Overview of reactor core neutron transport codes

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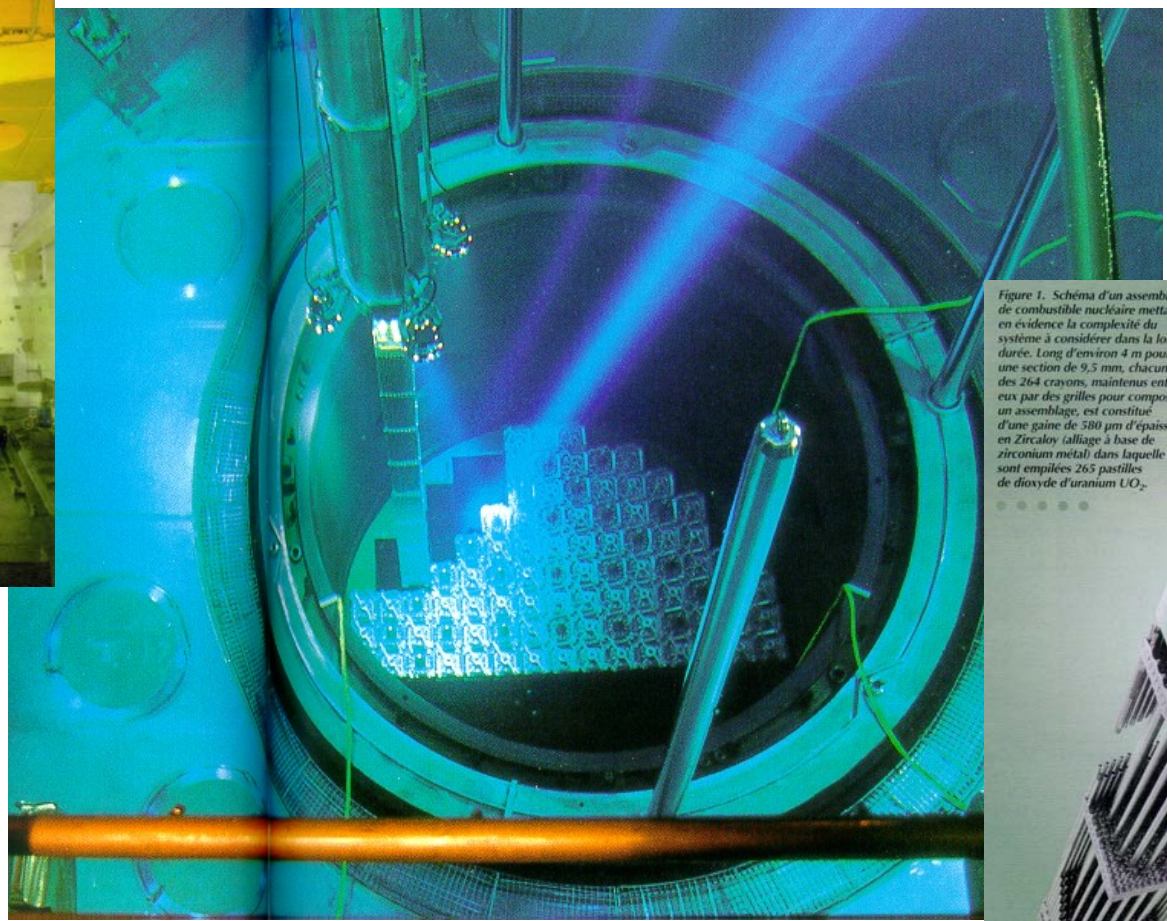
Outline

- The big picture
  - Geometry is challenging
  - The physics is challenging
- Basic nuclear data
- First order form of the integro-differential NTE
- Multigroup approximation
- Divide and conquer approach:
  - Lattice level
  - Core level
- XS Multi-parameterization
- Current and future target accuracies
- Short discussion on Monte Carlo

The big picture: example of a PWR core



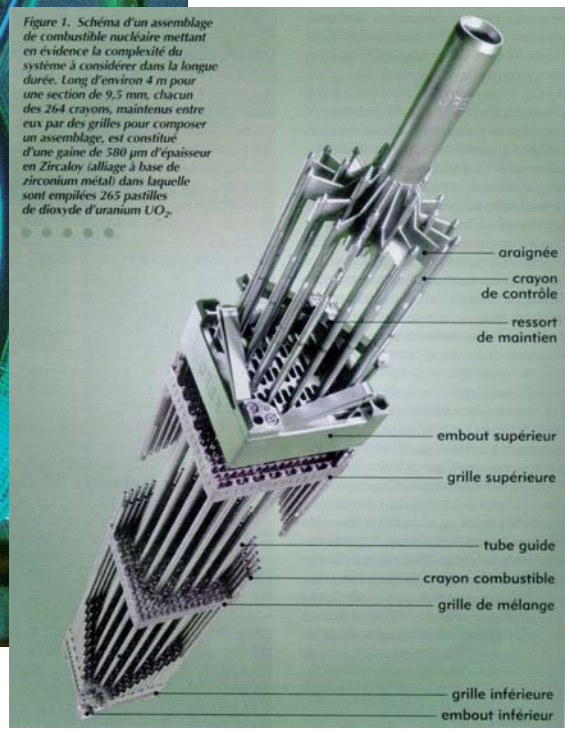
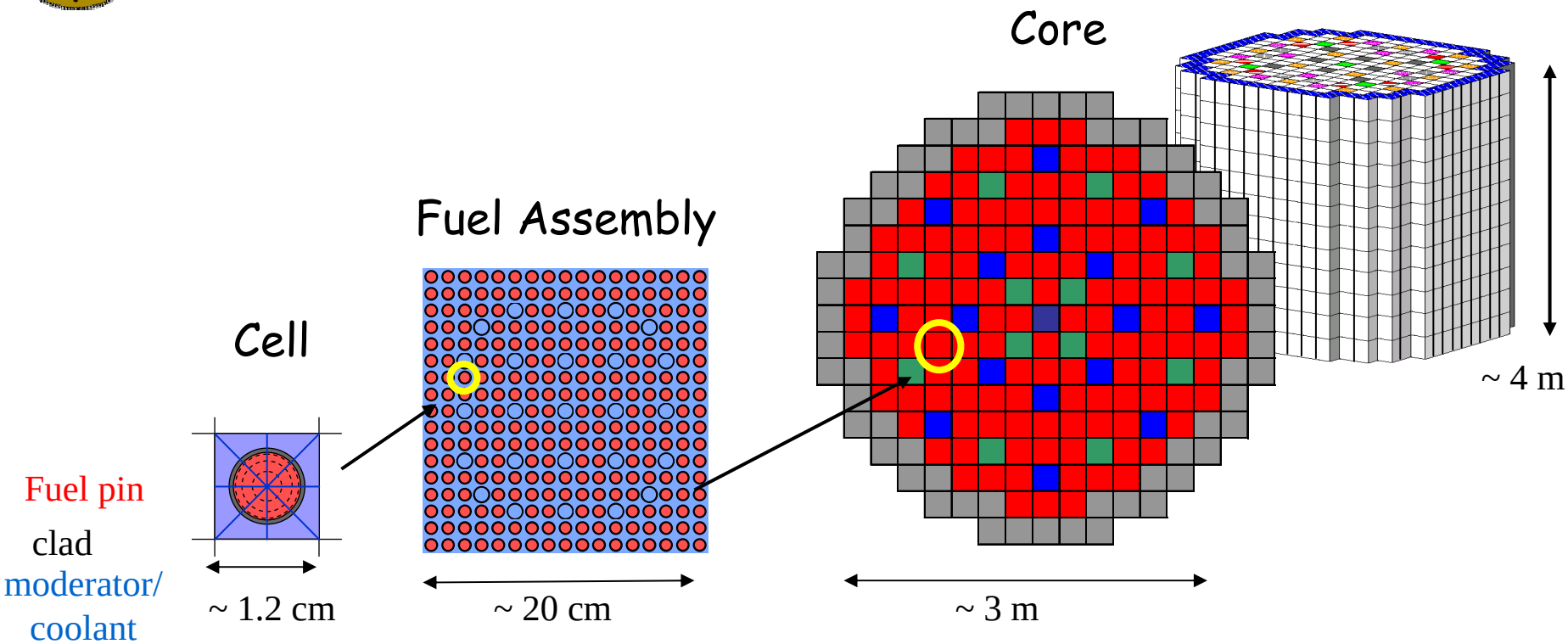


Figure 1. Schéma d'un assemblage de combustible nucléaire mettant en évidence la complexité du système à considérer dans la longue durée. Long d'environ 4 m pour une section de 9,5 mm, chacun des 264 crayons, maintenus entre eux par des grilles pour composer un assemblage, est constitué d'une gaine de 580 µm d'épaisseur en Zircaloy (alliage à base de zirconium métal) dans laquelle sont empilées 265 pastilles de dioxyde d'uranium UO_2.

