Serpent User's group meeting, Berkeley, CA, November 6-8, 2013

Generation of One-Group Cross Sections for coupled MC codes

D. Kotlyar, E. Fridman, E. Shwageraus

Department of Nuclear Engineering,

Ben Gurion University of the Negev

Outline

- Introduction
  - Depletion problem description
- Multi-group approach
  - Choosing the number of groups
  - Generating self shielded cross sections
  - Calculating background cross section
- Results
  - Number of groups vs. CPU time
- Summary and conclusions

Depletion problem

- Solve Bateman eq. for each nuclide in each burnable zone:

$$\frac{dN_j(t)}{dt} = -\lambda_j N_j(t) - \phi\sigma_j N_j(t) + \sum_{k=1}^{k=n} \lambda_k BR_{k\to j} N_k(t) + \phi\left(\sigma_{k\to j} N_k(t)\right)$$

Disappearance due to decay

Disappearance due to neutron absorption

Rate of amount change of nuclide **i**

Buildup due to decay of other nuclides

Buildup due to absorption in other nuclides

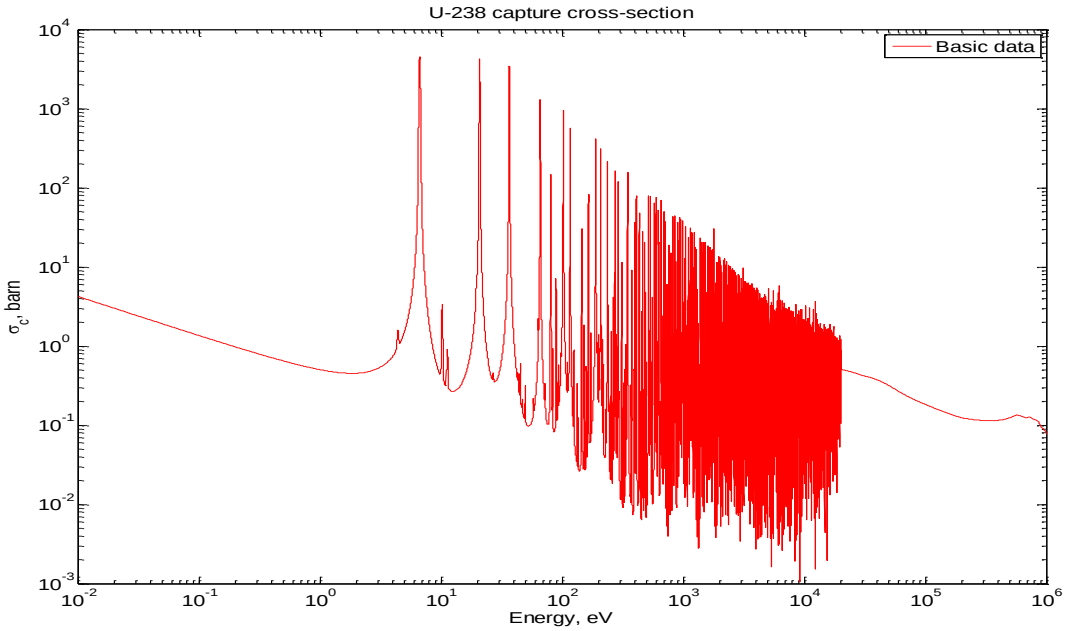
- Required data:
  - Decay constants ⇒ available directly from ENDF
  - Fission product yields ⇒ available directly from ENDF
  - One-group cross sections ⇒ MC transport solution
  - Fluxes ⇒ MC transport solution

One-group cross section generation

- **Direct tally** method
  - MC transport to obtain 1G reaction rates:
    - For every reaction type;
    - In every isotope;
- **Multi-group (MG)** method
  - MC transport to obtain fine spectrum (>10K groups)
  - External collapsing procedure into 1G
    - Requires separate lib of pre-generated MG cross-sections for each isotope and reaction type
- **Main trade-offs**
  - Direct tally ⇒ requires more CPU time (up to ×30)
  - MG ⇒ requires more data storage space

