

22.211 Lecture 18

Overview of lattice physics

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April 12, 2023



Outline

1 Objectives

2 Lattice methods

3 Spectrum Correction

4 Code Examples

5 Case Matrix

6 Validation

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5 Case Matrix

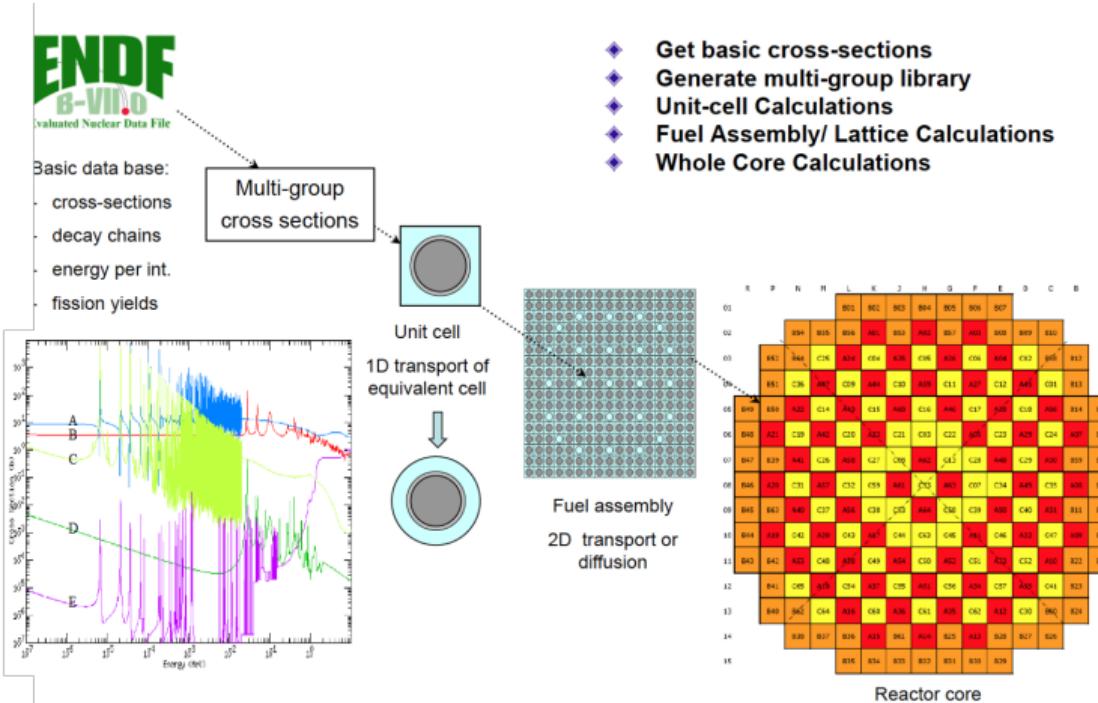
6 Validation



Objectives

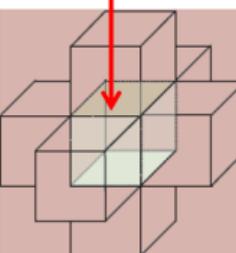
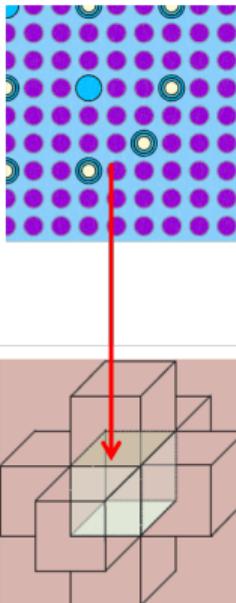
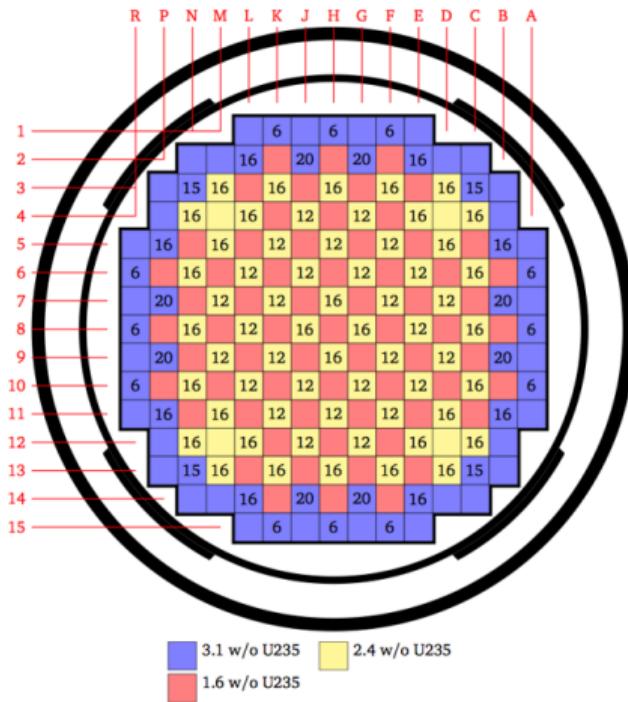
- Big picture of lattice code
- Data generation and data flow
- Energy structure
- Resonance self-shielding
- Transport solver
- Depletion
- Case matrix
- Analysis of control mechanisms

Big Picture



- ◆ Get basic cross-sections
- ◆ Generate multi-group library
- ◆ Unit-cell Calculations
- ◆ Fuel Assembly/ Lattice Calculations
- ◆ Whole Core Calculations

PWR



```
'NEW' 'cmslink.lib'/  
'CAS' 'baffle.cax',,'RAD'/  
'STA'/  
'CAS' 'radref.cax',,'RAD'/  
'STA'/  
'CAS' 'radbar.cax',,'RAD'/  
'STA'/  
'CAS' 'botref.cax',,'BOT'/  
'STA'/  
'CAS' 'topref.cax',,'TOP'/  
'STA'/  
  
'ADF' 'ON'/  
  
'CAS' 'C4.160w00.cax'/  
'STA'/  
'CAS' 'C4.240w00.cax'/  
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'STA'/  
'CAS' 'C4.240w16.cax'/  
'STA'/  
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'STA'/  
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'STA'/  
  
'END'
```

Burnable Absorbers

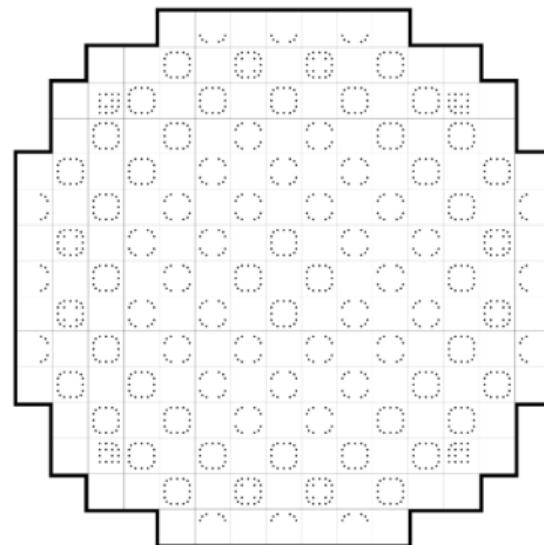
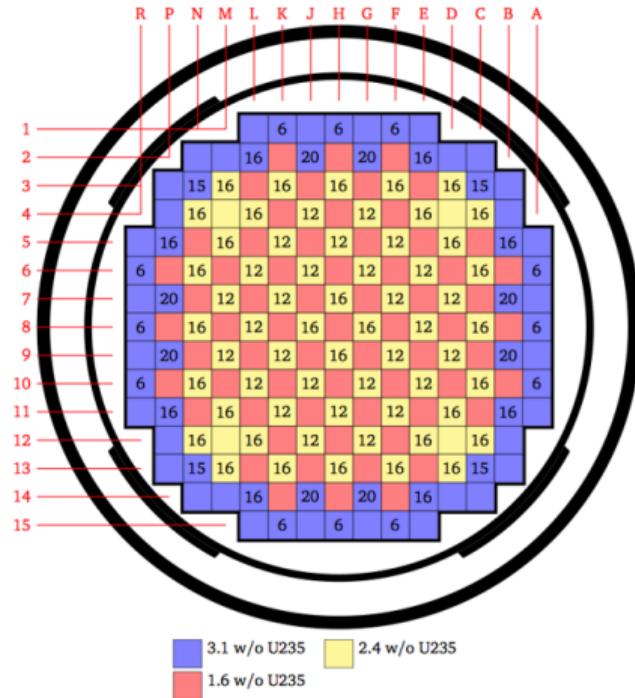


Figure 25: Detailed scale view of burnable absorber pins in cycle 1, showing proper rotations.

Control Rods

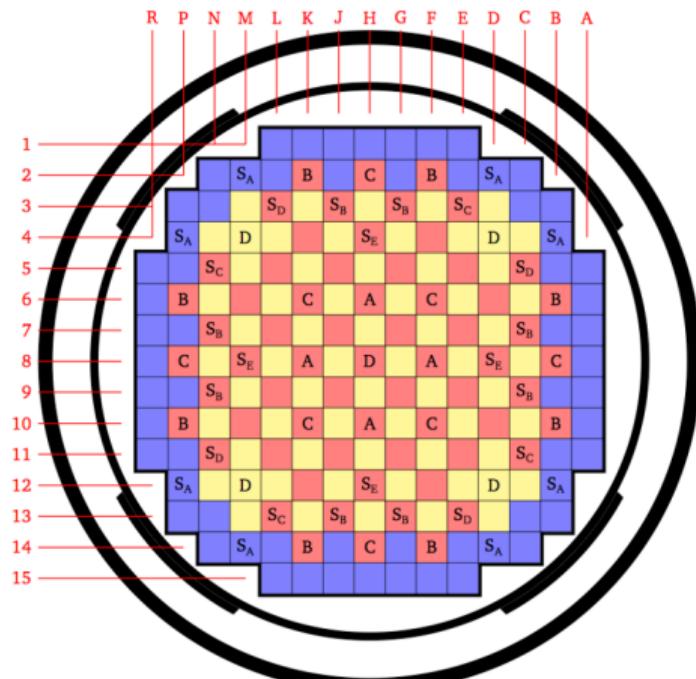
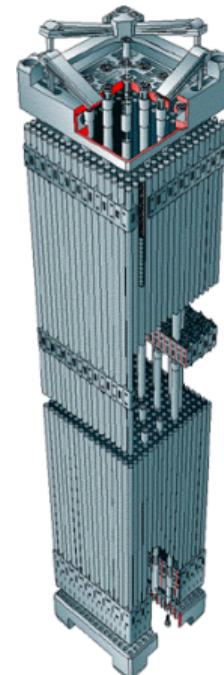
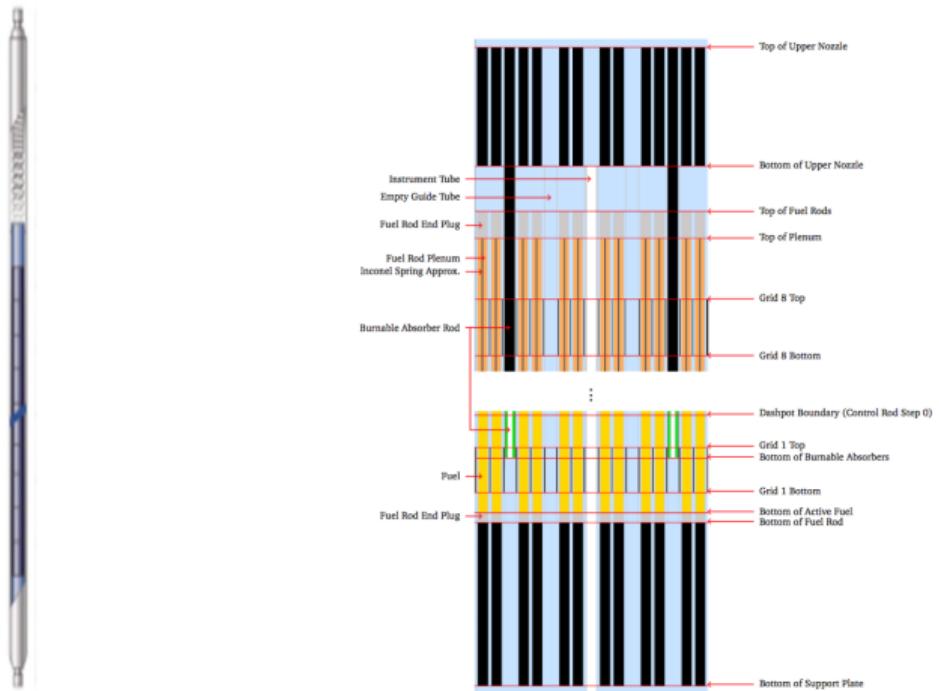