Geometry is challenging



meshes per cell
6 to 48

cells per assembly:
264+25

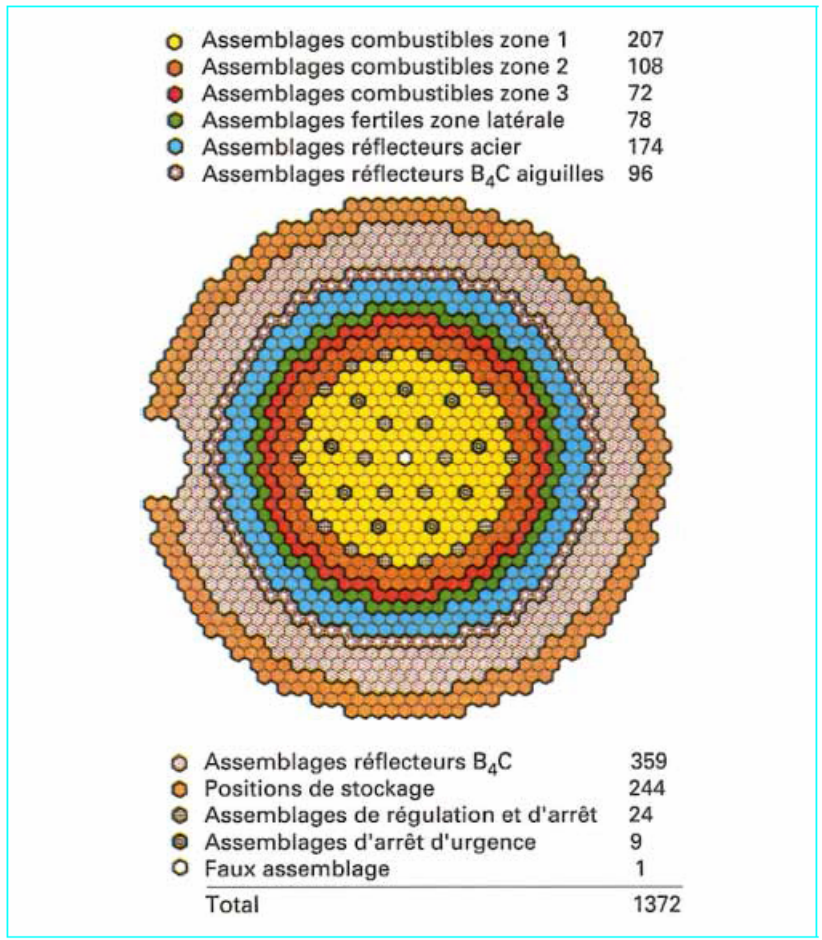
fuel assemblies in a LWR: 157 to 215

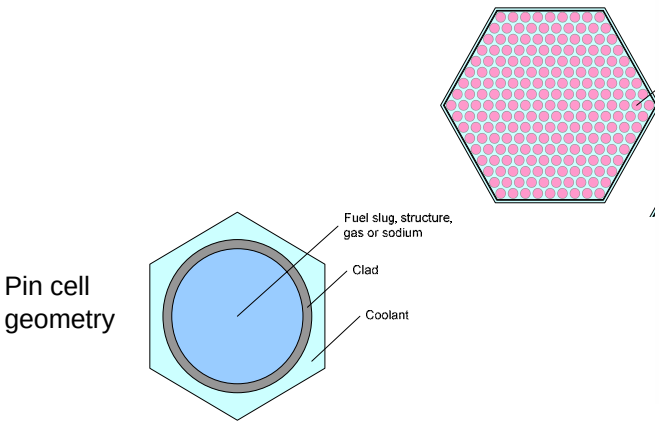
30 to 40 axial planes

- about 50,000 fuel pins (and actually 30 millions of fuel pellets)
- about 10 to 100 millions of 3-D spatial meshes
- excluding any intricacies related to radial reflector, upper/lower plena geometrical modeling

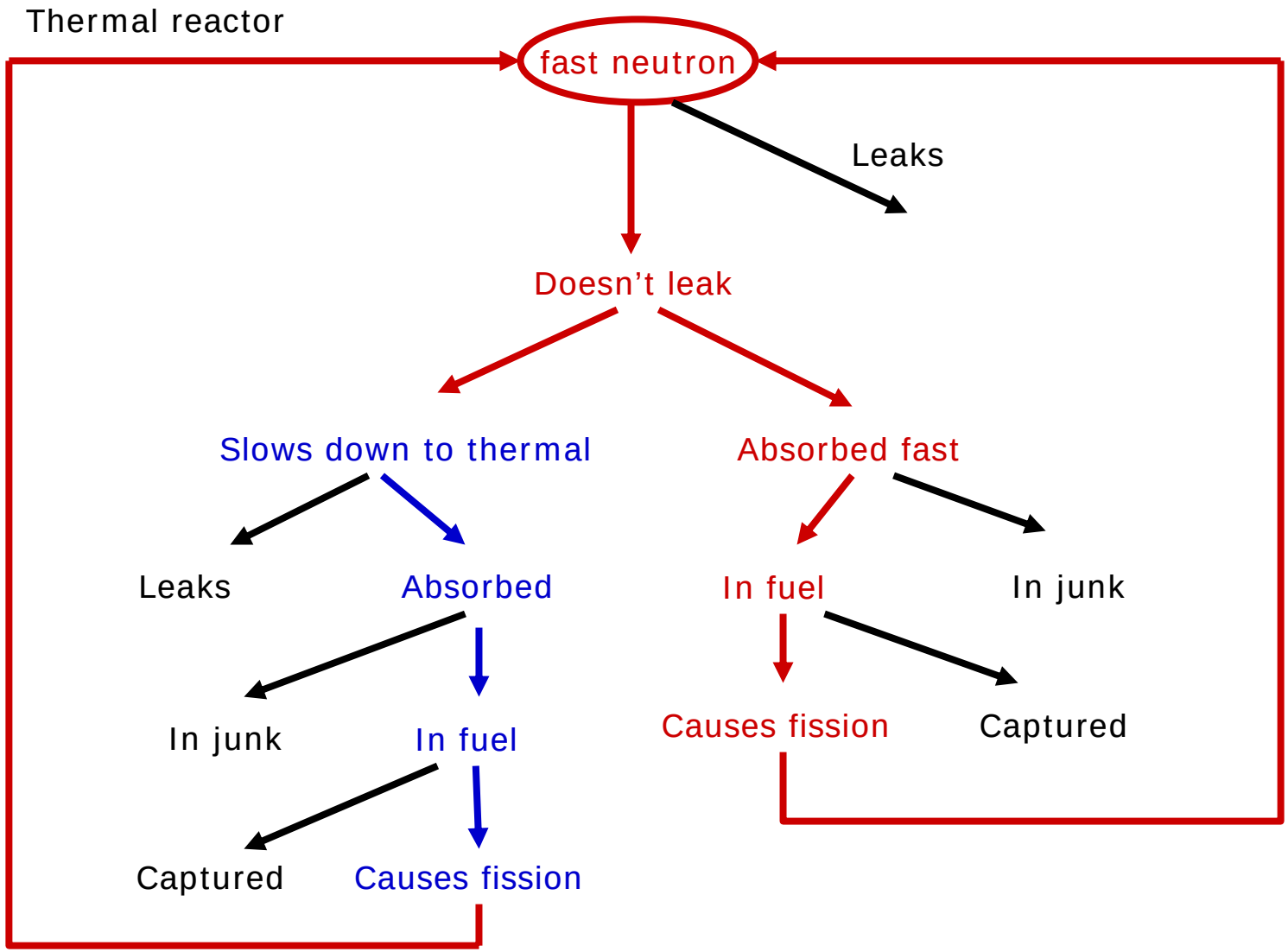
Geometry is challenging

- "EFR":
  - 271 pins per FA
  - ~400 FAs in core rings 1/2/3
  - Blanket FAs: 0 to 164