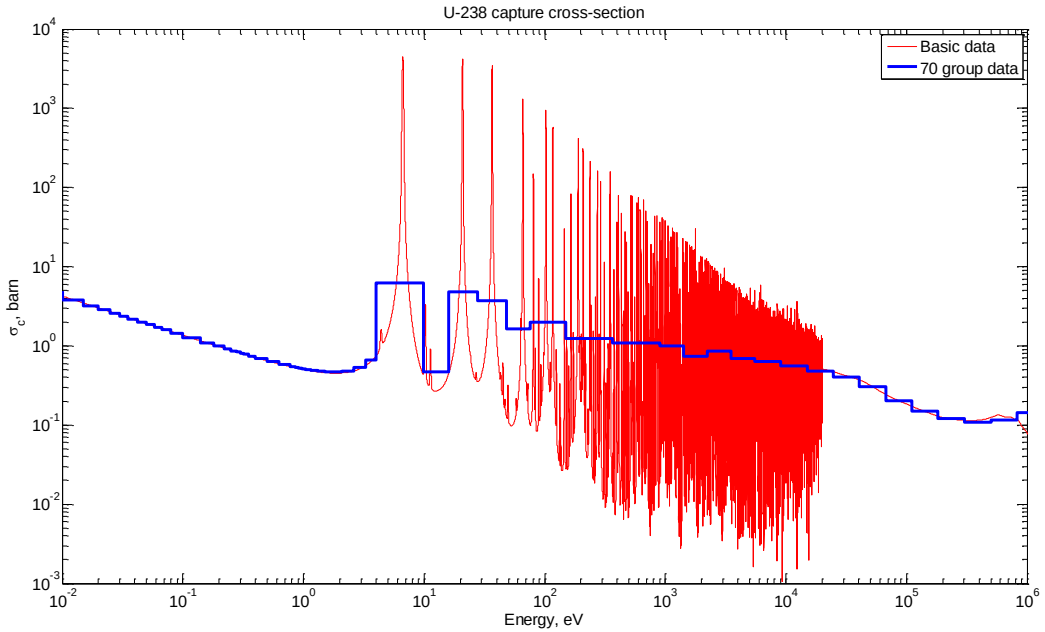
Preparation of MG data sets (1)

- Basic data libraries
  - Reaction cross sections: *(n,γ), (n,f), (n,xn), etc*
    - *Cover entire neutron energy range (up to 25 MeV)*
  - Examples:
    - Joint European Data Files (JEFF)
    - Evaluated Nuclear Data Files (ENDF)



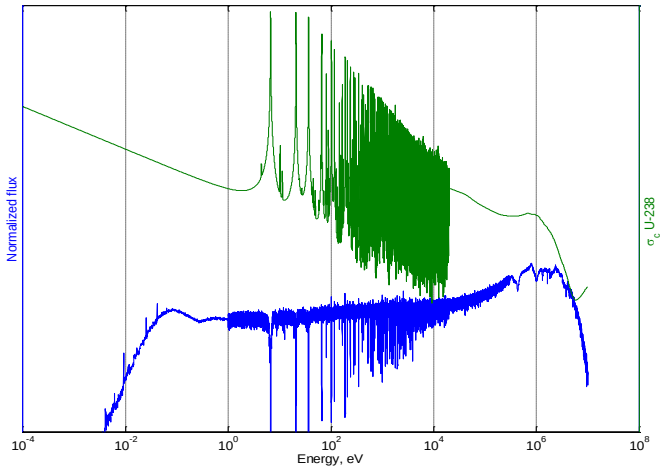
Preparation of MG data sets (2)

- Routine reactor calculation practices:
  - Basic point wise data is not used directly
  - Use pre-generated microscopic cross-sections in limited no. of groups
    - *Typical energy range covered: 0.0001 eV – 25 MeV*
  - **NJOY** is used to generate MG XS in few groups
    - *Group XS become spectrum dependent*
    - *Require tabulation against T and Bondarenko "background"*