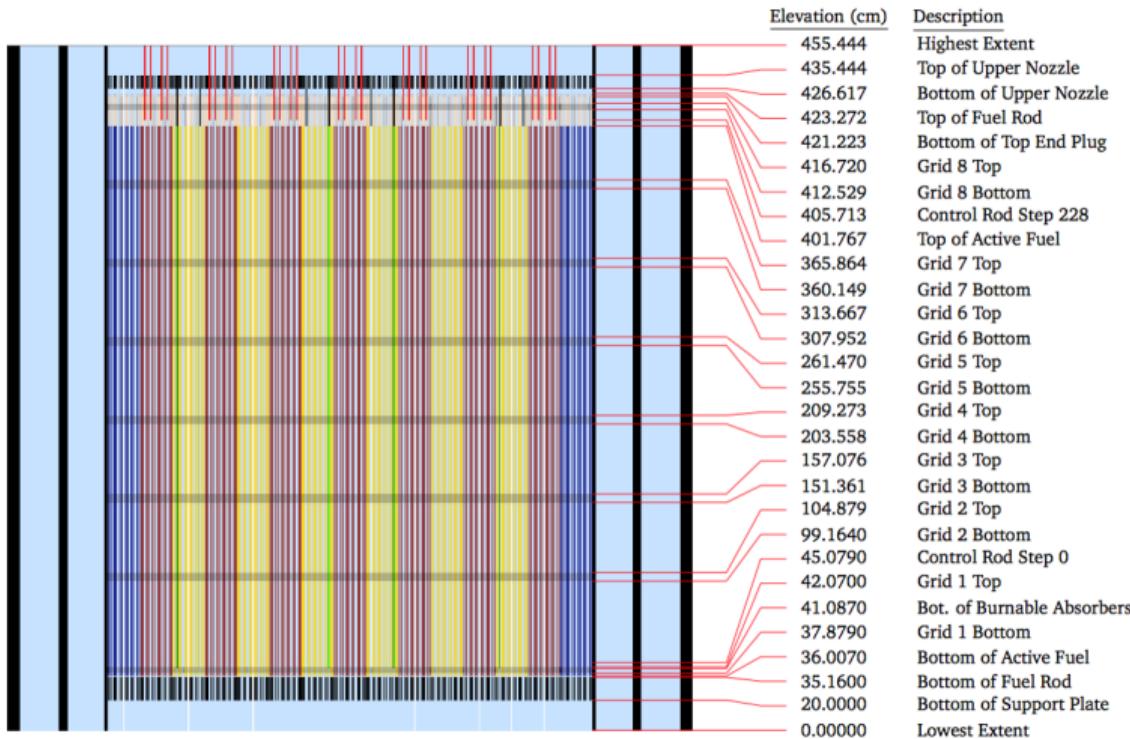
Figure 27: Control rod and shutdown bank positions. Source: 1

- S_A to S_E are shutdown rods
- All shutdown rods are pulled at startup
- Startup sequence pulls out rods A 2/3 of the way
- Rods B start pulling out while A are removed rest of the way
- Rods C start pulling out when B is 2/3 of the way out ...
- Follow 1/M plot using ex-core detectors
- PWR typically operate with all rods out at full power, with D bank in "bite" position

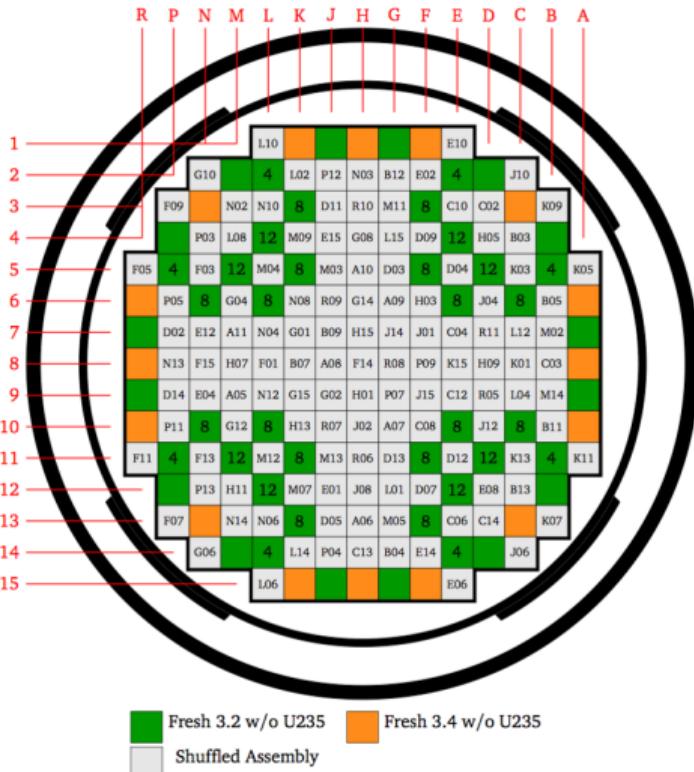
Axial Heterogeneity



Axial Heterogeneity



Core Shuffling



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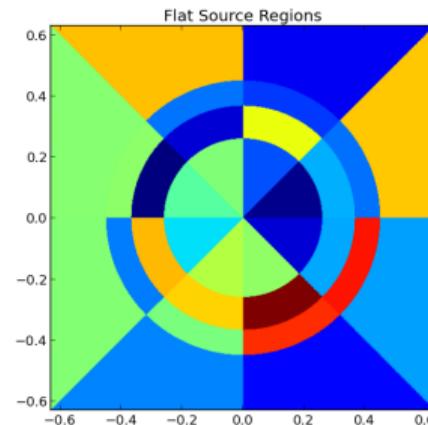
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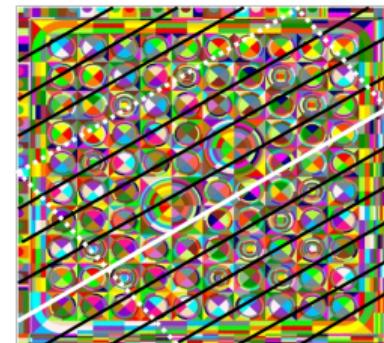
Lattice

A lattice calculation consists of a 2D transport solution of an assembly with reflective boundary conditions. It is either done as a 1-step process with 100's of groups or a 2-step process for resonance self-shielding on unique pins in 100's of group followed by an assembly calculation in 10's of groups.



Approximations

- Reflective boundary conditions
- Leakage correction using homogeneous buckling search
- 2D calculation (LWRs are quite homogeneous axially)
- Resonance models



These approximations work well for LWRs, but may not necessarily extend to other reactor types.

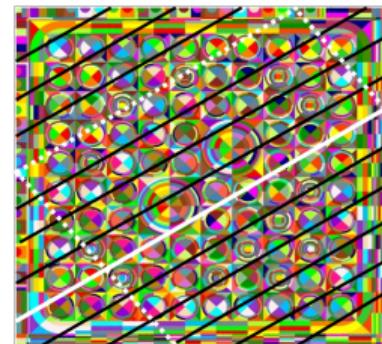
Questions addressed at lattice level

Lattice mechanical design

- Number of pins in assembly
- Pin diameter
- Clad/Duct thickness, material
- Number/size of water rods
- Control rod material

Neutronic lattice design

- Pin enrichment layout
- Burnable absorber material and layout



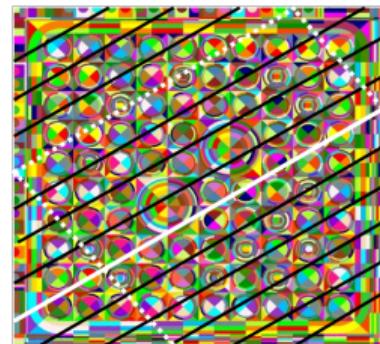
Questions addressed at lattice level

Isotopic mass flows

- Pu production for recycle
- Residual U for recycle
- Isotopes for heat load analysis
- Isotopes for radiotoxicity

Parametrize data as a function of

- Fuel burnup
- History parameters (void, boron, ...)
- Cooling intervals



Questions addressed at lattice level

Reactivity Coefficients

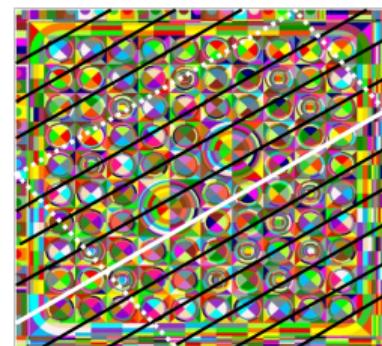
- Moderator temperature
- Doppler
- Power, Boron, Control rod, ...

