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# Nuclear Data Uncertainty Propagation by the XSUSA Method in the HELIOS2 Lattice Code

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# Introduction

- Uncertainty evaluation is becoming standard practice
- Covariance data more widely available in evaluated data libraries
- International expert groups (UAM) providing benchmarks
- Regulators are beginning to require uncertainty estimations (!)
  - Including fuel cycle analyses and depletion (!)
- Few commercial codes have capability to estimate uncertainty

# XSUSA

- Sampling-based uncertainty and sensitivity analysis code
- Developed at GRS
- Perturbation vectors generated by random sampling
  - Uncertainty and correlation both considered
  - Fundamental reactions used in sampling – (n,n), (n,n’), (n,2n), (n,$\gamma$), (n,p), (n,d), (n,t), (n,$^{3}$He), (n,$\alpha$), (n,f), total $\nu$, $\chi$
- Output in 44-group SCALE6.1 structure
- Perturbation vector length = 1000

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# HELIOS2

- General-geometry lattice code
- Collision probabilities and Method of Characteristics transport
- Multi-group nuclear data libraries (177 and 49 groups)
- Depletion (CRAM) and branching calculations
- Very flexible modeling capabilities
- Widely used in commercial, research, and regulatory environments

# XSUSA + HELIOS2 = Code Modifications

- Read perturbation vectors produced by XSUSA
- Two primary challenges
  - Energy group boundary mismatches
    - Map 44-group SCALE to selected HELIOS group structure
  - Nuclear data library details
    - HELIOS2 library is highly processed ➡ summed reactions
    - Total scattering matrices, absorption and fission
    - Use ratios of fundamental-to-summed XS to define weighted sums of perturbations

$$f_i = \sum_{j \in i} \frac{\sigma_j}{\sigma_i} f_j$$

    - Ratios provided as supplementary data library

# Application to Depletion

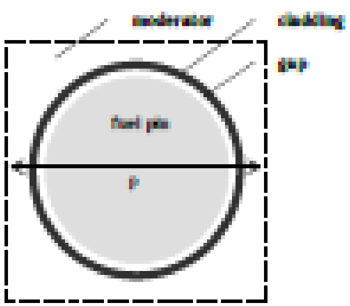
- Weighting factors processed once per case
- Perturbation factor summation performed once per depletion calculation
  - Perturbation applied at each step in depletion
  - Also applied to any branch calculations
- 1001 depletion calculations performed (base + 1000 perturbations)

# Testing – UAM Benchmarks

- Initial tests – pin-cell models
  - Depletion (no boron)
  - Edit $k_{eff}$, 2-group macro XS, isotope concentrations
- Additional tests – assembly models
  - BOC controlled and uncontrolled
  - Depletion (constant 900ppm boron)
  - Edit $k_{eff}$, 2-group macro XS and ADF, $\beta$ and inverse velocity, isotopes concentrations, burnup and power maps
- Models tested
  - TMI-1 (PWR)
  - Peach Bottom 2 (BWR)
  - Kozloduy-6 (VVER)

# Models – TMI-1

**Figure 4: Configuration of TMI-1PWR unit cell**




p – pitch of the unit cell

| Parameter | Value |
|---|---|
| Unit cell pitch, [mm] | 14.427 |
| Fuel pellet diameter, [mm] | 9.391 |
| Fuel pellet material | $UO_2$ |
| Fuel density, [g/cm$^3$] | 10.283 |
| Fuel enrichment, w/o | 4.85 |
| Cladding outside diameter, [mm] | 10.928 |
| Cladding thickness, [mm] | 0.673 |
| Cladding material | Zircaloy-4 |
| Cladding density, [g/cm$^3$] | 6.55 |
| Gap material | He |
| Moderator material | $H_2O$ |

| Parameter / Reactor condition | HZP | HFP |
|---|---|---|
| Fuel temperature, [K] | 551 | 900 |
| Cladding temperature, [K] | 551 | 600 |
| Moderator (coolant) temperature, [K] | 551 | 562 |
| Moderator (coolant) density, [kg/m$^3$] | 766 | 748.4 |
| Reactor power ,[MWt] | 2 772 | 2 772 |