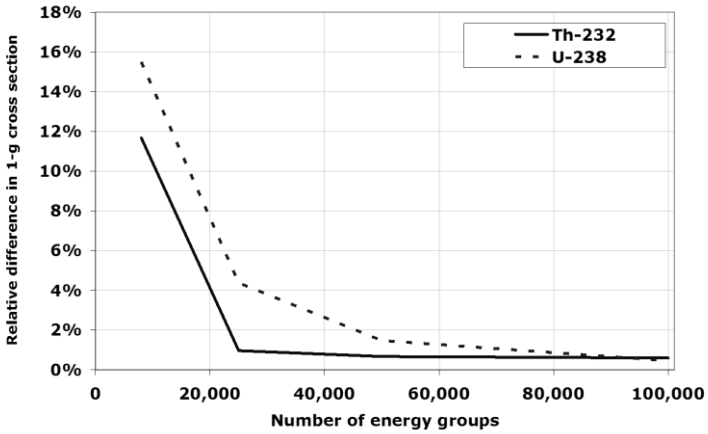


Generation of 1G cross-sections

- Presumably, if NG $\rightarrow \infty \Rightarrow$ infinite dilution XS can be used
  - Preserving the reaction rates:
    - $\bar{\sigma} = \frac{\int \sigma(E)\varphi(E)}{\int \varphi(E)} \Rightarrow \bar{\sigma} = \frac{\sum \sigma_i \varphi_i}{\sum \varphi_i}$



- Proved to be not true
  - Probabilistic treatment of unresolved res.
  - Even with NG $\rightarrow \infty$, ~ 1% systematic error
  - **Solution:**
    - tabulate against background XS
  - Background XS is not easy to obtain



Extension of MG approach

- **Simplified tabulation against σ_0** (Fridman et al., 2008)
  - Generate fine group XS for multiple values of σ_0
  - Tabulation is used only in the resonance region
  - Calculate energy and spatial components of σ_0
    - Use potential scattering XS data from ENDF
    - Ask user to provide basic fuel geometry (e.g. chord length)
  - Interpolate between σ_0 to obtain "shielded" in each group
  - The approach was proven to fix the systematic error problem

Simplified σ_0 model (a = γ = 1)

- The approach simplifies basic lattice physics

$$\sigma_{0,j} = \frac{\sum_{i=1}^{M} N_i \sigma_{p,i} + \frac{1/R}{1/a + 1/\gamma - 1}}{N_j}$$

  - Neglects Dancoff shadowing effect (γ = 1)
  - Neglects empirical correction to the Wigner rational approximation (Bell Factor, a = 1)

- **Procedure** for 1G XS generation
  - Collapsing of the MG set for different σ_0
  - Estimation of the σ_0 value
  - The σ_0 value is used to extract the 1G XS

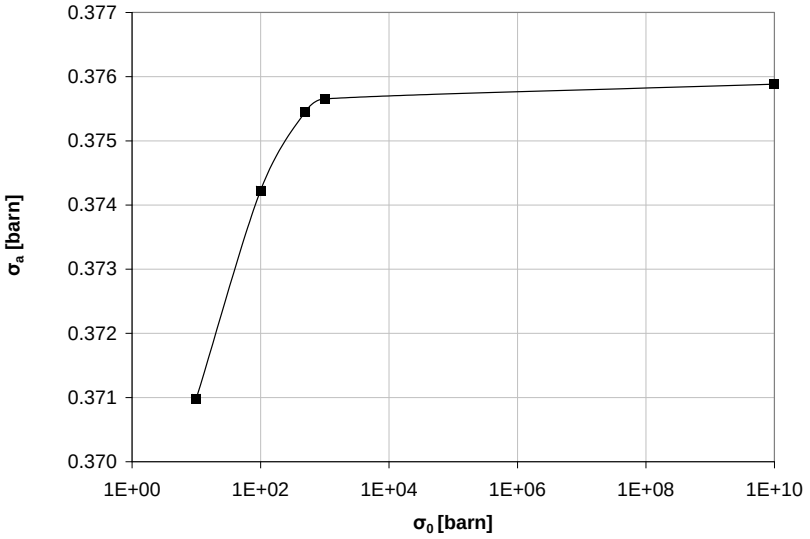
Simplified σ_0 model (a = γ = 1)