Thermal limits

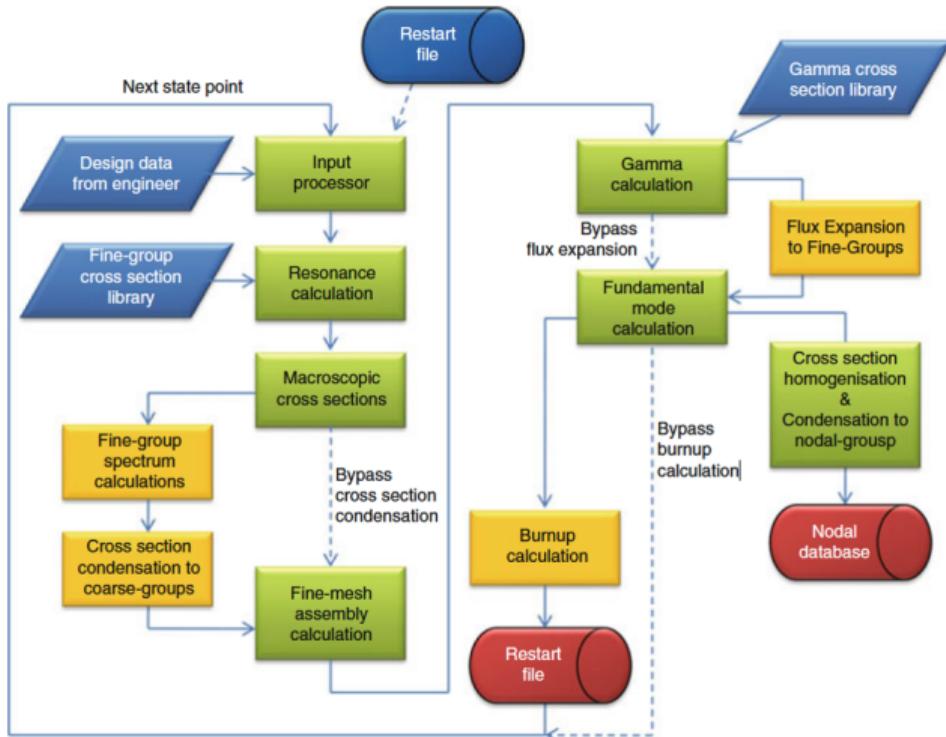
- Power peaking
- Burnup peaking
- CPR/DNBR

Operational parameter sensitivities

- Average void
- Boron concentration



Data flow



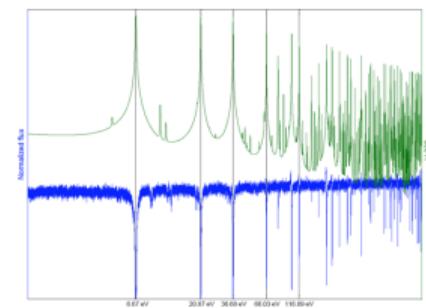
Energy Self-Shielding

Equivalence in dilution

- Ultra-fine group homogeneous calculations are used to generate tables of resonance integrals for each isotope as a function of dilution

Subgroup

- Ultra-fine group homogeneous or heterogeneous calculations are used to generate reference cross-sections and tables for each isotope
 - Optimization is used to find subgroup weights and levels that best match the reference solutions in each group for each isotope



Resonance calculation

Equivalence in Dilution

- IR source
- Dancoff correction
- Carlvik (or optimal) 2-term approximation of P_e
- Read resonance integral for each background xs in pre-generated table
- Repeat for each region and each isotope

Subgroup

- Solve fixed source transport equation for each subgroup level and each isotope using IR source
- Calculate effective absorption cross section for each region
- Reverse lookup fission and scattering cross-section from resonance integral table

Fine group library

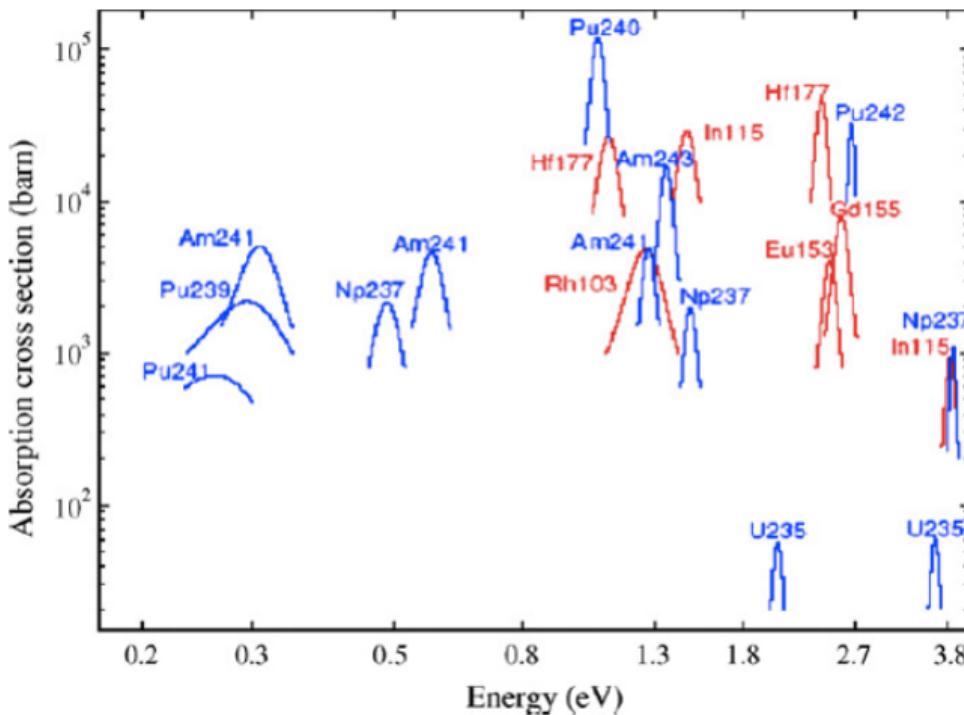
- Group structure depends on choice of self-shielding model
- Important resonances can be mapped out explicitly with very fine group structures
- More groups implies a larger library and a slower runtime

	CASMO-5 E7R0-LIB	CASMO-4 E4-LIB
# energy groups	586	70
# of fast groups	128	14
# groups with resonance data	41	13
# narrow groups in low eV range	375	-----
# thermal groups	42(below .625 eV)	43 (below 4 eV)
# nuclides/materials	446	103
# nuclides treated as reson. absorbers	112	21
# of nuclides with Pn data	66	0
# of nuclides with fission yield data	27	7
# nuclides with burnup data	285	57

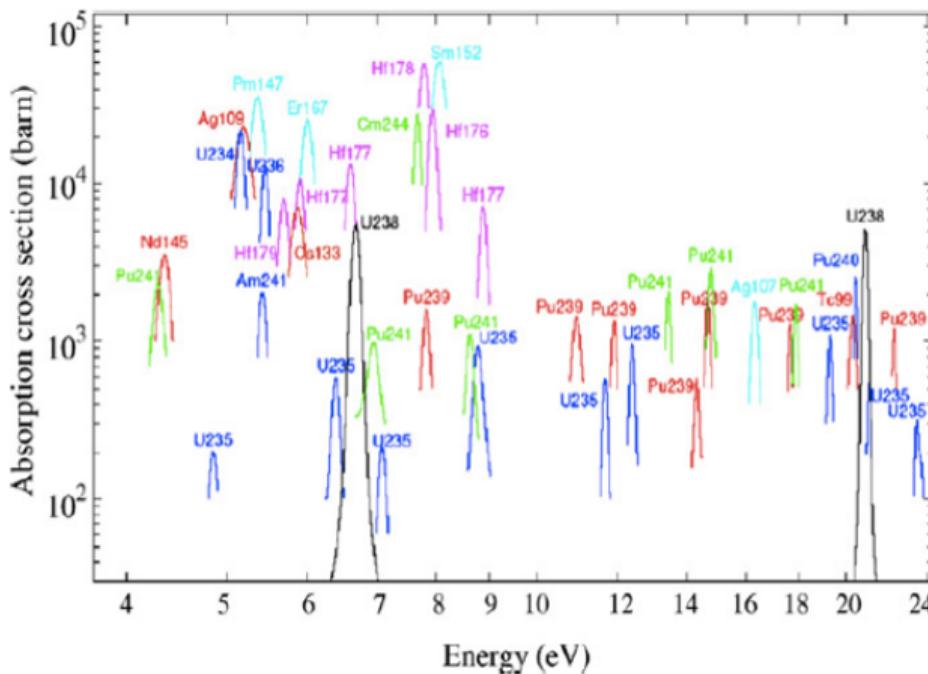
Fine group libraries

- WIMS 69-groups (LWR)
 - Designed for equivalence in dilution
 - Requires use of resonance interference factors
- SHEM 281/361 groups (LWR)
 - Map out resonances up to 22 eV with great accuracy
 - Subgroup method is used above 22 eV
- Westinghouse 6064 groups (LWR)
 - Map out the entire resonance range with high accuracy
 - No resonance self-shielding approximation needed
- CEA 1968 groups (fast reactors)
 - fine detail in resolved range to capture interference effects
 - Subgroups for resolved and unresolved ranges

Mapping out low energy resonances

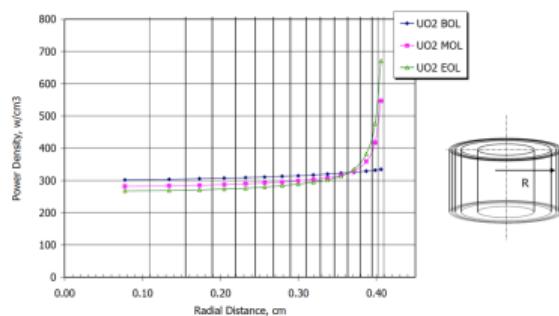
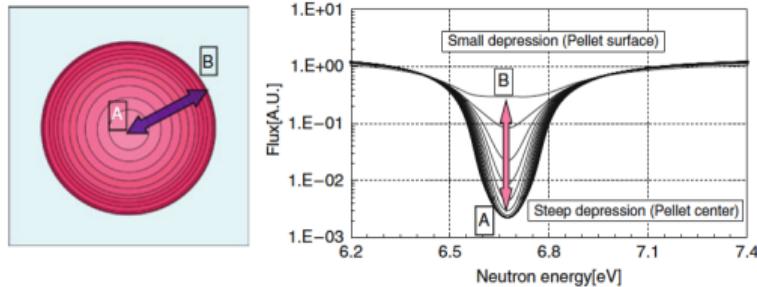


Mapping out low energy resonances



Spatial self-shielding

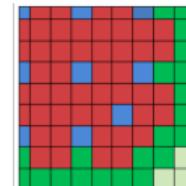
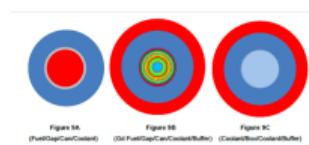
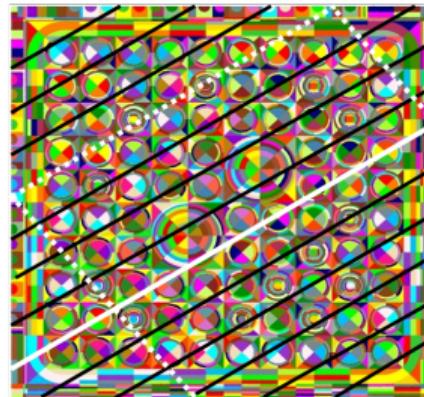
Spatial self-shielding effect is large inside the pellet. Flux shape varies considerably from the surface to the center.