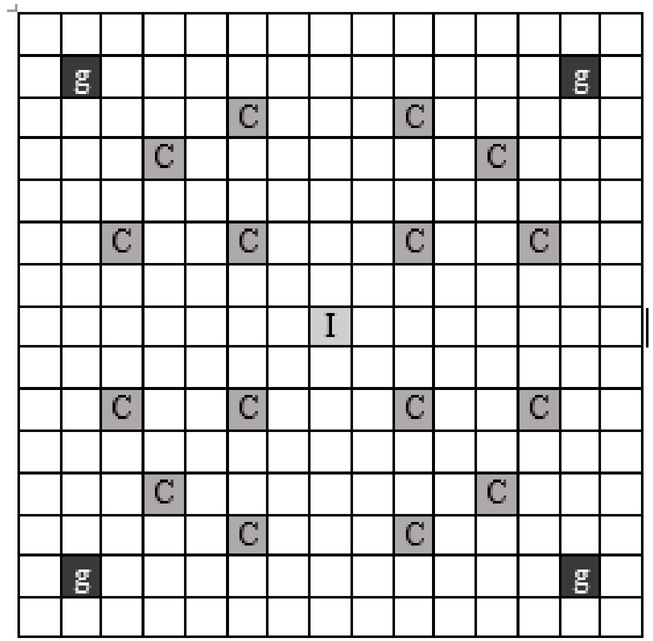



Figure from NEA/NSC/DOC(2013)

# Results – TMI-1 Pin-cell

## Macros and Relative Uncertainties

| Value | BOC | | MOC | | EOC | |
|---|---|---|---|---|---|---|
| | Result | Uncertainty | Result | Uncertainty | Result | Uncertainty |
| $k_{eff}$ | 1.41274 | 0.4967 | 1.08170 | 0.6053 | 0.89421 | 0.7667 |
| D (gr. 1) | 1.078 | 1.1773 | 1.079 | 1.1628 | 1.082 | 1.1690 |
| D (gr. 2) | 3.321E-01 | 0.1991 | 3.245E-01 | 0.2013 | 3.265E-01 | 0.2175 |
| $\Sigma_a$ (gr. 1) | 1.129E-02 | 0.9614 | 1.229E-02 | 1.0085 | 1.274E-02 | 1.0798 |
| $\Sigma_a$ (gr. 2) | 1.157E-01 | 0.2361 | 1.295E-01 | 0.7543 | 1.178E-01 | 1.4582 |
| $\nu\Sigma_f$ (gr. 1) | 9.690E-03 | 0.5026 | 7.127E-03 | 0.8494 | 5.404E-03 | 1.6274 |
| $\nu\Sigma_f$ (gr. 2) | 2.101E-01 | 0.4411 | 1.968E-01 | 0.9707 | 1.562E-01 | 1.9303 |
| $\Sigma_f$ (gr. 1) | 3.843E-03 | 0.3670 | 2.692E-03 | 0.6604 | 1.953E-03 | 1.5058 |
| $\Sigma_f$ (gr. 2) | 8.620E-02 | 0.3244 | 7.435E-02 | 0.7788 | 5.619E-02 | 1.7867 |
| $\Sigma_{s0}$ (gr. 1) | 5.337E-01 | 0.9614 | 5.318E-01 | 0.9387 | 5.300E-01 | 0.9399 |
| $\Sigma_{s0}$ (gr. 2) | 1.222 | 0.1470 | 1.233 | 0.1457 | 1.238 | 0.1461 |