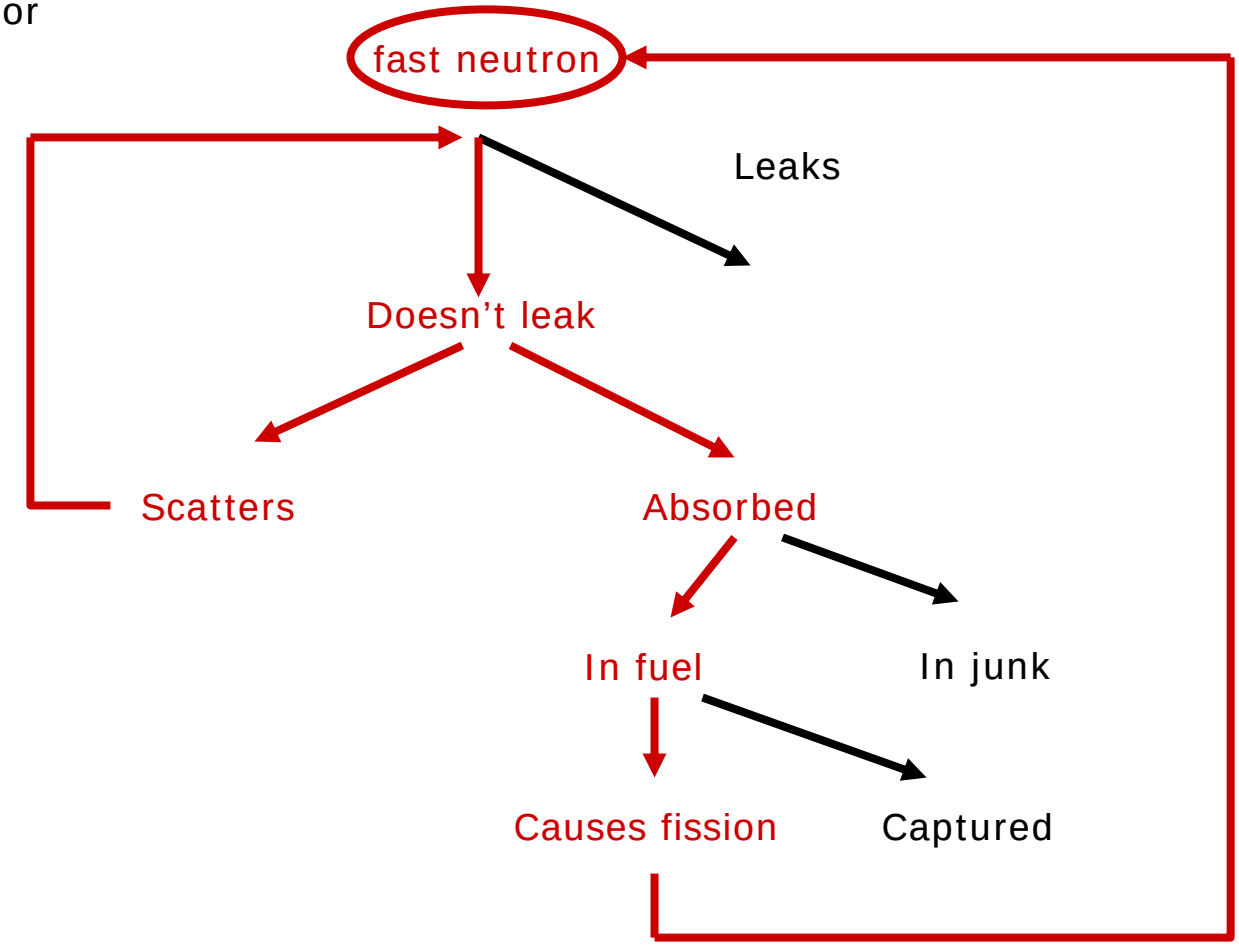


Nature is challenging: simplified neutron life cycles

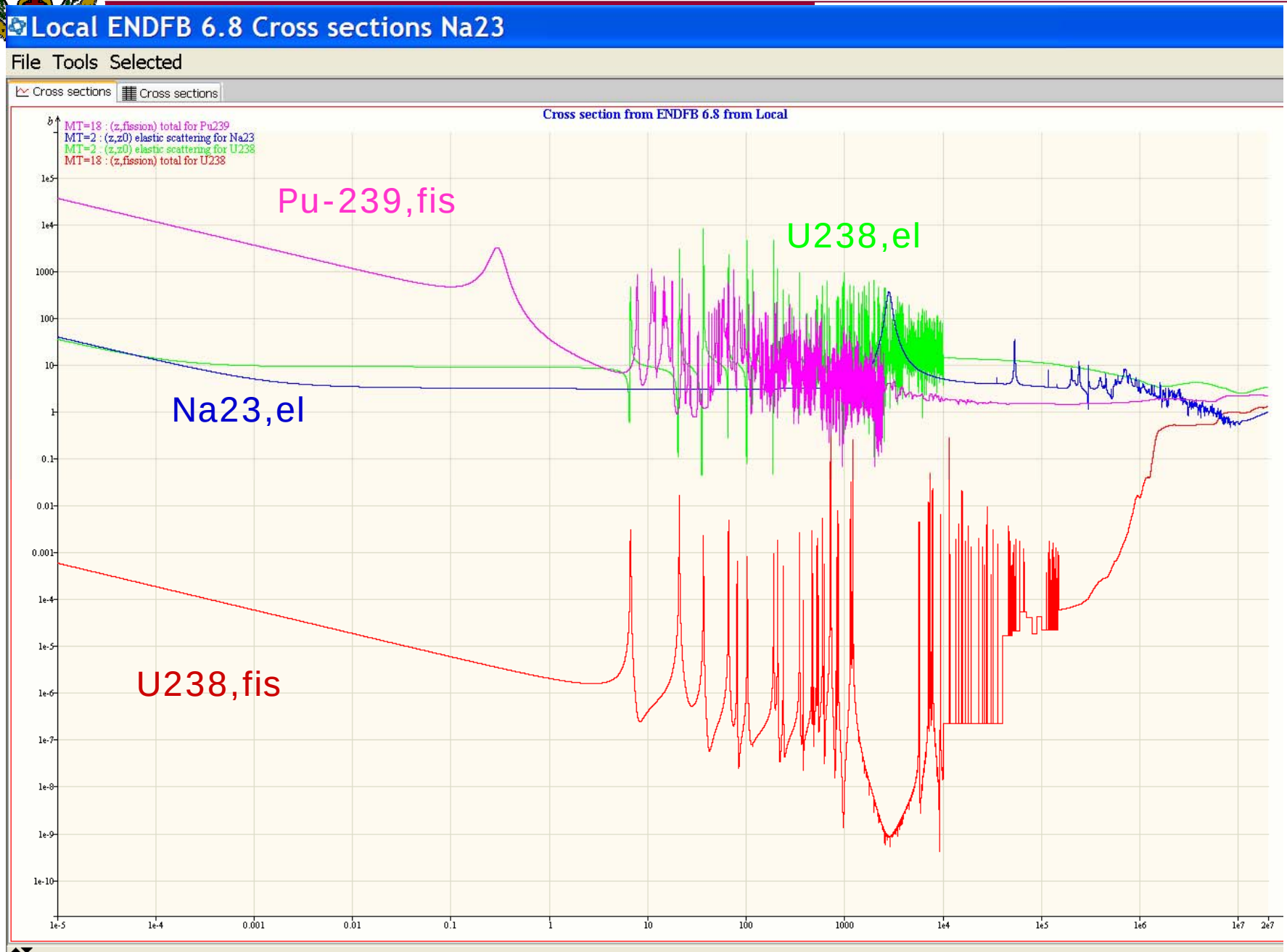


Nature is challenging: simplified neutron life cycles

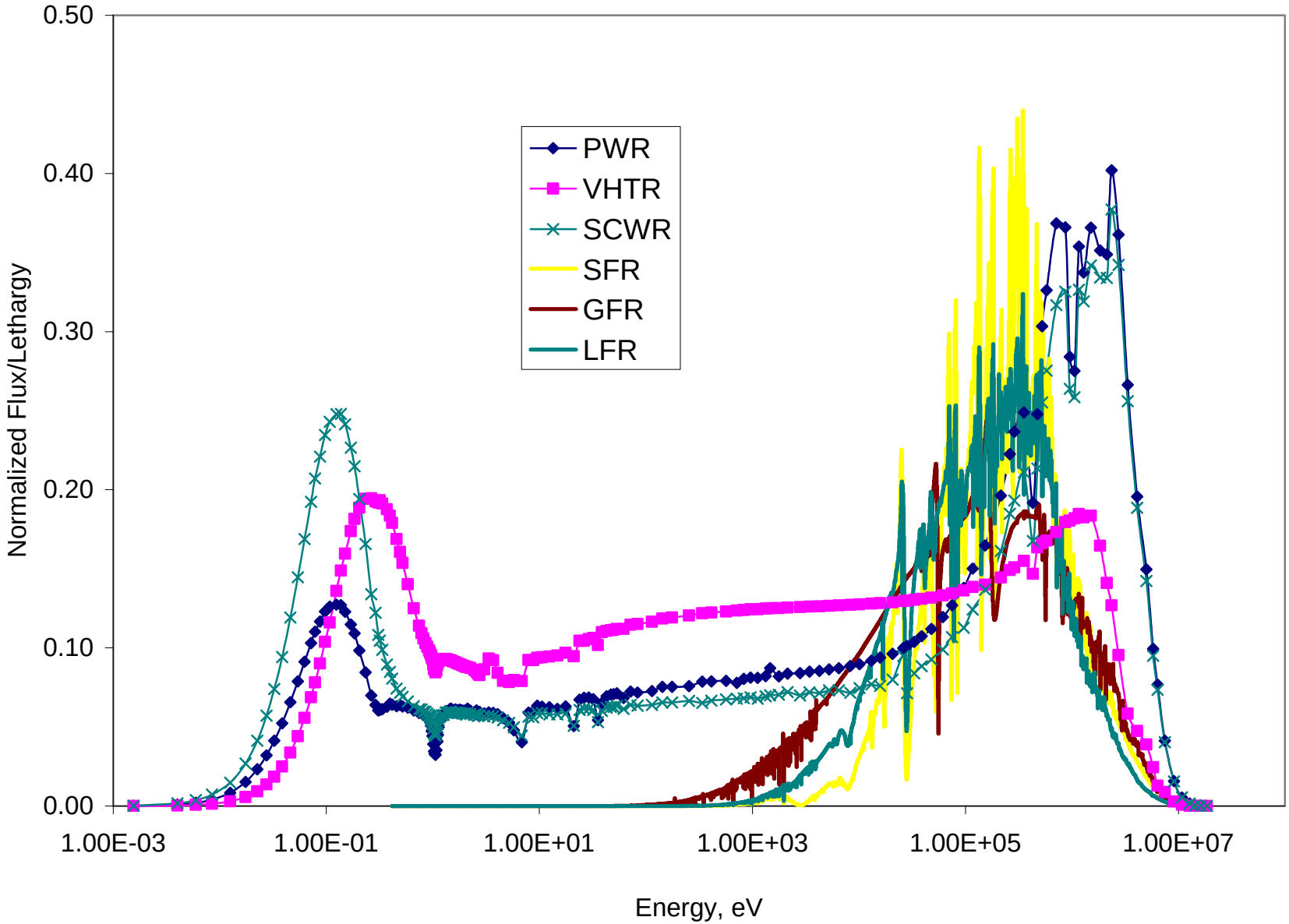
Fast reactor



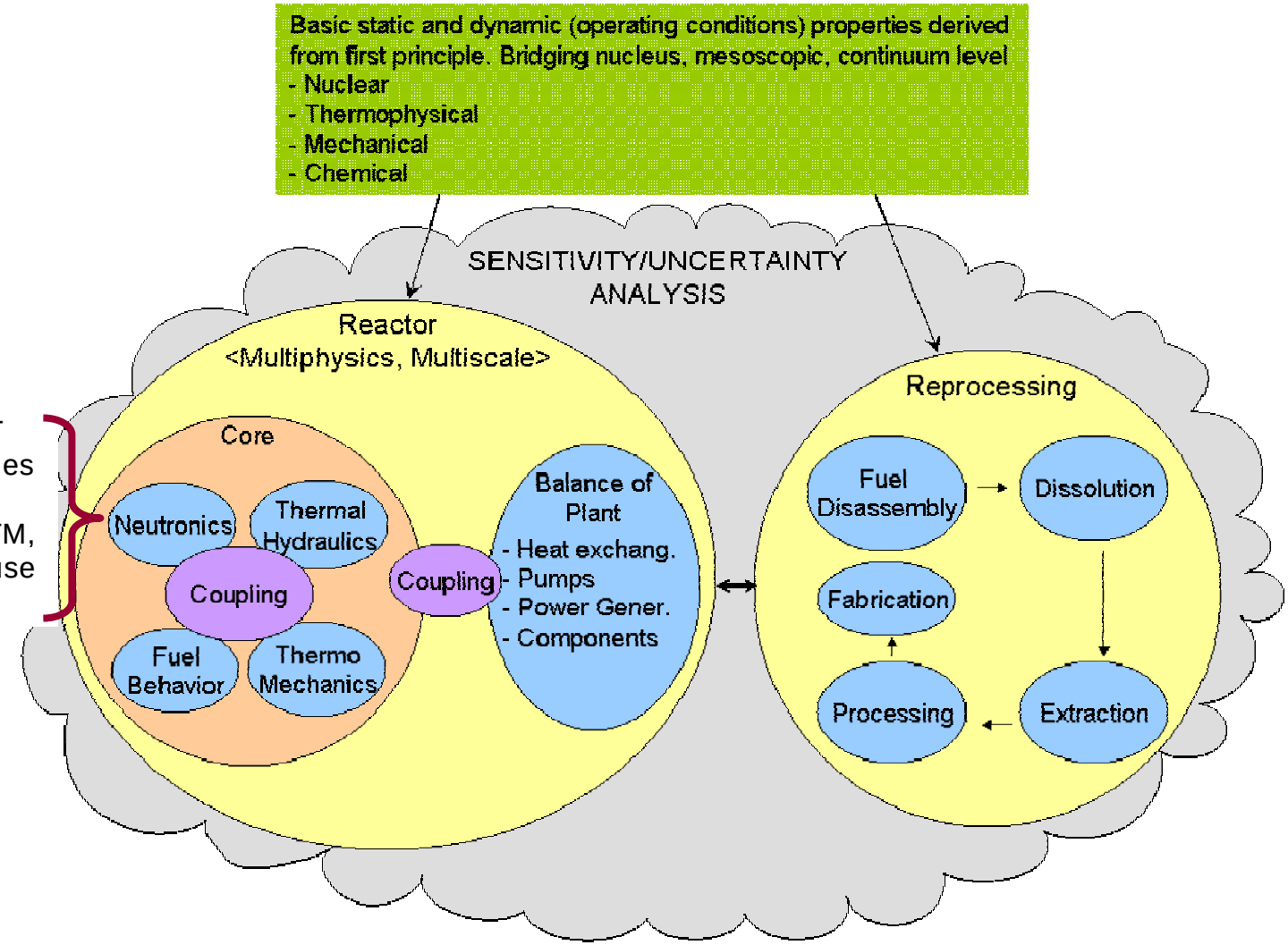
Nature is challenging



Nature is challenging : Typical spectrum per reactor type



Nature is challenging : coupled problem



XS depends on T and atom densities (which change because of TH, TM, ... but also because fuel depletes)

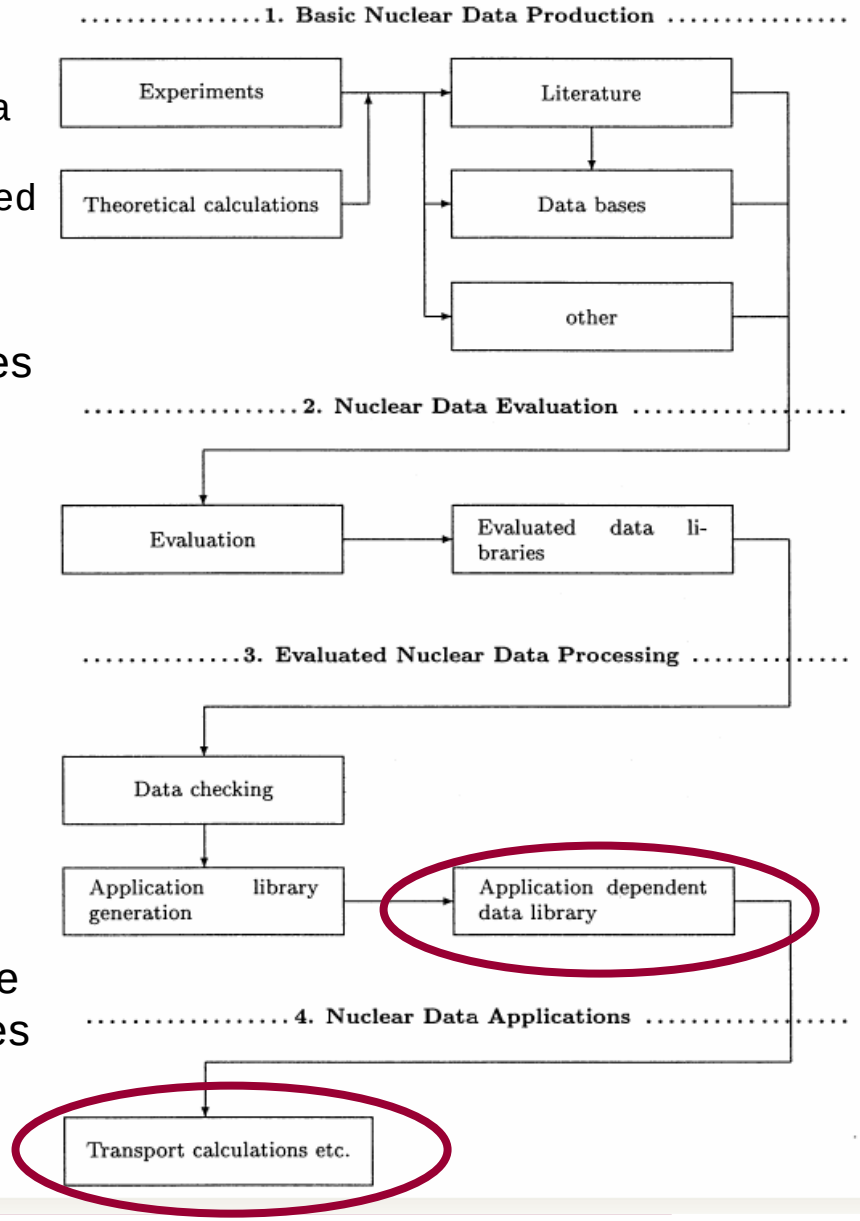
Basic nuclear data

- Activities related to nuclear data:
  - Problem dependant data are often given in a multigroup format where an “appropriate” weighting function has been used to collapsed the data in energy group

- Examples of evaluated nuclear data libraries

Country	Data file
Russia	BROND-2.2
China	CENDL-2
U S A	ENDF/B-IV
	ENDF/B-V
	ENDF/B-VI
	ENDL-84
OECD/ NEA	JEF-2.2
	EFF-2.4
	JEFF-3
Japan	JENDL-3.2

- “cross section data” is often applied to wide range of specific data at the different stages of data processing and reactor applications...!



Basic nuclear data

- Microscopic cross sections (XS): $\sigma_{xyz}(E)$