Transport solution

- MOC method
- CPM method
- Interface current
- Homogenized pin cell SN

$$\psi_{k,g}(s'') = \psi_{k,g}(s') e^{-\tau_{k,i,g}} + \frac{Q_{i,g}}{\sum_{tig}} (1 - e^{-\tau_{k,i,g}})$$



Leakage correction by searching for critical buckling of the homogeneous assembly

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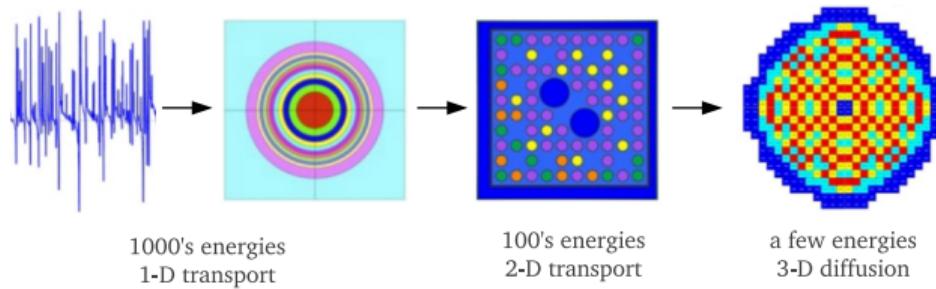
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Big Picture Condensation Process



Another approach

We can also take a similar approach in transport theory and solve either the P_N equations or the B_N equations. We start from the homogeneous Helmholtz equation

$$\nabla^2 \psi(\vec{r}) + B^2 \psi(\vec{r}) = 0$$

with a solution

$$\psi(\vec{r}) = \psi_0 e^{i\vec{B} \cdot \vec{r}}$$

where the buckling is a measure of curvature of the system. We can thus approximate the flux shape by

$$\psi(\vec{r}, E, \hat{\Omega}) = \varphi(E, \hat{\Omega}) e^{i\vec{B} \cdot \vec{r}}$$

Transport Equation

We can then substitute in the transport equation.

$$\begin{aligned}\hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}) + \Sigma(E) \psi(\vec{r}, E, \hat{\Omega}) = \\ \int_{4\pi} d^2\Omega' \int_0^\infty dE' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}') \\ + \frac{\chi(E)}{4\pi k_{\text{eff}}} \int_0^\infty dE' \nu \Sigma_f(E') \phi(\vec{r}, E').\end{aligned}$$

After substitution

$$\begin{aligned}\hat{\Omega} \cdot \nabla \left[\varphi(E, \hat{\Omega}) e^{i\vec{B} \cdot \vec{r}} \right] + \Sigma(E) \left[\varphi(E, \hat{\Omega}) e^{i\vec{B} \cdot \vec{r}} \right] \\ = \int_{4\pi} d^2\Omega' \int_0^\infty dE' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \left[\varphi(E', \hat{\Omega}') e^{i\vec{B} \cdot \vec{r}} \right] \\ + \frac{\chi(E)}{4\pi k_{\text{eff}}} \int_0^\infty dE' \nu \Sigma_f(E') \left[\varphi(E') e^{i\vec{B} \cdot \vec{r}} \right],\end{aligned}$$

where

$$\hat{\Omega} \cdot \nabla \left[\varphi(E, \hat{\Omega}) e^{i\vec{B} \cdot \vec{r}} \right] = (\hat{\Omega} \cdot i\vec{B}) \varphi(E, \hat{\Omega}) e^{i\vec{B} \cdot \vec{r}}$$

Final Form

after a few simplifications

$$\begin{aligned} & \left[\Sigma(E) + \hat{\Omega} \cdot i\vec{B} \right] \varphi(E, \hat{\Omega}) \\ &= \int_{4\pi} d^2\Omega' \int_0^\infty dE' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(E', \hat{\Omega}') \\ &+ \frac{\chi(E)}{4\pi k_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E'). \end{aligned}$$

Flux Expansion

We then expand the angular flux in terms of Spherical Harmonics

$$\varphi(E, \hat{\Omega}) = \sum_{l=0}^1 \sum_{m=-l}^l \varphi_{lm}(E) Y_{lm}(\theta, \psi)$$

defined as

$$Y_{lm}(\theta, \psi) = \sqrt{\frac{2l+1}{4\pi}} \frac{(l-m)!}{(l+m)!} P_l^m(\mu) e^{im\psi}$$

Only taking the first two terms yields (P_1 approximation)

$$\varphi(E, \hat{\Omega}) = \frac{1}{4\pi} [\varphi(E) + 3\hat{\Omega} \cdot J(E)]$$

Scattering kernel

We can also expand the scattering kernel using a Legendre polynomial expansion.

$$\begin{aligned}\Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) &= \sum_{l=0}^1 \frac{2l+1}{4\pi} \Sigma_{s,l}(E' \rightarrow E) \\ &\times \left[P_l(\mu) P_l(\mu') + 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu) P_l^m(\mu') \cos m(\psi - \psi') \right]\end{aligned}$$

The last term goes to zero assuming azimuthal symmetry of the scattering kernel.

After substitution

$$\begin{aligned} \left[\Sigma(E) + \hat{\Omega} \cdot i\vec{B} \right] \varphi(E, \hat{\Omega}) &= \int_0^\infty dE' \left\{ \frac{1}{4\pi} \Sigma_{s,0}(E' \rightarrow E) \varphi(E') \right. \\ &\quad \left. + \frac{3}{4\pi} \Sigma_{s,1}(E' \rightarrow E) J(E') \cdot \hat{\Omega} \right\} \\ &\quad + \frac{\chi(E)}{4\pi k_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E') \end{aligned}$$

First equation

Integrate over all angles

$$\begin{aligned} & \int_{4\pi} d^2\Omega \left[\Sigma(E) + \hat{\Omega} \cdot i\vec{B} \right] \frac{1}{4\pi} \left[\varphi(E) + 3\hat{\Omega} \cdot J(E) \right] \\ &= \int_{4\pi} d^2\Omega \left\{ \int_0^\infty dE' \left[\frac{1}{4\pi} \Sigma_{s,0}(E' \rightarrow E) \varphi(E') \right. \right. \\ &\quad \left. \left. + \frac{3}{4\pi} \Sigma_{s,1}(E' \rightarrow E) J(E') \cdot \hat{\Omega} \right] \right. \\ &\quad \left. + \frac{\chi(E)}{4\pi k_{eff}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E') \right\}. \end{aligned}$$

After simplifications - First equation

$$\begin{aligned}\Sigma(E)\varphi(E) + iBJ(E) &= \int_0^\infty dE' \Sigma_{s,0}(E' \rightarrow E) \varphi(E') \\ &\quad + \frac{\chi(E)}{k_{eff}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E')\end{aligned}$$

where

$$J(E) = \frac{1}{B} [\vec{B} \cdot J(E)]$$

Two ways to get second equation

- PN approach

$$\int_{4\pi} \hat{\Omega} d^2\Omega$$

- BN approach

$$\int_{4\pi} \frac{1}{\Sigma(E) + \hat{\Omega} \cdot i\vec{B}} d^2\Omega$$

Second equation

The second equation for P_N becomes

$$\frac{iJ(E)}{B} = \frac{1}{\Sigma(E)} \left\{ \frac{1}{3} \varphi(E) + \int_0^\infty dE' \Sigma_{s,1}(E' \rightarrow E) \frac{iJ(E')}{B} \right\}$$

and for B_N

$$\frac{iJ(E)}{B} = \frac{1}{\Sigma(E)\gamma[B, \Sigma(E)]} \left\{ \frac{1}{3} \varphi(E) + \int_0^\infty dE' \Sigma_{s,1}(E' \rightarrow E) \frac{iJ(E')}{B} \right\}$$

with (for buckling near zero)

$$\gamma \approx 1 + \frac{4}{15} \left(\frac{B}{\bar{\Sigma}} \right)^2 - \frac{12}{175} \left(\frac{B}{\bar{\Sigma}} \right)^4 \dots$$

Final Equations

$$\Sigma(E)\varphi(E) + iB^2 \frac{J(E)}{B} = \int_0^\infty dE' \Sigma_{s,0}(E' \rightarrow E) \varphi(E') \\ + \frac{\chi(E)}{k_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E')$$

$$\frac{iJ(E)}{B} = \frac{1}{\Sigma(E)\gamma[B, \Sigma(E)]} \left\{ \frac{1}{3}\varphi(E) + \int_0^\infty dE' \Sigma_{s,1}(E' \rightarrow E) \frac{iJ(E')}{B} \right\}$$

and we can define the diffusion coefficient

$$D(B, \Sigma(E)) = \frac{1}{B} \frac{iJ(E)}{\varphi(E)}$$



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What can we do with this?

There are two main goals for this equation:

- Leakage correction: Reactors operated with $k = 1$ but individual lattice calculations often deviated from 1. Thus we can homogenize our cross sections and do a critical buckling search. We then use this new spectrum to condense our cross sections in energy.
- Diffusion coefficients: We can compute the flux and current for a given buckling and define diffusion coefficients.

Condensation example

Using the following 2 group x.s. for a 17x17 pwr assembly with 1.6% enrichment:

- $D_1 = 1.42$
- $\Sigma_{a,1} = 0.0076$
- $\nu\Sigma_{f,1} = 0.0044$
- $\Sigma_{r,1} = 0.0191$
- $\Sigma_{s,1 \rightarrow 2} = 0.0115$
- $D_2 = 0.35$
- $\Sigma_{a,2} = 0.051$
- $\nu\Sigma_{f,2} = 0.073$
- $B_g^2 = 0.00308$

With buckling

$$k = \frac{\nu \Sigma_{f1}}{\Sigma_{r1} + D_1 B_g^2} + \frac{\Sigma_{s1 \rightarrow 2}}{\Sigma_{r1} + D_1 B_g^2} \frac{\nu \Sigma_{f2}}{\Sigma_{a2} + D_2 B_g^2}$$

- $k = 1.003209$
- $\frac{\phi_1}{\phi_2} = 2.727$

Without buckling

$$k = \frac{\nu \Sigma_{f1}}{\Sigma_{r1}} + \frac{\Sigma_{s1 \rightarrow 2}}{\Sigma_{r1}} \frac{\nu \Sigma_{f2}}{\Sigma_{a2}}$$

- $k = 1.188735$
- $\frac{\phi_1}{\phi_2} = 2.67$

Collapse to 1 group

Flux collapsing all cross sections and diffusion coefficient, and computing the homogeneous problem with 1 group data and leakage:

With buckling

$$k = \frac{\nu \Sigma_f}{DB_g^2 + \Sigma_a}$$

Without buckling

$$k = \frac{\nu \Sigma_f}{DB_g^2 + \Sigma_a}$$

- $k_{inf} = 1.1851$
- $k = 1.003209$

- $k_{inf} = 1.188735$
- $k = 1.00832$

Neglecting leakage during condensation results in 500 pcm difference!