# Results – TMI-1 Assembly

## Macros and Relative Uncertainties

| Value | BOC | | EOC | |
|---|---|---|---|---|
| | Result | Uncertainty | Result | Uncertainty |
| $k_{eff}$ | 1.30160 | 0.4752 | 0.84446 | 0.7749 |
| D (gr. 1) | 1.088 | 1.1610 | 1.092 | 1.1495 |
| D (gr. 2) | 3.181E-01 | 0.1912 | 3.147E-01 | 0.2031 |
| $\Sigma_a$ (gr. 1) | 1.071E-02 | 0.9358 | 1.199E-02 | 1.0798 |
| $\Sigma_a$ (gr. 2) | 1.166E-01 | 0.2089 | 1.104E-01 | 1.4582 |
| $\nu\Sigma_f$ (gr. 1) | 8.9868E-03 | 0.5086 | 4.896E-03 | 1.6274 |
| $\nu\Sigma_f$ (gr. 2) | 1.861E-01 | 0.4408 | 1.306E-01 | 1.9303 |
| $\Sigma_f$ (gr. 1) | 3.552E-03 | 0.3619 | 1.771E-03 | 1.5058 |
| $\Sigma_f$ (gr. 2) | 7.637E-02 | 0.3241 | 4.709E-02 | 1.7867 |
| ADF (gr. 1) | 1.022 | 0.0318 | 1.031 | 0.0616 |
| ADF (gr. 2) | 7.816E-01 | 0.0507 | 7.617E-01 | 0.2796 |

# Results – TMI-1 Assembly $\beta_{eff}$

| Delayed Group | BOC | | EOC | |
|---|---|---|---|---|
| | Result | Uncertainty | Result | Uncertainty |
| 1 | 2.049E-04 | 0.0691 | 1.156E-04 | 0.3925 |
| 2 | 1.123E-03 | 0.1707 | 9.235E-04 | 0.4756 |
| 3 | 1.105E-03 | 0.2332 | 7.624E-04 | 0.7887 |
| 4 | 3.230E-03 | 0.3453 | 2.076E-03 | 1.1367 |
| 5 | 1.034E-03 | 0.7436 | 8.291E-04 | 1.5011 |
| 6 | 3.460E-04 | 0.5232 | 2.391E-04 | 1.4125 |

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# Results – TMI-1 Assembly EOC Isotopics

| Isotope | Concentration | Uncertainty | Isotope | Concentration | Uncertainty |
|---|---|---|---|---|---|
| U-235 | 1.60E-04 | 2.1533 | Tc-99 | 7.15E-05 | 0.4695 |
| U-236 | 1.58E-04 | 1.4460 | Ru-101 | 7.29E-05 | 0.6678 |
| U-238 | 2.07E-02 | 0.0364 | Ag-109 | 6.84E-06 | 1.3663 |
| Pu-239 | 1.36E-04 | 2.1696 | I-129 | 1.15E-05 | 0.3654 |
| Pu-240 | 6.75E-05 | 2.4003 | Xe-135 | 7.56E-09 | 3.4407 |
| Pu-241 | 4.19E-05 | 1.9089 | Cs-137 | 8.45E-05 | 0.0339 |
| Pu-242 | 2.39E-05 | 3.6290 | Ce-144 | 1.43E-05 | 0.0806 |
| Am-241 | 1.69E-06 | 3.4094 | Nd-148 | 2.42E-05 | 0.3975 |
| Am-243 | 6.58E-06 | 7.3024 | Sm-149 | 9.55E-08 | 2.7349 |
| Cm-242 | 6.92E-07 | 1.6264 | Eu-155 | 5.62E-07 | 5.4565 |
| Cm-244 | 3.36E-06 | 7.9305 | Gd-158 | 1.44E-06 | 4.8844 |
| Mo-95 | 6.90E-05 | 0.3587 | | | |

# Summary and Future Work

- Successful linking of XSUSA and HELIOS2
- Results comparable with previously compiled results
- Future work
  - Comprehensive validation with UAM benchmarks
  - Few-group macros as input to core simulator
  - Extensions to XSUSA
    - Additional energy structures (esp. SCALE6.2 56-group)
    - Individual uncertainties for $\nu_d$
  - Formal release of HELIOS2 modifications

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