- The approach simplifies basic lattice physics

$$\sigma_{0,j} = \frac{\sum_{i=1}^{M} N_i \sigma_{p,i} + \frac{1/R}{1/a + 1/\gamma - 1}}{N_j}$$

  - Neglects Dancoff shadowing effect (γ = 1)
  - Neglects empirical correction to the Wigner rational approximation (Bell Factor, a = 1)

- **Procedure** for 1G XS generation
  - Collapsing of the MG set for different σ_0
  - Estimation of the σ_0 value
  - The σ_0 value is used to extract the 1G XS



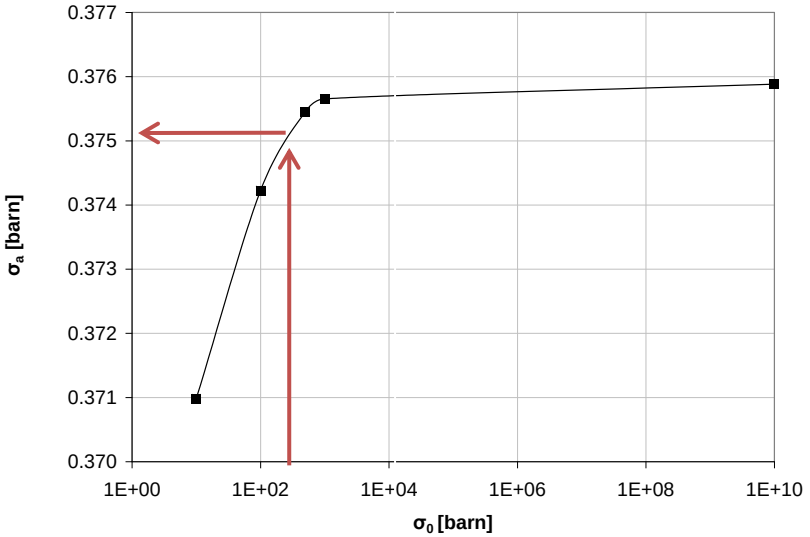
Simplified σ_0 model (a = γ = 1)

- The approach simplifies basic lattice physics

$$\sigma_{0,j} = \frac{\sum_{i=1}^{M} N_i \sigma_{p,i} + \frac{1/\bar{R}}{1/a + 1/\gamma - 1}}{N_j}$$

  - Neglects Dancoff shadowing effect (γ = 1)
  - Neglects empirical correction to the Wigner rational approximation (Bell Factor, a = 1)

- **Procedure** for 1G XS generation
  - Collapsing of the MG set for different σ_0
  - Estimation of the σ_0 value
  - The σ_0 value is used to extract the 1G XS



- In LWRs: a ~ 1.2, γ ~ 0.8
  - $\Rightarrow$ cancellation of errors $\Rightarrow$ does not always work

Open questions

- How to make MG approach universally applicable?
- Can it be extended beyond unresolved resonances range?
- Can the number of groups be reduced?
- Will this save CPU time?

Reconstruction of σ_0 from MC statistics

- MCNP collects some RR statistics (table 140)
- **Can be used to reconstruct σ_0**

$$\sigma_{0,j} = \frac{\sum_{i=1}^{M} N_i \sigma_{p,i} + \frac{1/R}{1/a + 1/\gamma - 1}}{N_j}$$

1. Calculate 1G σ_a for nuclide *j*

$$\overline{\sigma_a^j} = \frac{w_c^j + w_f^j \left[\frac{\#}{SN}\right]}{\phi\left[\frac{\#}{cm^2 \cdot SN}\right] \cdot V\left[cm^3\right] \cdot N_j\left[\frac{\#}{b \cdot cm}\right]}$$