- Differential microscopic XS:

$$\sigma_s\left((\Omega,E)\rightarrow(\Omega',E')\right)=\sigma_s\left(E\right)\times f_s\left(\Omega\bullet\Omega',E\rightarrow E'\right)$$

$$\sigma_f\left((\Omega,E)\rightarrow(\Omega',E')\right)=\sigma_s\left(E\right)\times\frac{1}{4\pi}f_f\left(E\rightarrow E'\right)\cong\sigma_s\left(E\right)\times\frac{\chi\left(E'\right)}{4\pi}$$

- Interaction in a medium is given by the macroscopic XS [probability of interaction per unit particle track length]

$$\Sigma_{xyz}(E)=\sum_{iso=1}^{NISO}N_{iso}\sigma_{xyz,iso}(E)$$

(steady state) Integro-differential Neutron transport equation

- First order form of the integro-differential neutron transport equation (NTE)

$$\Omega \cdot \vec{\nabla}\Psi(\mathbf{r},\Omega,E) + \Sigma(\mathbf{r},E)\Psi(\mathbf{r},\Omega,E) = \int_0^\infty dE' \int_{(4\pi)} d\Omega' \Sigma_s(\mathbf{r},\Omega'\bullet\Omega, E' \to E)\Psi(\mathbf{r},\Omega',E') + \frac{1}{\mathrm{K}_{eff}} \frac{\chi(E)}{4\pi} \int_0^\infty dE' \nu\Sigma_f(\mathbf{r},E') \int_{(4\pi)} d\Omega' \Psi(\mathbf{r},\Omega',E')$$

where the angular (energy-dependent) neutron flux is: $\Psi(\mathbf{r},\Omega,E) = \mathrm{v}(E)\, n(\mathbf{r},\Omega,E)$

