delta\chi_i^g$ in the denominator, not the change in χ_i^g after the renormalization.

Sampling Fission in MCNP

- In multigroup or continuous-energy mode, MCNP first samples the neutron's distance to collision in the material, then samples what type of collision occurred.

- If it is fission, then it samples for the fissioning nuclide at incoming neutron energy g' using probabilities $N_i \nu\sigma_{f,i}^{g'} / \nu\Sigma_f^{g'}$, $i = 1,\ldots,I$, where I is the number of fissionable nuclides.

- Then it samples for the outgoing energy group g from that nuclide's χ vector (in multigroup).

- Given a fission event and incoming group g', then, the probability of choosing nuclide i and outgoing group g is $\chi_i^g N_i \nu\sigma_{f,i}^{g'} / \nu\Sigma_f^{g'}$.

- The overall probability of choosing outgoing group g is the sum over all fissionable nuclides: $\sum_{i=1}^{I} \chi_i^g N_i \nu\sigma_{f,i}^{g'} \Big/ \nu\Sigma_f^{g'}$.

If only the vector χ is available for each nuclide, the material χ matrix is

$$\overline{\overline{\chi}} = \begin{bmatrix} \frac{\sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \frac{\sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \frac{\sum_{i=1}^{I} \chi_i^1 N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \\ \frac{\sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \frac{\sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \frac{\sum_{i=1}^{I} \chi_i^2 N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^1}{\nu\Sigma_f^1} & \frac{\sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^2}{\nu\Sigma_f^2} & \cdots & \frac{\sum_{i=1}^{I} \chi_i^G N_i \nu\sigma_{f,i}^G}{\nu\Sigma_f^G} \end{bmatrix}$$

Fission in PARTISN

- PARTISN version 8 is now available from RSICC.
  - Uses keyword `fissdata` in block 3 to specify whether to use a χ vector or matrix for all nuclides.
  - Only useful at Los Alamos.

- For external users, PARTISN uses fission χ vectors.

- The material fission $\overline{\chi}$ vector is composed of elements χ^g computed from the isotopic fission vectors $\overline{\chi_i}$ with elements χ_i^g using

$$\chi^g = \frac{\sum_{i=1}^{I} \chi_i^g N_i \sum_{g'=1}^{G} \nu\sigma_{f,i}^{g'}}{\sum_{i=1}^{I} N_i \sum_{g'=1}^{G} \nu\sigma_{f,i}^{g'}}$$

Main Conclusion

- Even when you input multigroup fission χ vectors for nuclides, MCNP uses a material fission χ matrix!
- If you compare with PARTISN or with analytic solutions and don't account for this, you will be surprised.

Isn't this Obvious?

- None of the differences arise if:
  - + the test material has only one nuclide
  - + PARTISN uses a fission χ matrix

- The differences may be masked if different nuclear data are used in the comparison…
  - + Such as "continuous energy" vs. multigroup.

- Some combination of these probably explains why previous comparisons of Monte Carlo and deterministic sensitivities to χ did not seem to find this effect.

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Analytical Benchmark Test Set For Criticality Code Verification

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Abstract

A number of published numerical solutions to analytic eigenvalue (k_{eff}) and eigen-function equations are summarized for the purpose of creating a criticality verification benchmark test set. The 75-problem test set allows the user to verify the correctness of a criticality code for infinite medium and simple geometries in one-

5.2.2 Two-Group U-D_2O Reactor.

Two-Group Anisotropic Macroscopic Cross Sections

Tables 53 and 54 gives the two-group, linearly anisotropic cross sections for the U-D_2O system.