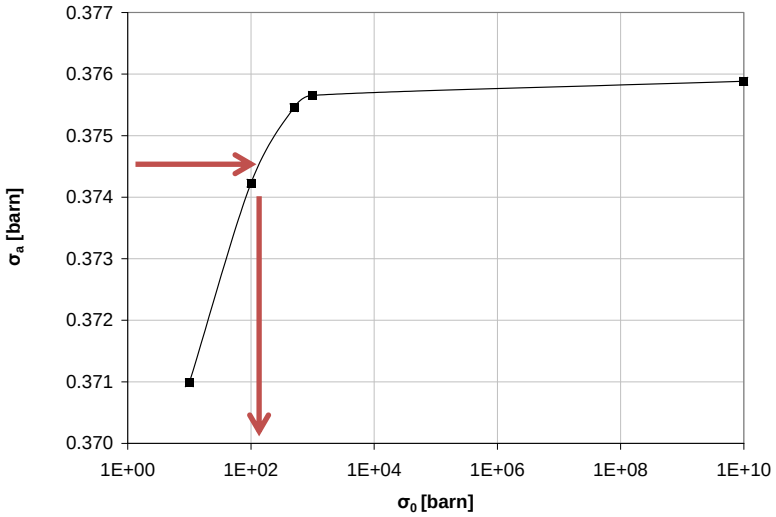
2. Collapsing of the MG set for different σ_0
3. Reconstruction of $\sigma_{0,j}$
4. Calculation of R^*_j
5. Calculation of the average
6. The average $\overline{R*}$ is to calculate the σ_0 and, the 1-g XS for all the nuclides

Reconstruction of σ_0 from MC statistics

- MCNP collects some RR statistics (table 140)
- **Can be used to reconstruct σ_0**

$$\sigma_{0,j} = \frac{\sum_{i=1}^{M} N_i \sigma_{p,i} + \frac{1/\bar{R}}{1/a + 1/\gamma - 1}}{N_j}$$

1. Calculate of 1-g σ_a for nuclide *j*
2. Collapse MG set for different σ_0
3. Reconstruct $\sigma_{0,j}$
4. Calculation of R^*_j
5. Calculation of the average $\overline{R*}$
6. The average $\overline{R*}$ is to calculate the σ_0 and, the 1-g XS for all the nuclides



Reconstruction of σ_0 from MC statistics

- The model relies on statistical data to calculate (**a,γ**)
- **Procedure** for 1-g XS generation

$$\sigma_{0,j} = \frac{\sum_{i=1}^{M} N_i \sigma_{p,i} + \frac{1/R}{1/a + 1/\gamma - 1}}{N_j}$$

1. Calculate of 1-g σ_a for nuclide *j*
2. Collapse MG set for different σ_0
3. Reconstruct $\sigma_{0,j}$
4. Calculation of R^*_j

$$\sigma_{0,j} = \frac{\sum_{i=1}^{M} N_i \sigma_{p,i} + 1/R^*_j}{N_j}$$

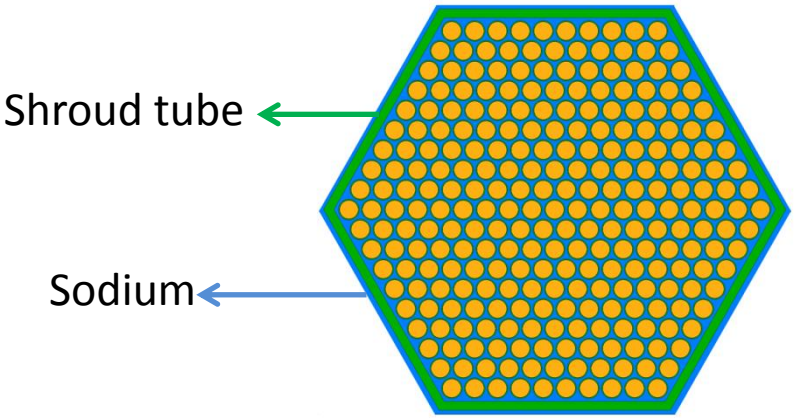
5. Calculation of the average $\overline{R*}$