Another common mistake

Often the temptation exists to flux collapse Σ_{tr} instead of D .

$$D = \frac{D_1\phi_1 + D_2\phi_2}{\phi_1 + \phi_2} \quad \Sigma_{tr} = \frac{\Sigma_{tr,1}\phi_1 + \Sigma_{tr,2}\phi_2}{\phi_1 + \phi_2}$$

$$k_{2group} = 1.003209$$

$$k_{1group,Dflux} = 1.003209 \quad k_{1group,\Sigma_{tr}flux} = 1.0535$$

Never flux collapse Σ_{tr} !

Real lattice code

```

***** K-INF = 1.18619 * (FUNDAMENTAL MODE CALC. SKIPPED)
*****
***** C A S M O - 4E 10.00.01 REV:00 CREATED:2011/10/07 **STUDSVIK** EXECUTED:2014/04/14 10:23:18 S
***** 168 enrichment with no bp
***** BURNUP= 0.800 V= 0.8 TF= 568.0 TM= 568.0 BOR= 0.8 EPHM= 0 ECH= 0.800

C A S M O - 4 S U M M A R Y -----
BURNUP = 0.800 MWD/KG K-INF = 1.18619

***** POWER DISTRIBUTION PEAK: LL = 1.039 ( 188.2 W/CM), HSF = 1.039 ( 65.4 W/CM2)
0.800
1.039 1.022
1.037 1.021 1.022
0.800 1.036 1.038 0.800
1.034 1.019 1.021 1.039* 1.029
1.029 1.015 1.016 1.037 1.039* 0.800
0.800 1.021 1.023 0.800 1.026 1.018 0.970
1.007 0.992 0.992 1.084 0.986 0.970 0.954 0.942
0.977 0.975 0.972 0.972 0.965 0.954 0.944 0.936 0.933

***** GROUP DATA
DIFPF1 , DIFPF2 1.4101E+00 3.5089E-01 M2 " " 1.18619 1.18619
ABSI1 , ABSI2 7.7476E-03 5.0017E-01 XE2 MIC, MAC 5.0116E+01 5.0116E+01
NUFIS55 , NUFITS2 4.3830E-03 7.2628E-02 SM2 " " 4.9079E+04 1.3991E-20
REM0V1 , NU_1 9.1779E-02 2.4574E+00 BOR1 " " 1.3708E+01 3.3756E-24
KAPPA , XE-YIELD 3.2452E-11 6.5629E-02 BOR2 " " 4.4898E+02 4.4898E+02

```

```

+ 48 GROUP FUNDAMENTAL MODE: *  

+ 1.0000000000000000 M01: 0.00000000 M2: 0.0000000000000000 *  

+ K-EFF: 0.8088088088088082 B2M: 0.00308082 *  

+ BURNUP: 0.800E-0 8.0E-0 TF= 568.0 W= 560.0 BOR= 0.0 EFPH= 0 ECH= 0.000E+00  

+ C = 4.8000000000000000 REV:108 CREATED:28/11/18:07 **STUDSVIK** EXECUTED:28/11/18:13:18 STATEPOINT =  

+ 158 enrichment with no bc  

+ BURNUP= 0.800E-0 8.0E-0 TF= 568.0 W= 560.0 BOR= 0.0 EFPH= 0 ECH= 0.000E+00  

C S M D = 4 SUMMARY  

BURNUP = 0.800E-0 M01= 1.0000000000000000 M2= 0.0000000000000000 R2= 0.000E+00 B2= 3.000E-03  

+ POWER DISTRIBUTION PEAK: LL = 1.839 { 188.1 W/CM}, HSF = 1.839 { 65.4 W/CM}  

0.800  

1.839 1.822  

1.836 1.826 1.822  

0.800E-0 1.836 1.837 0.800E-0  

1.834 1.818 1.816 1.815 1.819 1.820  

0.800E-0 1.834 1.818 1.816 0.800E-0 0.800E-0  

0.800E-0 1.821 1.823 0.800E-0 1.825 1.800 0.978  

1.807 0.992 0.992 1.000 0.988 0.971 0.955 0.942  

0.978 0.975 0.972 0.972 0.965 0.955 0.944 0.937 0.933  

+ [100] BURN DATA K-INF XE, NDXE  

DIFP1 , DIFP2 1.4191E+00 5.5046E-01 M2 = 0.0000E+01 1.18493 1.18493  

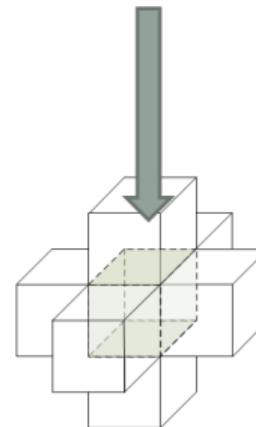
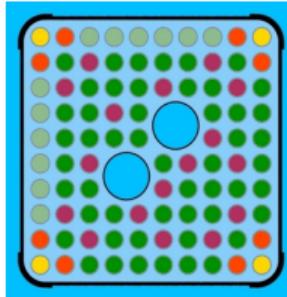
AB51 , AB52 7.5164E-01 5.0778E-02 XE2 MIC, MAC = 6.0546E-01 4.3998E-19  

AB53 , AB54 4.2030E-01 1.0000E-01 XE3 MIC, MAC = 1.6546E-01 1.6546E-01  

REMOVED , NU 1.9983E-02 2.4565E-08 BOR1 = 1.0000E+01 1.0000E+01  

KAPPA , XE-YIELD 3.2455E-11 5.6546E-02 BOR2 = 1.0000E+01 6.1744E-24  


```



Discontinuity factors

An alternative to SPH factors is to use assembly discontinuity factors. The original idea came from KWU in Germany, but was "perfected" by Prof. Smith during his PhD.

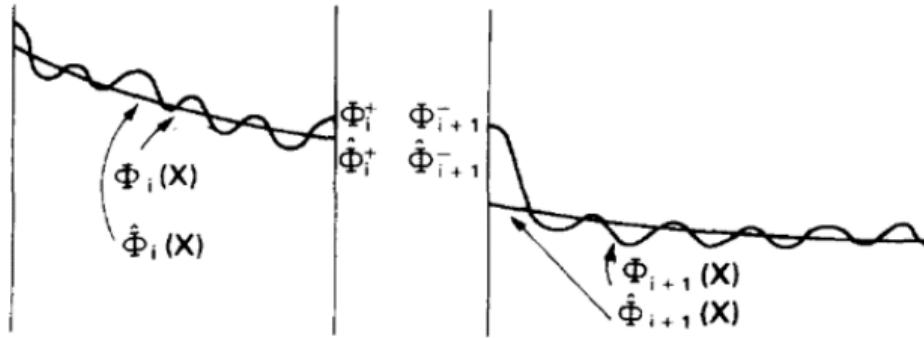
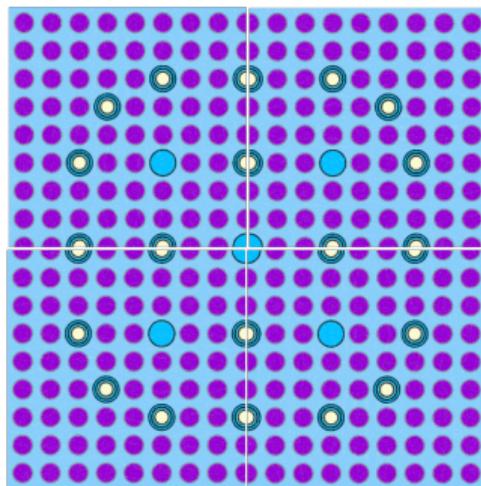
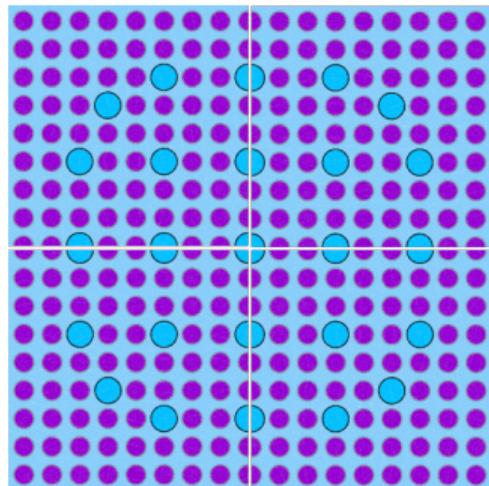


Fig. 4. One-dimensional nodal flux distributions.

The idea is to compute the discontinuity between the heterogeneous flux and the homogeneous flux at each boundary. The flux continuity thus becomes

$$DF^{i,+} \times \phi^{i,+} = DF^{i+1,-} \times \phi^{i+1,-}$$

Example



$$ADF_{int}^A = 1.04 \quad ADF_{ext}^A = 0.97 \quad ADF_{int}^B = 1.07 \quad ADF_{ext}^B = 0.90$$

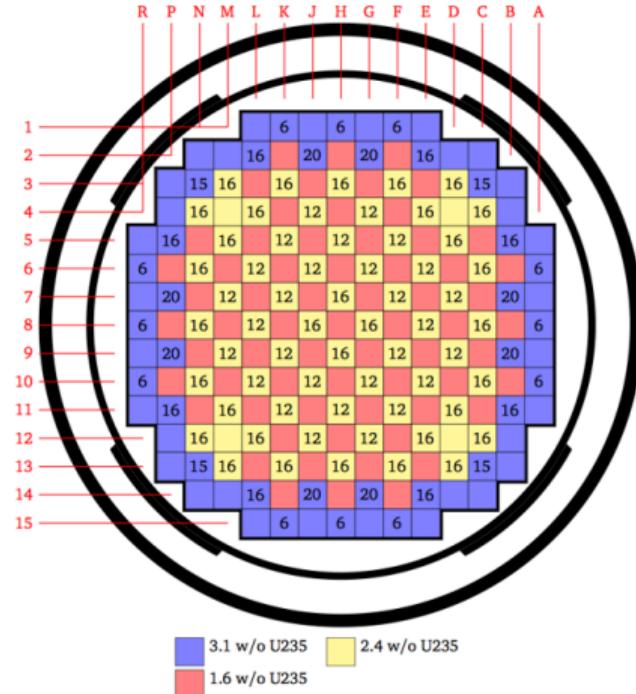
We get the ADF from the lattice calculation:

$$ADF = \frac{\phi_{surface}}{\bar{\phi}_{assembly}}$$

And we use it at the interfaces

$$\phi_{ext}^A ADF_{ext}^A = \phi_{ext}^B ADF_{ext}^B$$

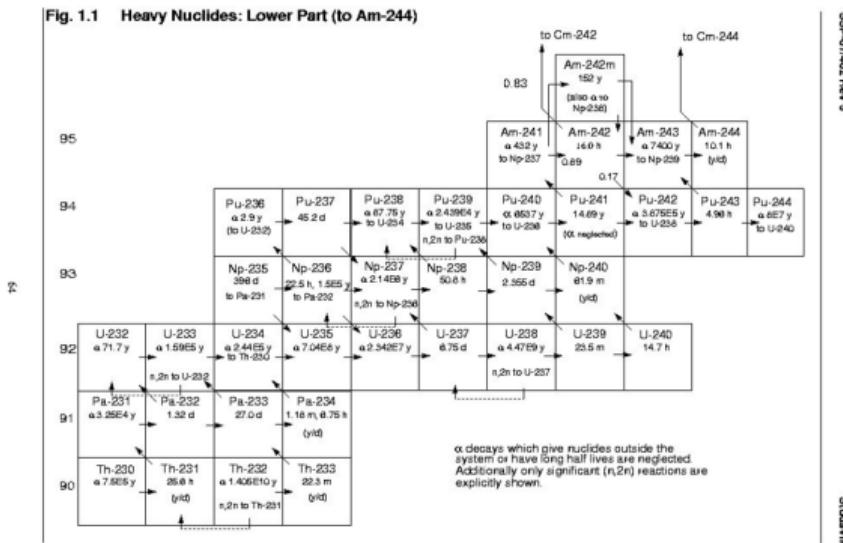
BEAVRS ADFs



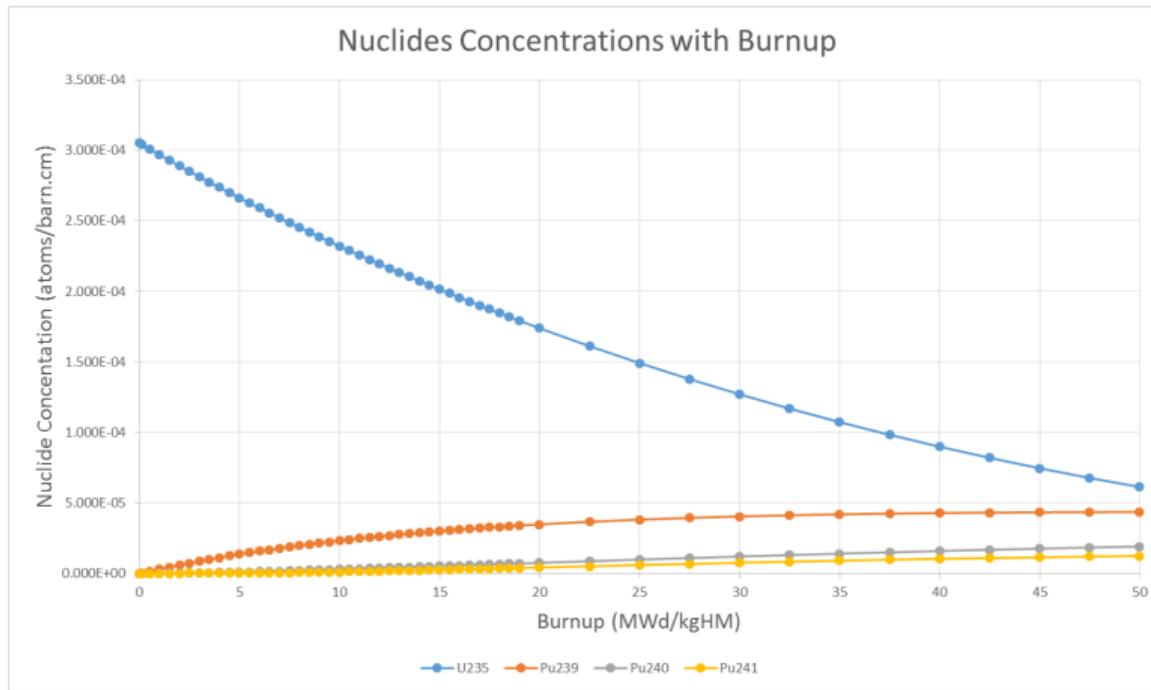
/ A00	1.0053E+00	9.7592E-01
/ B00	1.0044E+00	9.7128E-01
/ C00	1.0038E+00	9.6802E-01
/ B12	1.0029E+00	1.0314E+00
/ B16	1.0057E+00	1.0593E+00
/ C08	1.0201E+00	1.0605E+00
/ C12	1.0027E+00	1.0296E+00
/ C16	1.0053E+00	1.0569E+00
/ C20	1.0130E+00	1.1098E+00
/ C24	1.0232E+00	1.1700E+00

Depletion

Cross section data exists for roughly 400 isotopes, but decay data exists for upwards of 2000 isotopes. We must track the isotopes that are important from a neutronic standpoint but also all of the isotopes that we may need in analysis beyond the reactor.



Nuclide Concentrations



More details in Lecture 20!

Outline

1 Objectives

2 Lattice methods

3 Spectrum Correction

4 Code Examples

5 Case Matrix

6 Validation



Transport solver - 2D

- MOC: CASMO4/5 (Studsvik), MPACT (CASL), APOLLO2/3 (CEA), DRAGON (Canada), AEGIS (Japan), LANCER (GEH), HELIOS (Studsvik), WIMS (UK), TRITON/NEWT¹ (ORNL), POLARIS (ORNL)
- CPM - Interface Current: APOLLO2/3 (CEA), DRAGON (Canada), HELIOS (Studsvik), WIMS (UK), PARAGON (W), ERANOS/ECCO (CEA)
- SN - Discrete Ordinates: ATTILA (USA), APOLLO2/3 (CEA), PARTISN (LANL), DENOVO (ORNL),

¹Short characteristics

Transport solver - Self-shielding

- Equivalence Theory: CASMO4 (70 groups), CASMO5 (586 groups), APOLLO2/3 (172/281 groups), DRAGON (172 groups), LANCER (118/190 groups), WIMS (172 groups), PARAGON (70 groups)
- Subgroups: HELIOS (44/177 groups), ERANOS/ECCO (1968 groups), MPACT (69/252 groups)
- Ultra-fine mesh: AEGIS ($>100,000$ groups to 172), PARAGON (~ 6000 groups), TRITON/NEWT ($>50,000$ groups to 44/238)

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Case Matrix

The lattice calculation will generate a set of homogenized 2 group parameters with all branches and history effects.

- Branch: From a reference state, determines the impact to a cross section of a perturbation of fuel temperature, boron concentration, moderator temperature, control rod position, ...
- History: Measures the impact to a cross section at a given state from having an history (temperature, boron, ...) different than the reference state.

Example - Fuel temperature

- Reactivity coefficients are computed by comparing the branch case for a given history
- In this case the lattice is depleted at $T=900K$ with branches to $T=1000K$
- The history effect is computed by a separate depletion with $T=1000K$

EXP	TFU 900	Branch 1000	TFU 1000	Branch delta	History
0.0000	1.3301	1.3270	1.3270	-0.0031	0.0000
0.1000	1.2906		1.2876		
0.5000	1.2820		1.2791		
1.0000	1.2757		1.2727		
2.0000	1.2664		1.2635		
3.0000	1.2571		1.2542		
4.0000	1.2474		1.2446		
5.0000	1.2376		1.2348		
6.0000	1.2277		1.2249		
7.0000	1.2179		1.2151		
8.0000	1.2083		1.2055		
9.0000	1.1988		1.1961		
10.0000	1.1895	1.1867	1.1868	-0.0028	0.0001
11.0000	1.1804		1.1777		
12.5000	1.1672		1.1645		
15.0000	1.1461		1.1436		
17.5000	1.1261		1.1236		
20.0000	1.1069	1.1041	1.1046	-0.0028	0.0005
22.5000	1.0884		1.0862		
25.0000	1.0704		1.0684		
27.5000	1.0530		1.0511		
30.0000	1.0360	1.0332	1.0343	-0.0028	0.0011
32.5000	1.0194		1.0178		
35.0000	1.0031		1.0018		
37.5000	0.9872		0.9860		
40.0000	0.9715	0.9689	0.9706	-0.0027	0.0018
42.5000	0.9562		0.9555		
45.0000	0.9413		0.9408		
47.5000	0.9267		0.9264		
50.0000	0.9125	0.9099	0.9124	-0.0025	0.0025
52.5000	0.8986		0.8988		
55.0000	0.8851		0.8855		
57.5000	0.8719		0.8725		
60.0000	0.8592	0.8569	0.8600	-0.0024	0.0032
62.5000	0.8470		0.8480		
65.0000	0.8352		0.8364		
67.5000	0.8238		0.8252		
70.0000	0.8130	0.8108	0.8145	-0.0022	0.0037

Case Matrix Cost

```
2D Quadrature:Polar Angle Integration: Optimum 3 Polar Angle          Flat source regions:      2588
2D Neutron calculation performed in 19 energy groups with sym=1/2 assembly
B.C.'s: West: Mirror, South: Mirror, East: Mirror, North: Mirror
All Groups: 1 TO 19 Azimuthal Angles: 64   Polar Angles: 3 Spatial Mesh: 0.0500 cm Tracks: 641979

Characteristics    Solution --Statepoint: 1 Assembly Ave Exp: 0.000

Iter   Eigen Del PCM     CPU     EPS-2D   EPS-Source   EPS-Flux   CMCO-Dev   Thermal
-----  -----  -----  -----  -----  -----  -----  -----  -----
1  1.11685  0.02  1.000000  1.000000  1.000000  1.000000  0
2  0.96080 -15605.4  0.96  41.953312  0.151620  0.002382  9.000000  2
3  1.00275  4195.0  0.96  0.160714  0.025408  0.000583  0.366065  2
4  1.00718  442.7   0.96  0.032054  0.005733  0.000145  0.055287  2
5  1.00842  123.8   0.97  0.013038  0.002433  0.000054  0.032478  2
6  1.00890  48.6    0.97  0.005643  0.001149  0.000022  0.008623  2
7  1.00911  20.9    0.96  0.002556  0.000536  0.000010  0.004094  2
8  1.00919  7.9     0.96  0.001106  0.000272  0.000005  0.002080  2
9  1.00925  6.0     0.97  0.000524  0.000031  0.000001  0.001023  2
10 1.00924  -0.7   0.96  0.000108  0.000022  0.000000  0.000203  2
11 1.00924  -0.1   0.95  0.000063  0.000020  0.000000  0.000115  2
Total CPU (Sec)           9.63
2D k-infinity: 1.00924
All regions contained at least 1 track.
```

A single state-point takes 5-10s. Typical depletion to 80 MWd/kg (70 state-points) requires approximately 10min. Typical case matrix for parametrization requires approximately 1700 state-points or 4-5 hours for a single lattice type.