Table 53
Fast Energy Group Cross Sections for Linearly Anisotropic Scattering (cm^{-1}) for U-D_2O

Material	ν_2	Σ_{2f}	Σ_{2c}	Σ_{22s_0}	Σ_{22s_1}	Σ_{12s_0}	Σ_{12s_1}	Σ_2	χ_2
D_2O	2.50	0.0028172	0.0087078	0.31980	0.06694	0.004555	-0.0003972	0.33588	1.0

Table 54
Slow Energy Group Cross Sections for Linearly Anisotropic Scattering (cm^{-1}) for U-D_2O

Material	ν_1	Σ_{1f}	Σ_{1c}	Σ_{11s_0}	Σ_{11s_1}	Σ_{21s}	Σ_1	χ_1
D_2O	2.50	0.097	0.02518	0.42410	0.05439	0.0	0.54628	0.0

Infinite Medium (UD2O-2-1-IN)

The test set uses the two-group linearly anisotropic D_2O cross section set from Tables 53 and 54 with $k_\infty = 1.000227$ (problem 72) and the group 2 to group 1 flux

Consider this k_∞ Problem

- Material is plutonium with density 14 g/cm^3

Nuclide	Density [atoms/(b·cm)]	Weight Fraction
Pu-239	0.03385770516	0.96
Pu-240	0.001404851530	0.04

- Geometry is a slab with width 1 cm
- 618-group MENDF71X collapsed to 8 energy groups
- PARTISN (discrete-ordinates) parameters: 0.0005-cm mesh; S_{256}; P_0 scattering expansion
- Nuclide cross sections were put in ACE format using the `simple_ace_mg.pl` utility
- MCNP parameters: 6,400,000 neutrons/cycle, 1000 active cycles (100 inactive)

Did PARTISN use a χ vector or matrix?

If vector, was weighting function f_i^g used?

Results for k_∞

Code	k_∞
PARTISN	2.9445993
MCNP6.2	2.94461 ± 0.00001

Basically the same k_∞

Results for $S_{k_\infty,\chi^1_{\mathrm{Pu}\,240}}$

Code	$S_{k_\infty,\chi^1_{\mathrm{Pu}\,240}}$
PARTISN	7.442050E-07
MCNP6.2	2.7656E-06 ± 1.50 %

S is 3.7 × different

Comparison of k_∞ Values

- Analytic

Equation	Value	Equation	Value
Vector, with f	2.94459933	Vector, $f = 1$	2.94460099
Matrix	2.94460193	Matrix	2.94460193
Difference	–0.00008814%	Difference	–0.00003192%

$$\text{Difference} = \frac{(R_1 - R_2)}{\frac{1}{2}(R_1 + R_2)}$$

- All χ vector, deterministic

Calculation	Value	Difference
Analytic[(a)]	2.9445993	N/A
PARTISN	2.9445993	–0.000001%

(a) Using the actual spectrum weighting function.

- Isotopic χ vector, material χ matrix, Monte Carlo

Calculation	Value	Difference	Difference ($N\sigma$)
Analytic	2.94460	N/A	N/A
MCNP	2.94461 ± 0.00001	0.000274%	0.81

Analytic Sensitivities Compared

- Constrained Sensitivities of k_∞ to χ, Analytic, Not Using the NDI Spectrum Weighting Function (Full Normalization) (%/%)

Isotope	Group	Vector χ, $f = 1$	Matrix χ	Difference
Pu-239	1	1.023819E-04	1.017157E-04	0.65285%
	2	1.033315E-03	1.026591E-03	0.65284%
	3	2.654926E-02	2.637802E-02	0.64707%
	4	–1.119365E-02	–1.112195E-02	0.64257%
	5	–1.031274E-02	–1.024650E-02	0.64446%
	6	–5.565518E-03	–5.529357E-03	0.65186%
	7	–5.786425E-04	–5.748772E-04	0.65283%
	8	–3.440293E-05	–3.417906E-05	0.65285%
Pu-240	1	2.037760E-06	2.762766E-06	–30.205%
	2	1.977692E-05	2.681326E-05	–30.205%
	3	4.854356E-04	6.581838E-04	–30.211%
	4	–2.050723E-04	–2.780627E-04	–30.215%
	5	–1.891339E-04	–2.564481E-04	–30.214%
	6	–1.018182E-04	–1.380452E-04	–30.206%
	7	–1.059340E-05	–1.436239E-05	–30.205%
	8	–6.323635E-07	–8.573494E-07	–30.205%