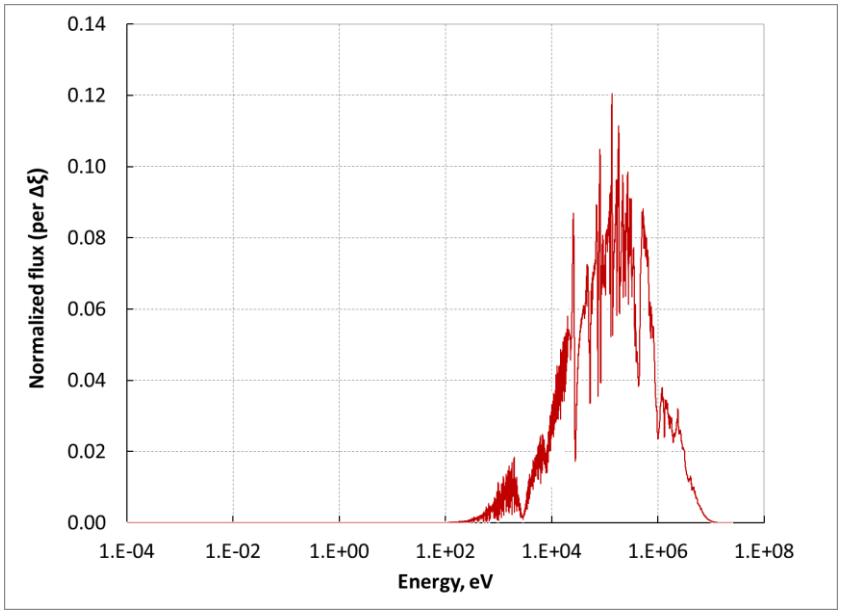
$$\overline{R^*} = \frac{\sum_{j=1}^{M} R^*_j \cdot w^j_a}{\sum_{j=1}^{M} w^j_a}$$

6. The average $\overline{R*}$ is to calculate the σ_0 and 1G XS for all the nuclides

Test case: SFR assembly

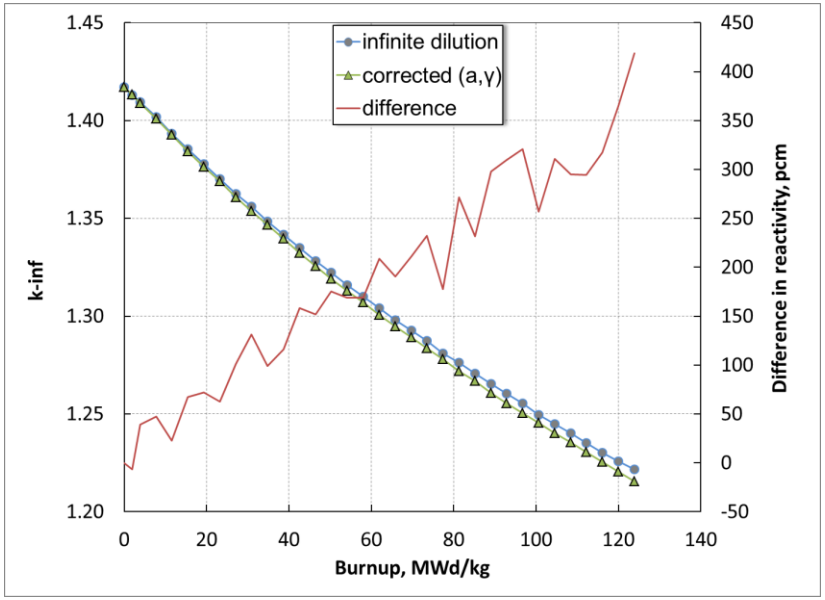
- **Sodium cooled fast reactor (Fiorini and Vasile, 2011)**
  - 38% of total absorption is in unresolved resonances
  - Self-shielding effect is of major importance
- **Input data**
  - Fuel: Pu MOX
  - Temperature = 300K
  - Power density = 206 W/cm^3
  - Number of fuel pins = 271