- The phase-space for the solution of the NTE possesses 6 dimensions ($\mathbf{r}$, $\mathbf{v}$ or $\mathbf{r}$, Ω and $\mathrm{v} = |\mathbf{v}|$)
  - **Spatial** discretization: **FV**, **FEM** (based either on the 1st form of the NTE or the 2nd order form).
  - **Angular** discretization: **collocation** of the angular flux on chosen directions Ω_m (short and long *characteristics* methods) or development of the angular on **spherical harmonics** basis.
  - **Energy** discretization: multigroup (averaging the NTE on an energy bin)

- Recall, about 10 to 100 millions of 3-D spatial meshes
- Multiply by G energy groups (~100's < G < 10,000's)
- Multiply by directions (100's to low 1,000's) or angular moments (10's to 100's)
- → a computational feat is needed to abide by "first-principles"

Integro-differential Neutron transport equation

- **First order** NTE (multigroup and within group)

$$\boldsymbol{\Omega}\cdot\vec{\nabla}\Psi^{g}(\mathbf{r},\boldsymbol{\Omega})+\Sigma^{g}(\mathbf{r})\Psi^{g}(\mathbf{r},\boldsymbol{\Omega})=\int_{(4\pi)}d\boldsymbol{\Omega}'\Sigma_{s}^{g\to g}(\mathbf{r},\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Psi^{g}(\mathbf{r},\boldsymbol{\Omega}')$$
$$+\sum_{\substack{g'=1\\ g'\neq g}}^{NG}\int_{(4\pi)}d\boldsymbol{\Omega}'\Sigma_{s}^{g'\to g}(\mathbf{r},\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Psi^{g'}(\mathbf{r},\boldsymbol{\Omega}') \qquad \text{for } 1\le g\le G$$
$$+\frac{1}{K_{eff}}\frac{\chi^{g}}{4\pi}\sum_{g'=1}^{NG}\nu\Sigma_{f}^{g'}(\mathbf{r})\int_{(4\pi)}d\boldsymbol{\Omega}'\Psi^{g'}(\mathbf{r},\boldsymbol{\Omega}')$$

$$\boldsymbol{\Omega}\cdot\vec{\nabla}\Psi(\mathbf{r},\boldsymbol{\Omega})+\Sigma(\mathbf{r})\Psi(\mathbf{r},\boldsymbol{\Omega})=\int_{(4\pi)}d\boldsymbol{\Omega}'\Sigma_{s}(\mathbf{r},\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Psi(\mathbf{r},\boldsymbol{\Omega}')+Q(\mathbf{r},\boldsymbol{\Omega})$$

- Even parity (**second order** formulation, within group)

$$-\boldsymbol{\Omega}\cdot\vec{\nabla}\frac{1}{\Sigma_{t-}(\mathbf{r})}\boldsymbol{\Omega}\cdot\vec{\nabla}\Psi^{+}(\mathbf{r},\boldsymbol{\Omega})+\Sigma_{t+}(\mathbf{r})\Psi^{+}(\mathbf{r},\boldsymbol{\Omega})=Q^{+}(\mathbf{r},\boldsymbol{\Omega})$$
$$+\sum_{\substack{\ell=0\\ \ell\ even}}^{L_{cut}^{+}}\Sigma_{s\ell}(\mathbf{r})\int_{(4\pi)}d\boldsymbol{\Omega}'P_{\ell}(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Psi^{+}(\mathbf{r},\boldsymbol{\Omega}')$$
$$+\sum_{\substack{\ell=1\\ \ell\ odd}}^{L_{cut}^{-}}(\boldsymbol{\Omega}\cdot\vec{\nabla})\left[\Sigma_{s\ell-}(\mathbf{r})\int_{(4\pi)}d\boldsymbol{\Omega}'P_{\ell}(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\boldsymbol{\Omega}'\cdot\vec{\nabla}\Psi^{+}(\mathbf{r},\boldsymbol{\Omega}')\right]$$

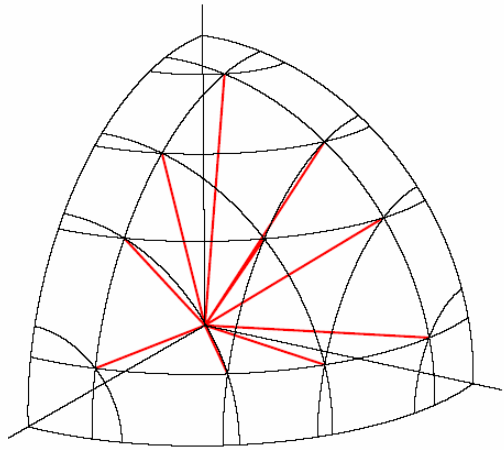
where $\Psi^{\pm}(\mathbf{r},\boldsymbol{\Omega})=\frac{1}{2}\left[\Psi(\mathbf{r},\boldsymbol{\Omega})\pm\Psi(\mathbf{r},-\boldsymbol{\Omega})\right]$

$$\Sigma_{s\ell-}(\mathbf{r})=\Sigma_{s\ell}(\mathbf{r})\Sigma(\mathbf{r})\Sigma_{t-}^{-1}(\mathbf{r})$$
$$\left[\Sigma(\mathbf{r})-\Sigma_{t+}(\mathbf{r})\right]\Psi^{+}(\mathbf{r},\boldsymbol{\Omega})=\sum_{\substack{\ell=L_{cut}^{+}+1\\ \ell\ even}}^{L_{max}}\Sigma_{s\ell}(\mathbf{r})\int_{(4\pi)}d\boldsymbol{\Omega}'P_{\ell}(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Psi^{+}(\mathbf{r},\boldsymbol{\Omega}')$$
$$\left[\Sigma(\mathbf{r})-\Sigma_{t-}(\mathbf{r})\right]\Psi^{-}(\mathbf{r},\boldsymbol{\Omega})=\sum_{\substack{\ell=L_{cut}^{-}+1\\ \ell\ odd}}^{L_{max}}\Sigma_{s\ell}(\mathbf{r})\int_{(4\pi)}d\boldsymbol{\Omega}'P_{\ell}(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Psi^{-}(\mathbf{r},\boldsymbol{\Omega}')$$

A few words on angular discretizations

- Collocation (discrete ordinates aka SN)
  - Requires a set of directions Ω_d and weights ω_d such that:

$$\Phi(\mathbf{r}) = \int_{(4\pi)} d\Omega' \Psi(\mathbf{r},\Omega') \approx \sum_{d=1}^{NDir} \omega_d \Psi(\mathbf{r},\Omega_d)$$



  - Iterations on the within source scatter

$$\Omega_d \cdot \vec{\nabla}\Psi^{i+1}(\mathbf{r},\Omega_d) + \Sigma(\mathbf{r})\Psi^{i+1}(\mathbf{r},\Omega_d) = \sum_{\ell=1}^{L} \Sigma_{s,\ell}(\mathbf{r}) \sum_{m=-\ell}^{\ell} Y^*_{\ell,m}(\Omega_d)\phi^i_{\ell,m}(\mathbf{r}) + Q(\mathbf{r},\Omega_d)$$

$$\phi^i_{\ell,m}(\mathbf{r}) = \int_{(4\pi)} Y_{\ell,m}(\Omega_d)\Psi^i(\mathbf{r},\Omega_d) \approx \sum_{d=1}^{Dir} \omega_d Y_{\ell,m}(\Omega_d)\Psi^i(\mathbf{r},\Omega_d)$$

    - Process needs to be accelerated when $\Sigma_{s,0} / \Sigma \cong 1$

  - Decouple angular directions from spatial discretization (in Cartesian geometries)

  - Short characteristics method: mesh sweeping done mesh cell by mesh cell
  - Long characteristics method: solve the transport equation for a trajectory along Ω_d crossing the domain from boundary to boundary.

A few words on angular discretizations

- PN method (spherical harmonics)
  - The angular is decomposed on the spherical harmonic basis

$$\Psi(\mathbf{r},\Omega) = \sum_{\ell=1}^{Nharm} \sum_{m=-\ell}^{\ell} Y^{*}_{\ell,m}(\Omega)\phi_{\ell,m}(\mathbf{r})$$

$$\text{where} \quad \phi_{\ell,m}(\mathbf{r}) = \int_{(4\pi)} d\Omega \; Y_{\ell,m}(\Omega)\Psi(\mathbf{r},\Omega)$$

  - Take the angular moment of the NTE

$$\int_{(4\pi)} d\Omega \; Y_{\ell,m}(\Omega)\left(\text{NTE}\right) \Rightarrow$$ spatial equations coupling several flux angular moments

Multigroup approximation

$$\int_{E_{g-1}}^{E_g} dE\,(\mathrm{NTE}) \Rightarrow$$

$$\Omega\cdot\vec{\nabla}\Psi^g(\mathbf{r},\Omega)+\Sigma^g(\mathbf{r})\Psi^g(\mathbf{r},\Omega)=\int_{(4\pi)} d\Omega'\,\Sigma_s^{g\to g}(\mathbf{r},\Omega'\bullet\Omega)\Psi^g(\mathbf{r},\Omega')$$

$$+\sum_{\substack{g'=1\\ g'\neq g}}^{NG}\int_{(4\pi)} d\Omega'\,\Sigma_s^{g'\to g}(\mathbf{r},\Omega'\bullet\Omega)\Psi^{g'}(\mathbf{r},\Omega') \qquad \text{for } 1\le g\le G$$

$$+\frac{1}{K_{eff}}\frac{\chi^g}{4\pi}\sum_{g'=1}^{NG}\nu\Sigma_f^{g'}(\mathbf{r})\int_{(4\pi)} d\Omega'\,\Psi^{g'}(\mathbf{r},\Omega')$$