Using the spectrum weighting function, these go to 1.8%

Using the spectrum weighting function, these go to –115%

Code Verification: SENSMG

- Constrained Sensitivities of k_∞ to χ, Deterministic Transport (Full Normalization) (%/%)

Isotope	Group	Analytic	SENSMG	Difference
Pu-239	1	1.035708E-04	1.035708E-04	–0.000035%
	2	1.045315E-03	1.045315E-03	0.000003%
	3	2.685757E-02	2.685757E-02	0.000011%
	4	–1.132364E-02	–1.132364E-02	0.000034%
	5	–1.043250E-02	–1.043250E-02	–0.000026%
	6	–5.630149E-03	–5.630149E-03	–0.000005%
	7	–5.853621E-04	–5.853621E-04	–0.000006%
	8	–3.480244E-05	–3.480244E-05	–0.000008%
Pu-240	1	7.442050E-07	7.442050E-07	0.000001%
	2	7.222675E-06	7.222675E-06	–0.000001%
	3	1.772846E-04	1.772846E-04	–0.000021%
	4	–7.489392E-05	–7.489392E-05	0.000000%
	5	–6.907309E-05	–6.907309E-05	–0.000005%
	6	–3.718477E-05	–3.718477E-05	–0.000002%
	7	–3.868789E-06	–3.868789E-06	0.000000%
	8	–2.309438E-07	–2.309438E-07	–0.000008%

Code Verification: MCNP (KSEN)

- Constrained Sensitivities of k_∞ to χ, Monte Carlo Transport (Full Normalization) (%/%)

Isotope	Group	Analytic CD	KSEN	Difference	Difference ($N\sigma$)
Pu-239	1	1.01716E-04	1.0212E-04 ± 1.04%	0.3975%	0.38
	2	1.02659E-03	1.0256E-03 ± 0.33%	–0.0966%	–0.29
	3	2.63780E-02	2.6405E-02 ± 0.12%	0.1023%	0.85
	4	–1.11220E-02	–1.1145E-02 ± 0.31%	0.2072%	0.67
	5	–1.02465E-02	–1.0243E-02 ± 0.16%	–0.0341%	–0.21
	6	–5.52936E-03	–5.5350E-03 ± 0.16%	0.1021%	0.64
	7	–5.74877E-04	–5.7564E-04 ± 0.29%	0.1327%	0.46
	8	–3.41791E-05	–3.3591E-05 ± 1.14%	–1.7205%	–1.54
Pu-240	1	2.76277E-06	2.7656E-06 ± 1.50%	0.1026%	0.07
	2	2.68133E-05	2.6776E-05 ± 0.44%	–0.1390%	–0.32
	3	6.58184E-04	6.5929E-04 ± 0.19%	0.1681%	0.88
	4	–2.78063E-04	–2.7880E-04 ± 0.48%	0.2652%	0.55
	5	–2.56448E-04	–2.5651E-04 ± 0.29%	0.0241%	0.08
	6	–1.38045E-04	–1.3822E-04 ± 0.29%	0.1267%	0.44
	7	–1.43624E-05	–1.4478E-05 ± 0.62%	0.8050%	1.29
	8	–8.57349E-07	–8.3399E-07 ± 2.39%	–2.7246%	–1.17

Main Conclusion

- Even when you input multigroup fission χ vectors for nuclides, MCNP uses a material fission χ matrix!
- If you compare with PARTISN or with analytic solutions and don't account for this, you will be surprised.

Main Conclusion + Other Conclusions

- Even when you input multigroup fission χ vectors for nuclides, MCNP uses a material fission χ matrix!
- If you compare with PARTISN or with analytic solutions and don't account for this, you will be surprised.
- Accounting for this, we verified SENSMG and MCNP's KSEN.