Other things to consider

- Thermal expansion
- Gamma transport / Energy deposition
- Isotopic tracking for all downstream applications
- Pre-built material composition (pay special attention to natural Boron)

CASMO Pin Cell Input

```
TTL *Pin cell example
TFU=293 TMO=293 BOR=550      *Statepoint parameters
FUE 1 10.1/3.2                *Fuel density/enrichment
PIC .49 .55 .81               *Pin cell radii
STA                           *Start execution
END                          *End of input
```

Line-by-line

- Line 1: TTL card provides a title to the file
- Line 2: TFU card defines the fuel temperature (293 K)
- Line 2: TMO card the moderator temperature (293 K)
- Line 2: BOR card defined the boron concentration (500 ppm of Natural Boron by weight)
- Line 3: FUE is the fuel composition card which is assigned material ID 1, followed by the density (10.1 g/cc). After the slash we find the enrichment of U-235 (weight percentage of U)
- Line 4: PIC card defines our unit pin cell model with radii defined from innermost to outermost. The last radius value (0.81) provides the equivalent radius for a square pin of equivalent area

The CASMO input is designed for simplicity, many specifications are assumed to be of a typical PWR or pre-defined for the desired process, such as UO₂ fuel, square lattice, reflective boundary conditions, clad material ...



CASMO PWR Assembly Input

```
TTL * + EX 3.1 PWR SIMULATE Library Generation
TFU=990 TMO=583 BOR=400 IDE='EX31'
SIM 'SEGNAM' 3.1
FUE 1 10.1/3.1
CRA 10.17/47000=80 49000=15 48000=5          * Ag-In-Cd
PWR 15 1.43 21.55
SPA 20.5,18.E-6,,7.9/718=57 347=43          * Inconel spacer
PDE 31
*
PIN 1 0.65 0.70/ 'MOD'   'BOX'           * Central IT PIN1
PIN 2 0.49 0.50 0.55                  * Simple fuel with clad
PIN 3 0.65 0.70/ 'MOD'   'BOX'           * Guide Tube PIN3
PIN 3 0.505 0.509 0.558 0.634 0.676 /
    'AIC' 'AIR' 'CRS' 'MOD' 'BOX'//1,'CR1' 'ROD' * Control rod PIN3
*
LPI
1
2 2
2 2 2
2 2 2 3
3 2 2 2 2
2 2 3 2 2 3
2 2 2 2 2 2
2 2 2 2 2 2 2
DEP -60
S3C
STA
END
```

Line-by-line

- Line 2: IDE card provide an identification name for a restart file
- Line 3: SIM card provides a name for the nodal code SIMULATE
- Line 5: CRA card defines the control rod absorbed material (Ag-In-Cd in this case)
- Line 6: PWR card defines a PWR assembly with a 15x15, 1.43 cm pin pitch and 21.55 cm assembly pitch
- Line 7: SPA card defines a grid space by units of mass per unit length (it will get homogenized with the coolant)
- Line 8: PDE defined the power density in MW / kgHM (kg of initial heavy metal)

Line-by-line

- Lines 10-14: PIN card defines 3 types of pins labeled 1, 2 and 3 for the instrument tube, the fuel and the guide tube (without and with control rod absorbers)
- Line 17: LPI card is the pin layout in 1/8 symmetry (by default but can be changed in the PWR card)
- Line 27: DEP is the depletion card that will deplete up to 60 MWd/kgHM (negative sign tells the code to use default spacing values, positive values define intervals)
- Line 28: STA card starts the computation
- Line 29: END terminates the execution

CASMO4 - ENDF6 Library

- 70 groups (13 resonance groups)
- Most nuclides only have 1 temperature 600K
- Important PWR nuclides have up to 6 temperatures
- Most nuclides only have an absorption cross-section
- Natural boron is split 18.3 % B-10

Outline

1 Objectives

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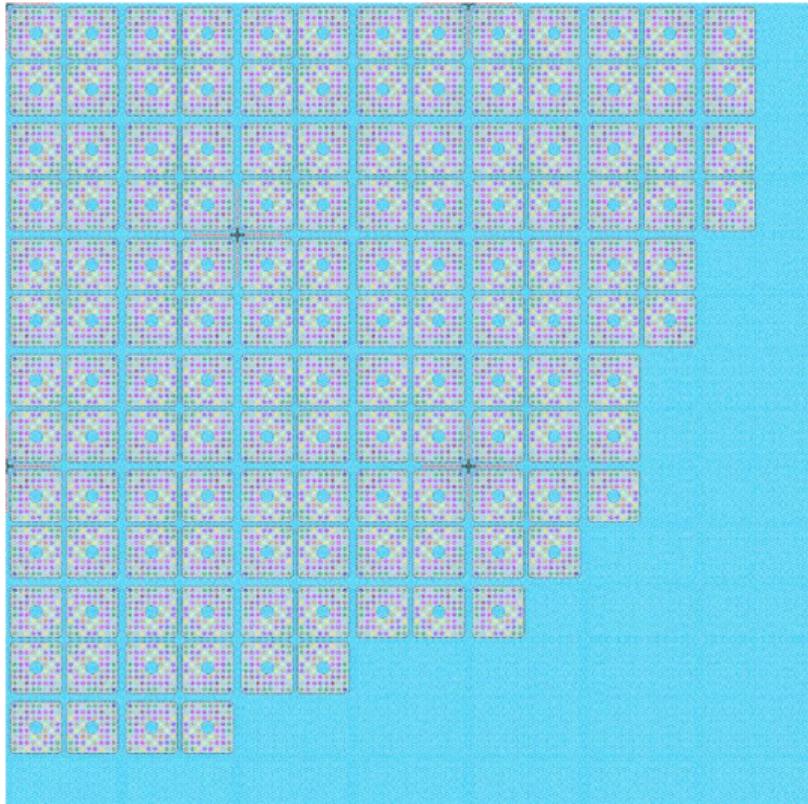
4 Code Examples

5 Case Matrix

6 Validation



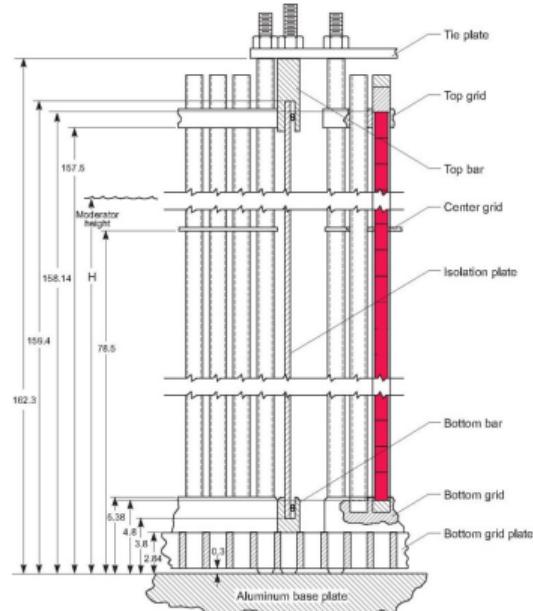
Lattice codes can solve more than lattices



B&W1484 series

Babcock & Wilcox performed series of measurements in the late 70's and early 80's, the 1484 series was performed in 1979.

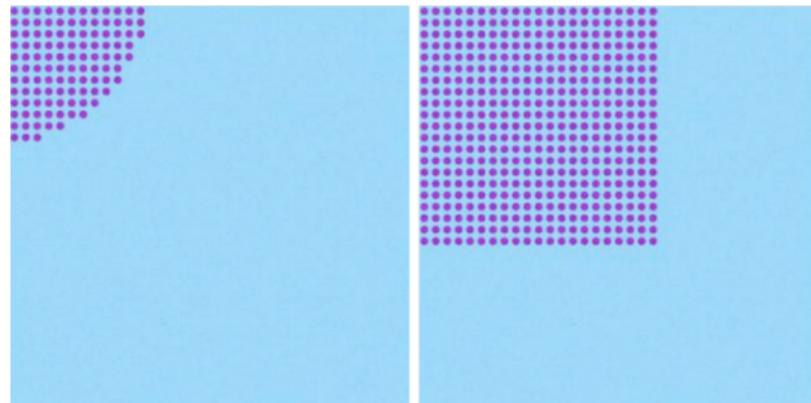
- Various absorbers (burnable absorbers, rods, plates, ...)
 - Criticality determined by moderator height
 - Various boron concentrations
 - Measured axial buckling





Core 1 and 2

The first two cores were very simple, but play a huge role in validating proper treatment of anisotropic scattering and transport cross section.



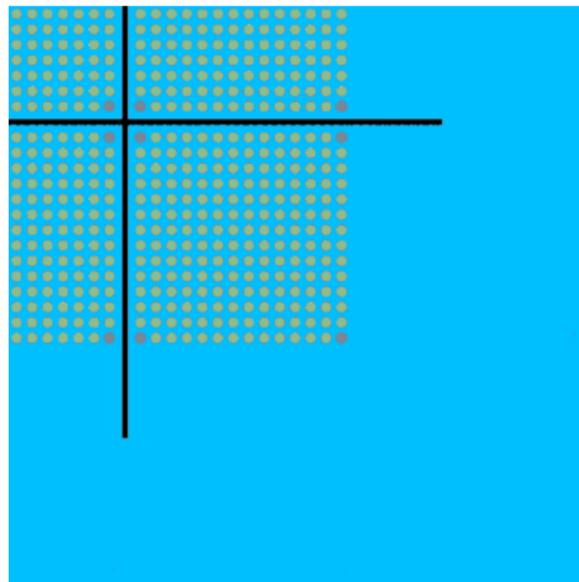
Core 1 has 35% leakage and no boron, while core 2 only has 15% leakage and 1037 ppm of boron.

How are the measurements performed?