- A key idea is to preserve the reaction rates (physically observable quantities)

$$\Sigma^g(\mathbf{r})\Phi^g(\mathbf{r})=\int_{E_{g-1}}^{E_g} dE\Sigma(\mathbf{r},E)\Phi(\mathbf{r},E) \quad \text{or} \quad \Sigma^g(\mathbf{r})=\frac{\int_{E_{g-1}}^{E_g} dE\Sigma(\mathbf{r},E)\Phi(\mathbf{r},E)}{\int_{E_{g-1}}^{E_g} dE\Phi(\mathbf{r},E)}$$

with $$\Phi(\mathbf{r},E)=\int_{(4\pi)} d\Omega'\,\Psi(\mathbf{r},\Omega',E)$$

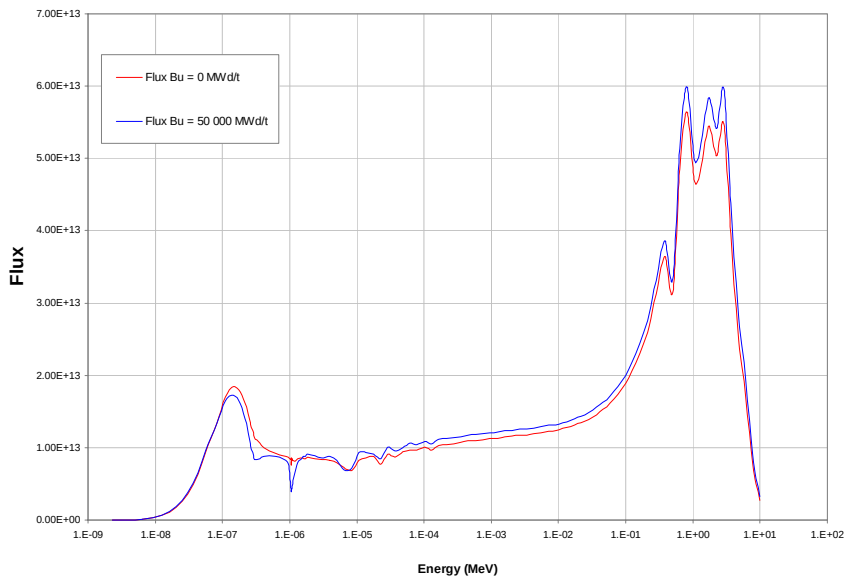
- Is this a “tour de force” where the unknown Psi is needed to compute the multigroup cross sections…???

Multigroup approximation

- An *a priori* knowledge of the reactor spectrum (weighting function *w* below) is required to prepare the multigroup cross section set:

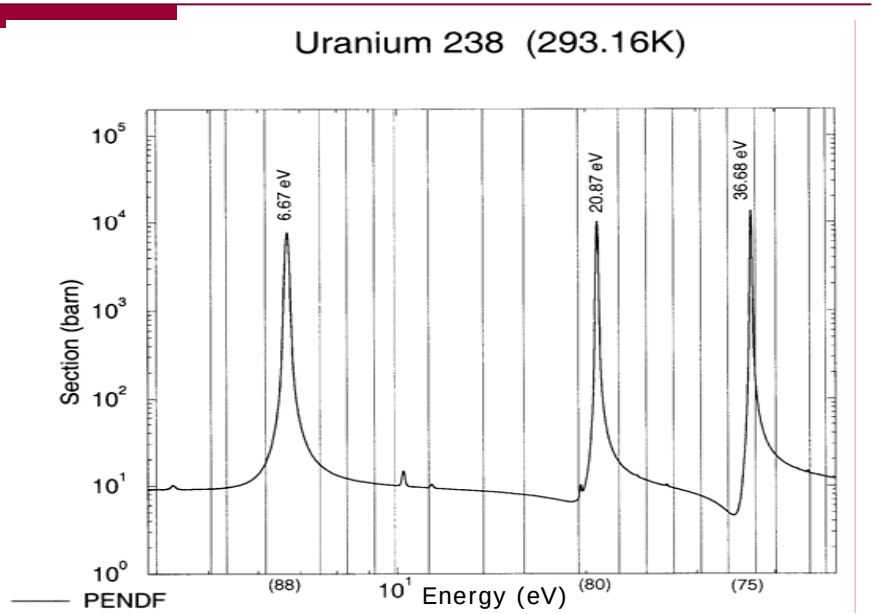
$$\sigma^g = \frac{\int_{E_{g-1}}^{E_g} dE\ \sigma(E)w(E)}{\int_{E_{g-1}}^{E_g} dE\ w(E)}$$

- E.g., for LWR, *w* is:
  - fission spectrum for E>1.3 MeV,
  - 1/E slowing down spectrum
  - Maxwellian distribution in the thermal range
  - Decent approximation when compared to a 172-g 2D UOX lattice calculation →

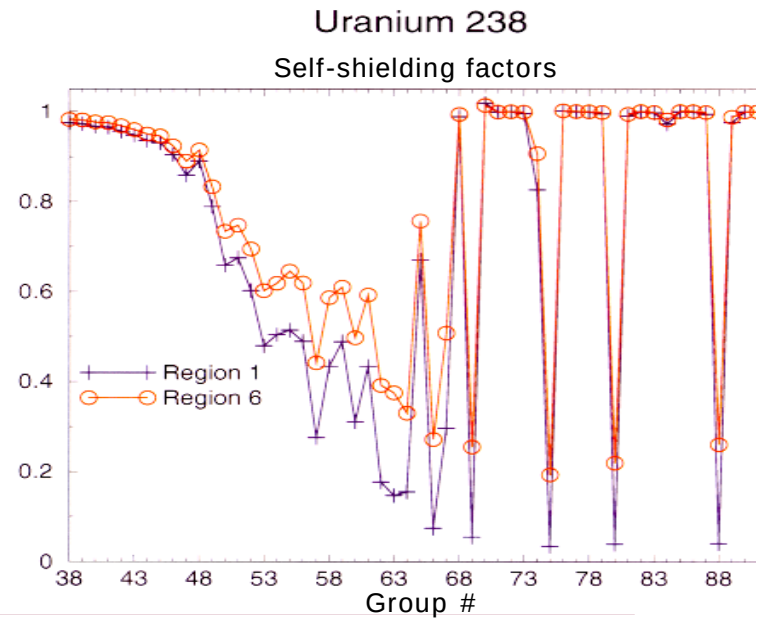


Multigroup approximation: self-shielding

- Issue:
  - The spectrum or weighting function *w* doesn't account for flux dip in resonances
  - Multigroup cross sections should be modified (self-shielded)



- Multigroup cross sections are prepared/tabulated with respect to
  - Temperature (Doppler broadening)
  - Dilution section σ_b
  - In subsequent lattice calculations, the cross section values will interpolated in these tables.



Divide and conquer

- In order to compute a reactor core, we currently rely on:
  1. Appropriate multigroup cross section libraries with 100's of energy groups:
     - ~200 g for thermal reactors,
     - ~2000 g for fast reactors

  2. A "divide and conquer" type of approach:

     - **Fuel assembly level** computations are performed with **high accuracy** (neutron transport calculations with 100's of groups, fine spatial discretization). Pin power form functions are stored for subsequent pin power reconstruction.

     - **Equivalence step**: spatial homogenization and group collapse of the assembly level results in order to generate few group cross section libraries for the core level calculation (few groups = 2 for thermal reactors, 232 for fast reactors). For LWRs, this step generated ADFs (assembly discontinuity factors)

     - **Full core level computations** during which the keff, reactivity, assembly averaged power distribution, etc …, are obtained.

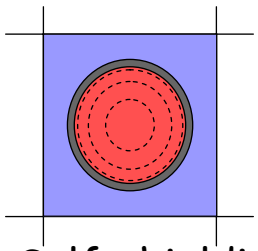
     - **Pin power reconstruction step** where the pin power is contained by combining the assembly level pin power form functions and the core level power distribution.

Divide and conquer

Evaluation $\sigma_{isot}(E)$

Library σ^{g}_{isot}

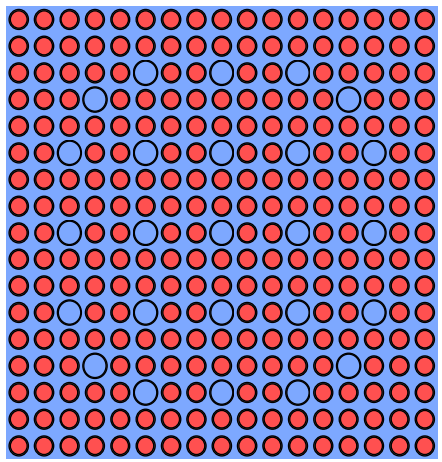
Assembly level



Self-shielding $\sigma^{g}_{isot,i} \rightarrow \Sigma^{g}_{i}$

NTE

Φ^{g}_{i}

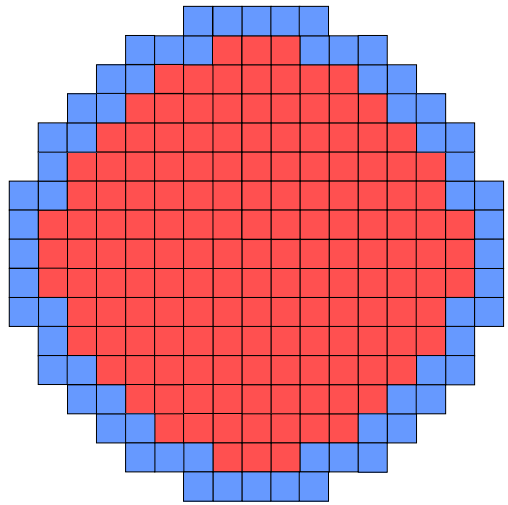


pin pow. fun.