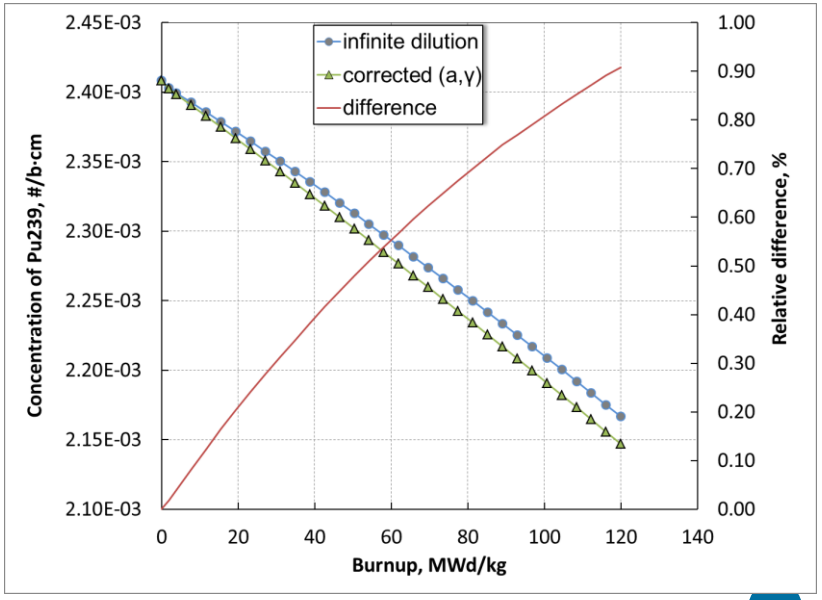




Results: effect of the XS correction

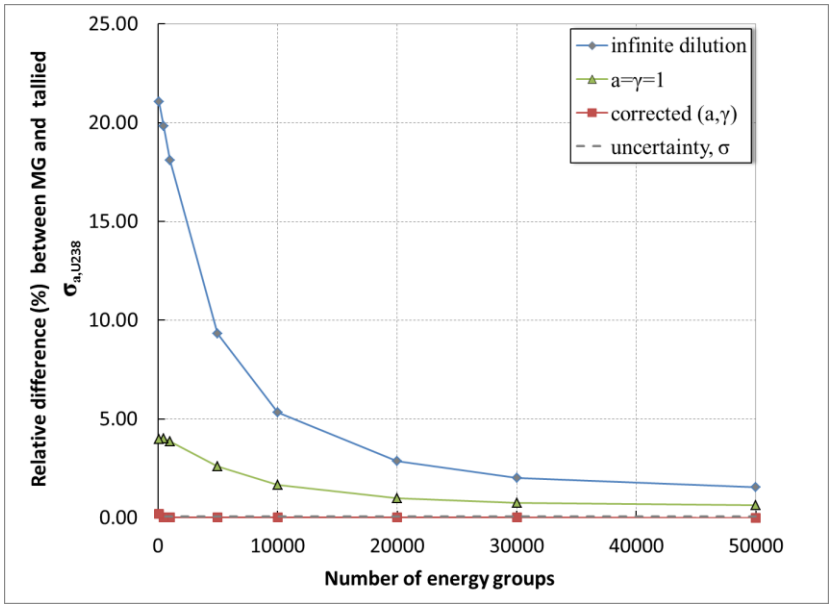
- Assembly depletion
  - BGCore
  - *50,000 energy groups*
- Two cases:
  1. Infinite dilution cross-sections
  2. Self-shielded cross-sections
     - here: ***corrected (a,γ)***
- Results:
  - systematic error in Case 1:
    - 400 pcm in reactivity
    - 1% error in Pu239 concentration
      - Due to the error in 1G XS of U238