Core	Run	Ldg. diagr. Fig. no.	Spacing between arrays, pin pitchens		No. of B,C pins	Moderator temp, °C	Moderator boron conc, ppm (±3)	Critical moderator ht, cm (±0.2)	Super- critical moderator ht, cm (±0.2)	ΔH , cm		$\frac{\Delta p}{\Delta H}$	\bar{h} , cm	$(\frac{\Delta p}{\Delta H})^{-1/2}$
			pin	pitchens						Δp , cm	ΔH , cm			
I	2245	12	--	--	21	0	143.88	147.12	98.5	6.95	3.24	2.15	145.5	0.775
II	2255	13	0	0	18.5	1037	144.29	--	--	--	--	--	--	--
III	2265	14	1	0	18	769	148.63	150.67	202	3.72	2.04	1.82	149.7	0.819
III	2266	14	1	0	18	764	144.88	149.88	64.5	9.70	5.00	1.94	147.4	0.802
III	2267	14	1	0	18	762	140.38	144.80	62.5	10.0	4.42	2.26	142.6	0.762
III	2268	14	1	0	18.5	753	131.32	133.80	95.0	7.20	2.48	2.90	132.6	0.701
III	2269	14	1	0	18	739	120.64	124.26	43.5	13.1	3.62	3.62	122.5	0.651
III	2270	14	1	0	18	721	110.04	111.84	78.0	8.40	4.67	110.9	0.598	
III	2271	14	1	0	18.5	702	100.32	102.09	55.5	11.0	1.77	6.21	101.2	0.544
IV	2282	15	1	84	17	0	145.68	148.94	110	6.33	3.26	1.94	147.3	0.802
V	2295	16	2	64	17.5	0	144.75	149.27	72.0	8.95	4.52	1.98	147.0	0.796
VI	2297	17	2	64	17.5	0	107.67	109.92	49.5	11.9	2.25	5.29	108.8	0.574
VII	2314	18	3	34	17.5	0	146.15	149.80	96.5	7.09	3.65	1.94	148.0	0.802
VIIa	2315	--	3	34	17.5	0	122.92	125.89	59.4	10.4	2.97	3.50	124.4	0.659
VIIb	2316	--	3	34	17.5	0	116.59	118.79	75.7	8.64	2.20	3.93	117.7	0.634
VIII	2317	19	3	34	17.5	0	111.49	113.78	56.7	10.8	2.19	4.72	112.6	0.596
IX	2321	20	4	0	17.5	0	129.65	131.87	100	6.88	2.22	3.10	130.8	0.686
IXa	2323	--	4	2	17.5	0	139.36	144.96	43.8	13.0	5.60	2.32	142.2	0.755

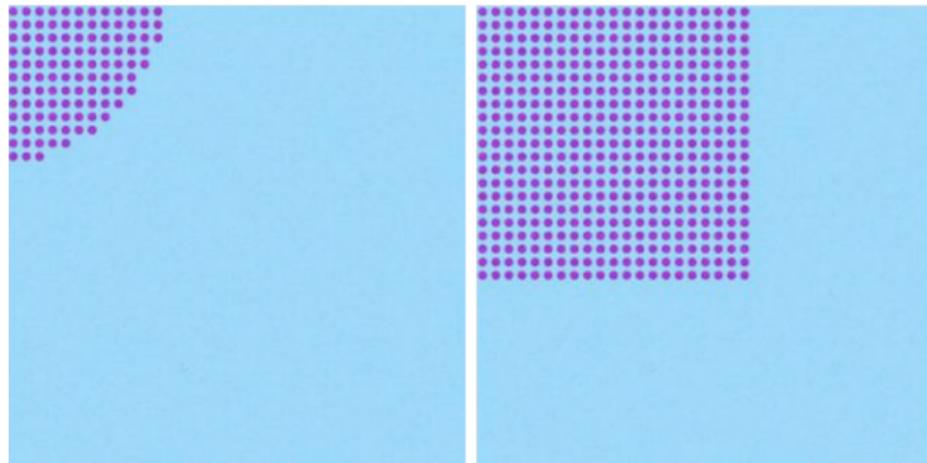
- ① Build configuration and add water until supercritical
- ② Measure worth of water addition
- ③ Adjust height to critical level
- ④ Extrapolate to common core height (145.0 cm in 1484 series)
- ⑤ Correct for temperature variations (20C)

How to model in 2D?



- Add DB_g^2 to the absorption cross section in each group

1484 Results - 70 groups



P_3 scattering; $k_{inf} = 0.99776$
 P_2 scattering; $k_{inf} = 0.99789$
 P_1 scattering; $k_{inf} = 0.99515$
 P_0 scattering; $k_{inf} = 1.09714$

P₃ scattering; k_{inf}=0.99973
 P₂ scattering; k_{inf}=0.99979
 P₁ scattering; k_{inf}=0.99894
 P₀ scattering; k_{inf}=1.03911

Dimple Critical

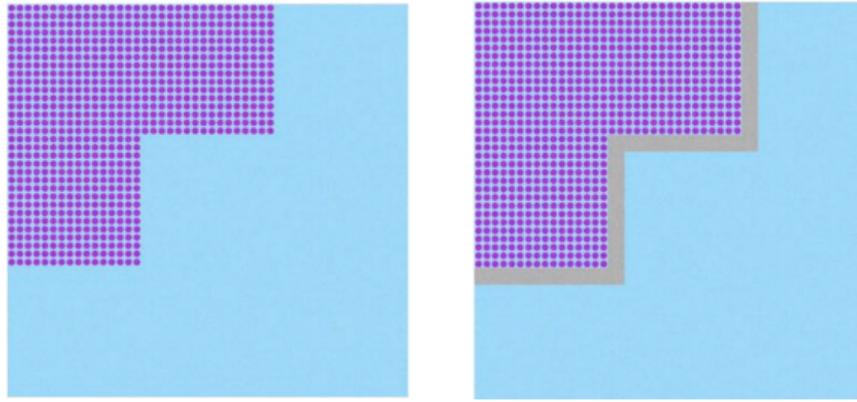


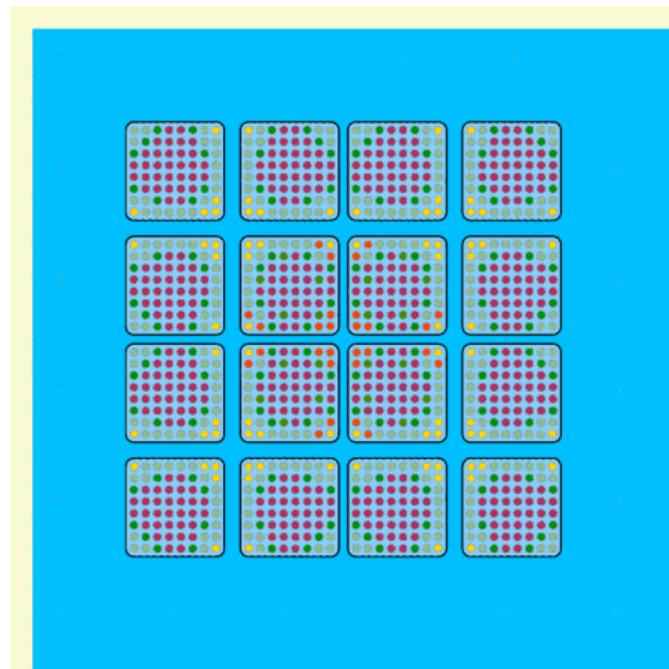
Table 3. CASMO-5 ENDF/B-VII.0 Results Dimple Criticals (95 groups, P0)

Core	Boron (PPM)	Geometry	CASMO-5 k-eff
S06A	0.0	Without Baffle	1.00126
S06B	0.0	With Baffle	1.00099
Average (All Cores)			1.00113
Standard Dev (All Cores)			0.00019

These are transport corrected P_0 results.

Temperature effects

Core	Condition	Total No. of Gd Pins	CASMO-5 k-eff
2:1	Cold	0	0.99880
2:1	Cold	0	0.99857
2:2	Cold	0	0.99896
2:2	Cold	0	0.99884
2:3	Cold	8	0.99911
2:3	Cold	8	0.99894
2:3	Warm	8	0.99900
2:3	Warm	8	0.99847
2:3	Hot	8	0.99791
2:3	Hot	8	0.99798
2:4	Cold	8	0.99865
2:4	Cold	8	0.99868
2:5	Cold	28	0.99927
2:5	Cold	28	0.99900
3:1	Cold	0	0.99910



Nuclear Data Libraries

- ENDF (USA): release 8 in 2018, managed by BNL
- ENDL (USA): managed by LLNL
- JEFF (EU): version 3.1.1
- JENDL (Japan)
- CENDL (China)
- TENDL: Based on nuclear models
- EXFOR: Experimental data

Most libraries are available in what's called the ENDF6 format. A newer format called GND is being released.

Library Impact - Actinides

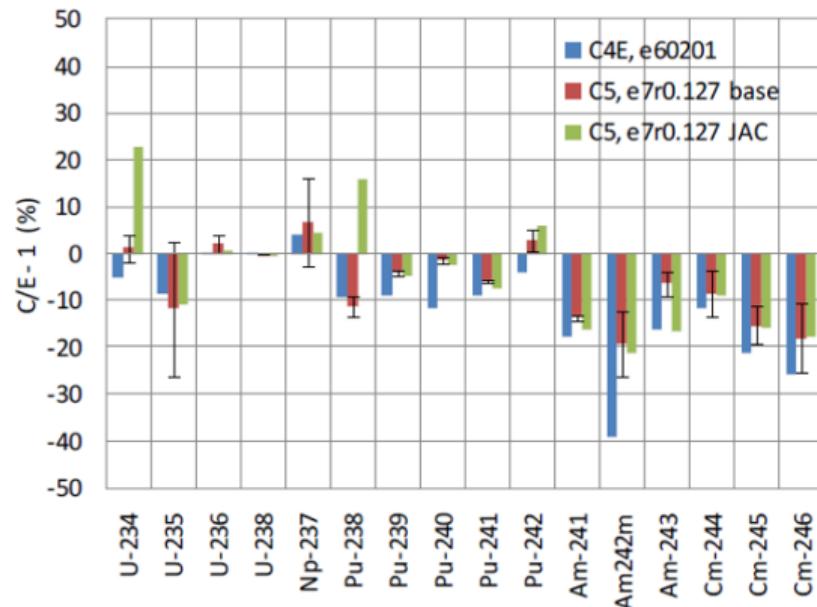


Figure 3: Actinide burnup results for UO₂ sample UR11.

Library Impact - Fission Products

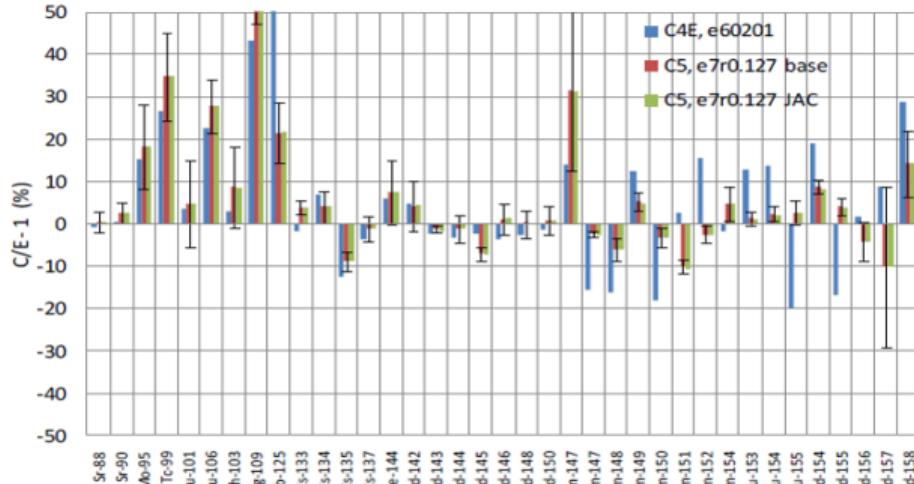


Figure 4: Fission product burnup results for UO₂ sample UR11.