Σ^{G}, ADF

Equivalence

Core level



Low-order few group Transport

Keff, power, etc...

Pin power reconstruction

Typical number of assembly level computations

Complete set of lattice calculations for a BWR includes:

- Depletion calculations:
- Each depletion has about 50 burnup points
- Depletions for 3 different voids (0, 40, 80%) both with/without control rods

- Branches from each depletion, for all independent variable, at 20 points:
- Void (3 points)
- Fuel temperature (3 points)
- Control rod (each type)
- Bypass void (3 points)
- Spacer type, detector type

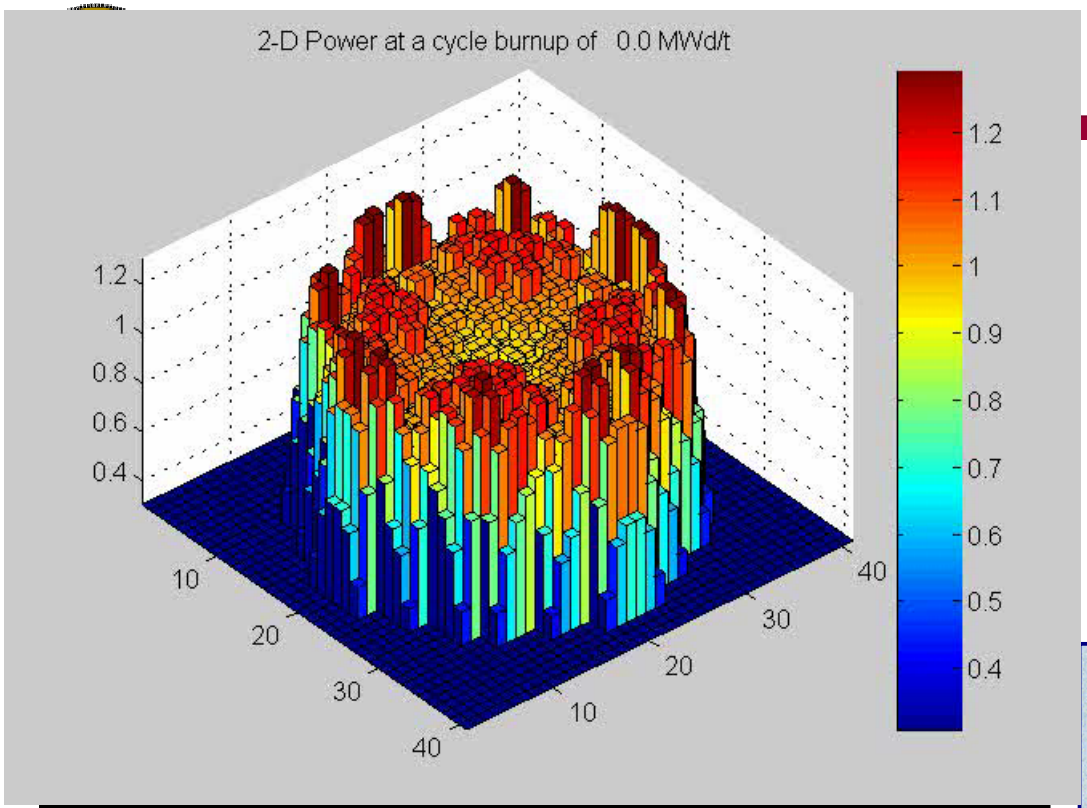
Complete (HFP at least) set of calculations includes:

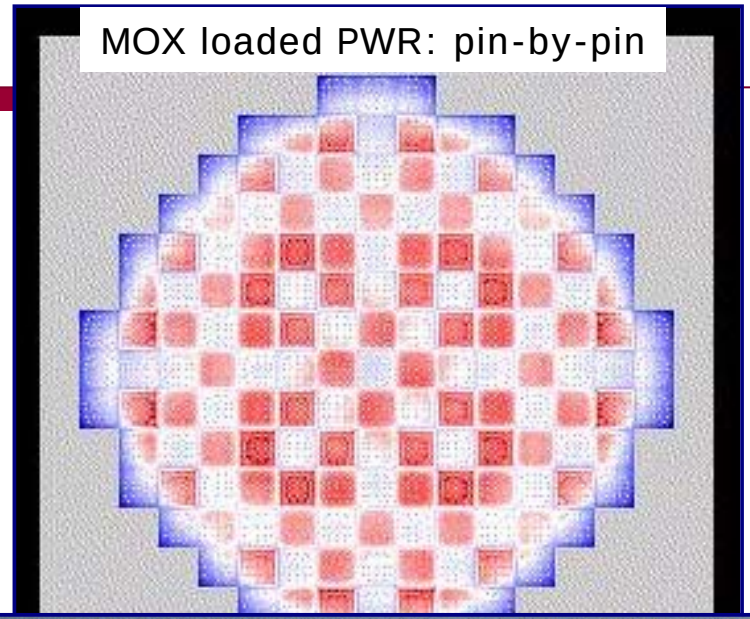
[50 x 3 x 2] + [20 x 3 x 2 x (3 + 3 + 1 + 3 + 2)] = **1740 total state points**

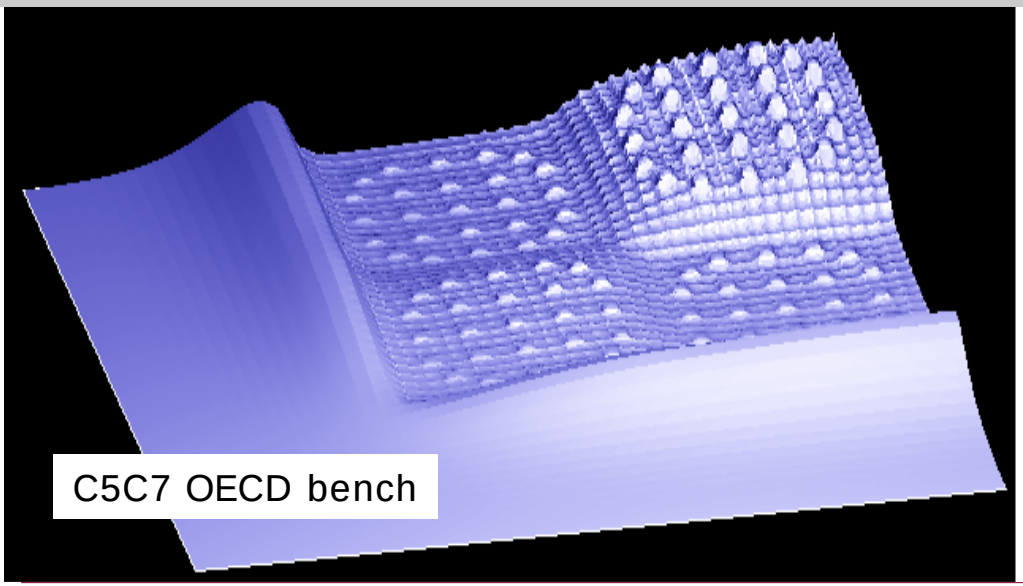
These **multi-parameterized** cross section libraries are subsequently used in core cycle depletion calculations

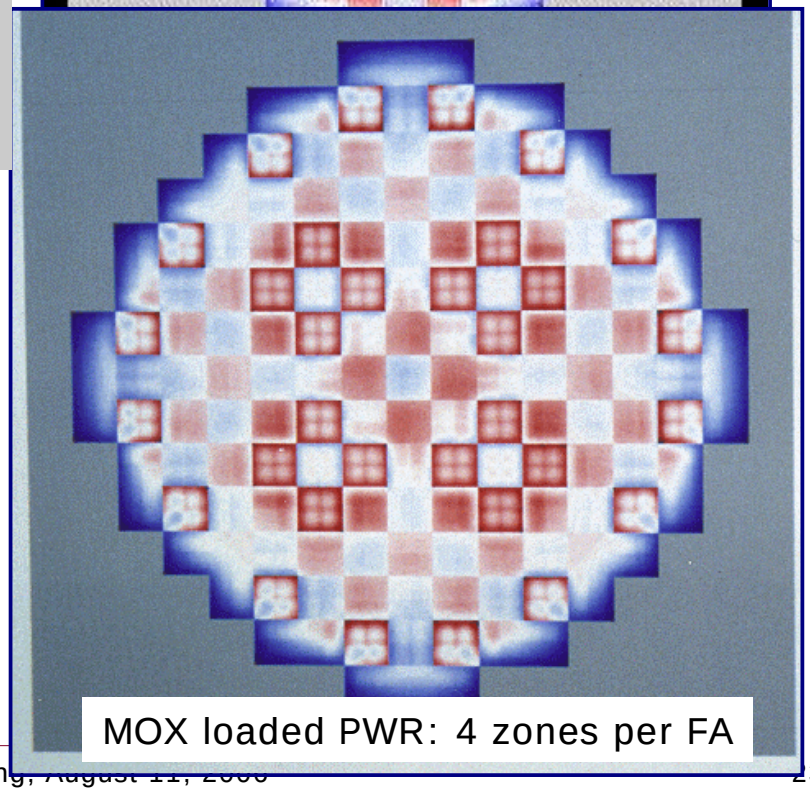
Accuracies

Current Operating Reactors (some due to K. Smith)		Future ?
Keff	~0.5%	0.1%
PWRs		
Axially-integrated reaction rates	~ 1.0% rms	
3-D reaction rates	~ 3.0% rms	1%
BWRs		
Axially-integrated reaction rates	~ 1.5% rms	
3-D reaction rates	~ 3.0-6.0% rms	1%
Rod worth	~2-8%	1%
Local nuclide densities		
Main elements	~5%	1%
Others	~5-20%	1-5%