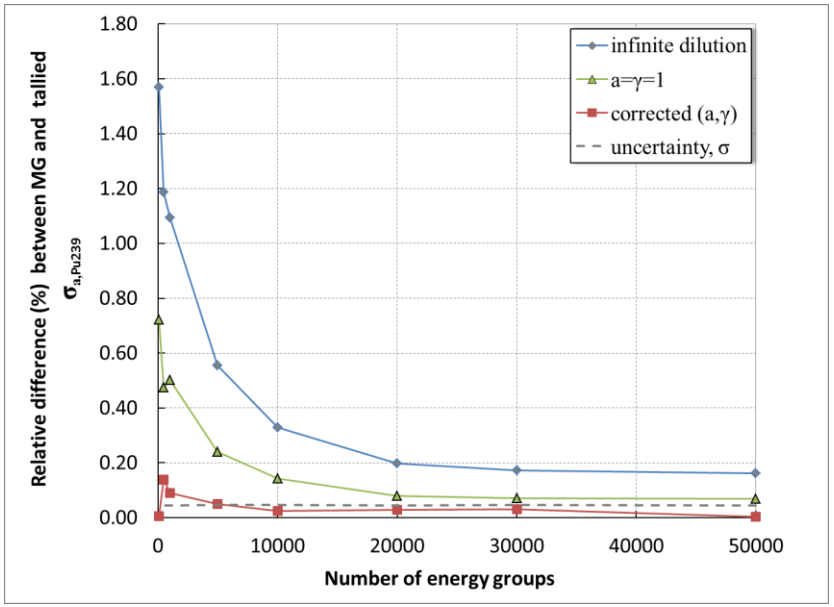




Results: No. of energy groups vs. accuracy

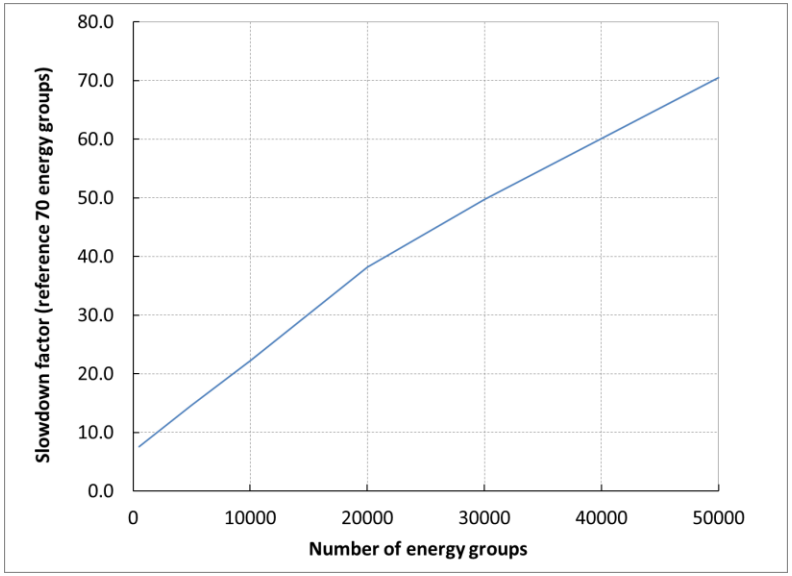
- No depletion
- Different collapsing methods:
  - Infinite dilution XS
  - Simplified σ_0 model *(a = γ = 1)*
  - σ_0 model with corrected a,γ values
- Reference: direct tally XS
- 30 independent MC simulations
  - 1G cross sections and statistical uncertainties (1σ)
- absorption reactions:
  - 39% in U238
  - 38% in Pu239





Storage requirements and CPU time

- Memory requirements strongly depends on the #EG
  - For a specific nuclide at a specific temperature
    - 70 EG require 27 Kbytes
    - 50,000 EG require 1677 Kbytes
  - We need ~340 nuclides at ~10 discrete T
    - 5.7 Gbytes ← 50,000 EG
    - 91 Mbytes ← 70 EG
- CPU time for data processing :
  - Loading the binary cross section data
  - Reading MCNP fluxes
- Reducing from 50,000 to 70 EG
  - × 70 speed-up



Conclusions and future work

- Direct tally approach is computationally intensive
- MG approach is a viable alternative
  - Generate universal MG sets of 1G XS
  - Collapse using fine group MC spectrum
- MG approach requires extension to be universally applicable
  - Accounting for self shielding requires accurate background XS
  - Background XS can be reconstructed from MC statistics
- The approach produces accurate shielded 1G XS
  - Even for very small number of energy-groups (e.g. 70)
- Full core analyses must include multi-zone division and TH
  - Considerable slow down of the overall calculation time

Thank you for your attention