2-D Power at a cycle burnup of 0.0 MWd/t
1.2
1
0.8
0.6
0.4
10
20
30
40
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4


MOX loaded PWR: pin-by-pin


C5C7 OECD bench


MOX loaded PWR: 4 zones per FA

Recent trends in methodology

- Eliminate or reduce the need for spatial homogenization of the fuel assembly
  - Homogenized Pin-by-pin core level computation
  - Pin-by-pin core level computation with limited homogenization (pin made of 2 regions: (1) coolant, (2) fuel+clad)

- Increase the number of energy groups
  - At the assembly level (10,000)
  - At the core level (e.g., fast reactors can now be computed with 2000 g)

- Avoid using diffusion theory at the core level
  - SN or PN transport (with N being limited by the computer)
  - Simplified PN transport

Monte Carlo simulations

- Def.:
  - Perform particle transport experiments in a random manner on a computer to estimate average behavior of a particle in phase space
- Advantages:
  - Precise geometric modeling
  - Energy continuous cross sections
- MC R&D needs:
  - Depletion
  - Temperature effects/coupling
  - Source convergence
- MC is primarily a V&V tool at BOL
  - Scale of problem:
    - Number of fuel Assemblies 200
    - Number of axial planes 100
    - Number of pins per assembly 300
    - Number of depletion regions per pin 10
    - Number of isotopes to be tracked 100
    - Total unknowns 6 billion tallies
    - **Source distribution** if far more difficult to converge for a full-core (dominance ratio > 0.995)

Summary and trends

- Moving away from the classical “divide & conquer” approach for full blown application of first principles

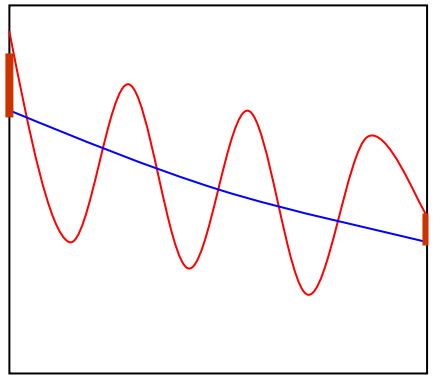
- Energy groups:
  - 10,000’s range to simplify or remove self shielding formalism

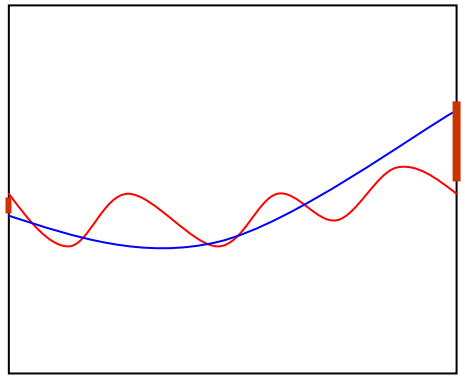
- Space-angle:
  - Even parity methods:
    - Nowadays exists in 3-D (Variant-ANL)
    - Intimate coupling of space and angle
    - Leads to the assembly and storing of use matrices
    - Well adapted for massively parallel libraries such as PETSc

  - SN methods:
    - Short characteristics:
      - Only SN mesh in 3-D nowadays (Attila –Transpire, IDT/Cronos-CEA)
      - Mesh is swept cell by cell (on regular grid, there exist efficient parallel sweeping schemes; on unstructured or curvilinear meshes: a topic of R&D)

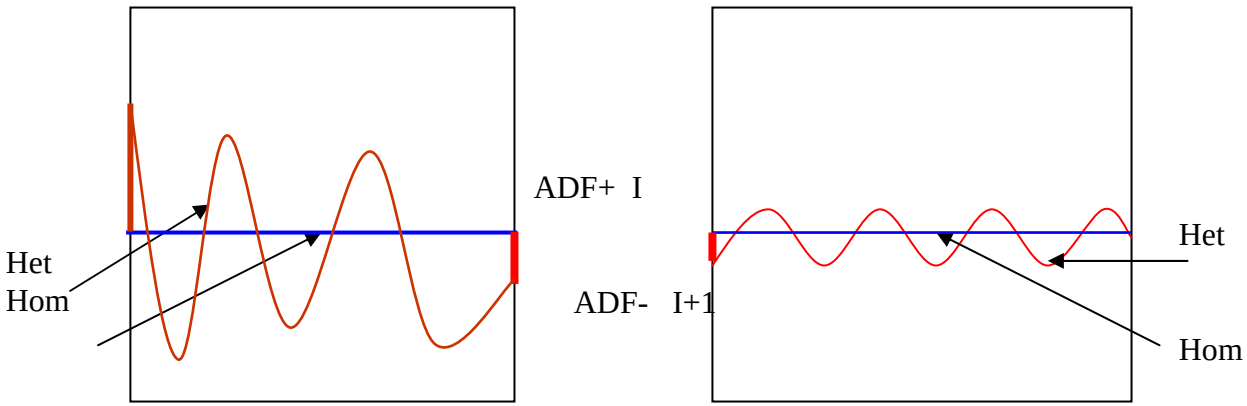
    - Long characteristics:
      - Each trajectory is independent (natural parallelism)
      - Hugh quantity of information to be stored for 3-D (topic of R&D)

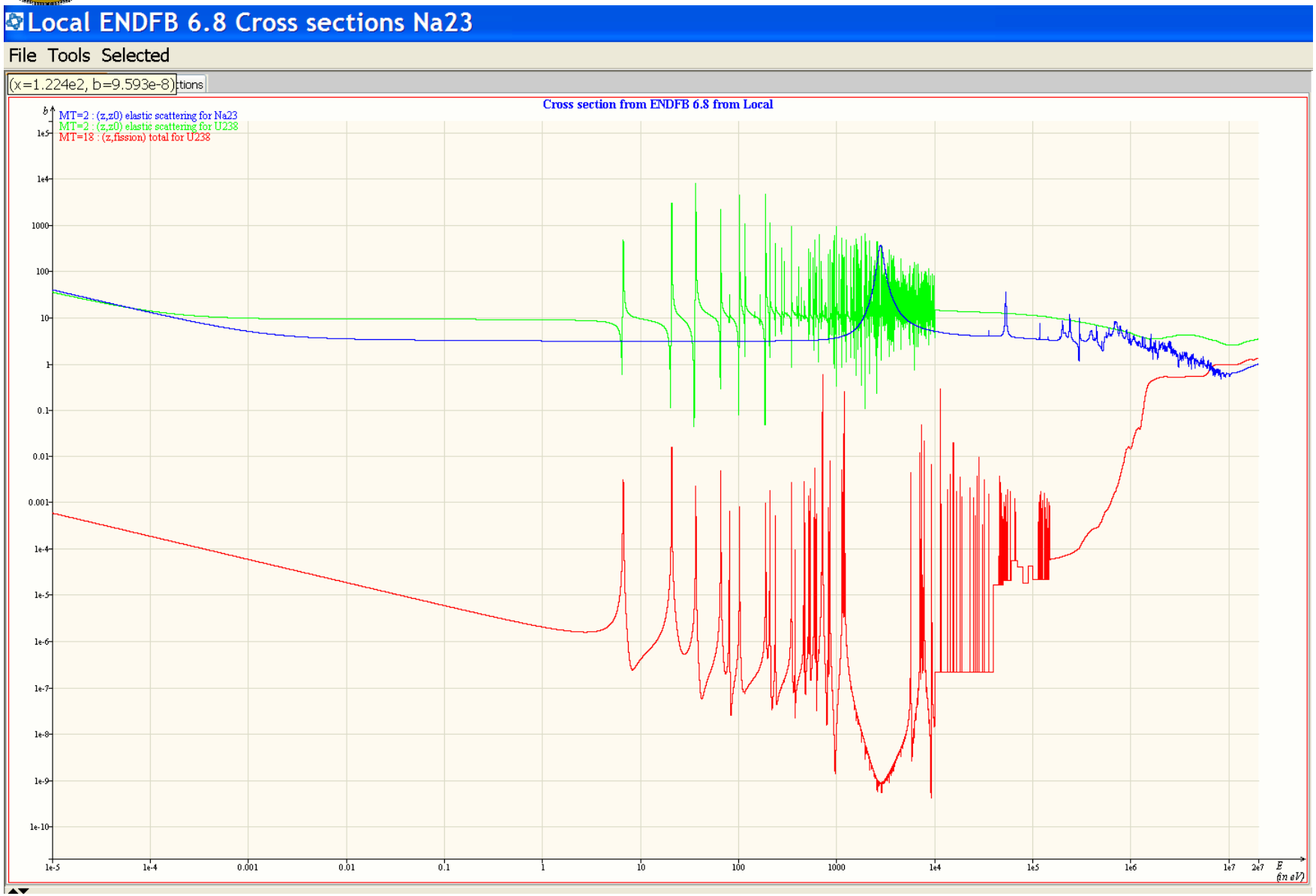
Discontinuity Factors





- Let + - heterogeneity factors be different (Discontinuity Factors)
- Approximate DF's from single-assembly lattice calculation (ADFs)




Local ENDFB 6.8 Cross sections Na23
File Tools Selected
(x=1.224e2, b=9.593e-8)
Cross section from ENDFB 6.8 from Local
MT=2 : (z,z0) elastic scattering for Na23
MT=2 : (z,z0) elastic scattering for U238
MT=18 : (z,fission) total for U238
b
E (in eV)