22.251 LAB Exercise 1
CASMO-4 Pin Cell Calculations

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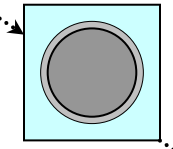
Core simulation sequence

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

Basic data base:

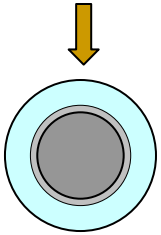
cross-sections, decay data

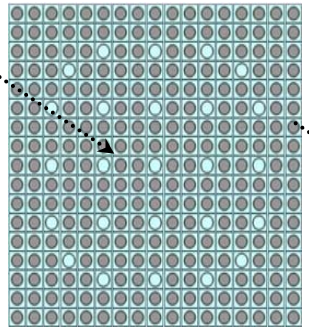
Multi-group cross sections



Unit cell

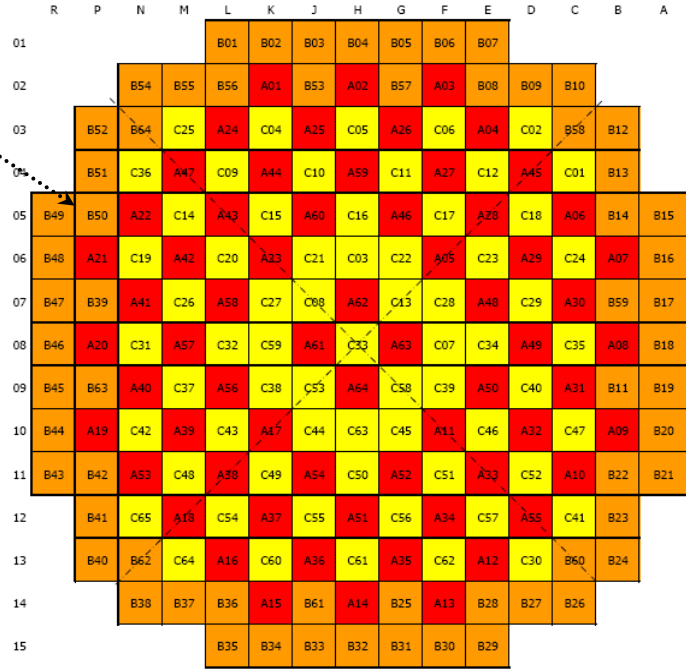
1D transport of equivalent cell





Fuel assembly

2D transport or diffusion



Reactor core

3D diffusion

LWR Core Simulations

- Lattice physics codes (e.g. CASMO) are used to prepare problem-dependent few group cross sections based on a smaller region (e.g. fuel assembly) for input to a whole-core program (e.g. SIMULATE).
- The CASMO few group cross sections are curve fitted to functions of important variables such as burnup, moderator temperature and void content, fuel temperature, soluble poison concentration …
- These workhorse codes (CASMO) are all deterministic. There is also growing use of stochastic “Monte Carlo” programs for these applications (MCNP will be introduced in later lab sessions), but code running times are still excessive for many purposes.

Computer codes

- Transport-burnup codes
  - Infinite lattice, fuel cell or assembly
  - Many energy groups
  - Region average cross-section data
  - Time (burnup) dependant
  - Operation condition dependent (Tf, Tm, Power, Xe, Boron conc.)
- Nodal Diffusion codes
  - 3D core power distribution
  - 2 energy groups
  - Account for thermal feedback

Reactor Theory Uses

- Slowing down
  - Energy spectrum calculation
  - Homogenization of heterogeneous regions
- Transport
  - Spatial power distribution where diffusion does not work
  - Preparation of region averaged cross-sections
- Diffusion
  - Nodal methods for 3D core power distribution
- Burnup
  - Evolution of nuclide concentrations with time

Current Code Sets Used for LWR Reload Analysis

Code supplier	Code set*	Users		
		Vendor	Licensee	Consultant
ABB-CE	PHOENIX/POLKA	✓	✓	
B&W/Framatome	CASMO**/NEMO	✓	✓	
General Electric	TGEBLA/PANACEA	✓	✓	
Siemens	CASMO**/MICROBURN	✓	✓	
Westinghouse	PHOENIX/ANC	✓	✓	
EPRI	CPM-2/NODE-P		✓	✓
EPRI	CPM-2/SIMULATE-E		✓	✓
EPRI	CPM-3/CORETRAN			✓
Studsvik	CASMO**/SIMULATE-3**		✓	✓
Scanpower***	HELIOS/RAMONA		✓	

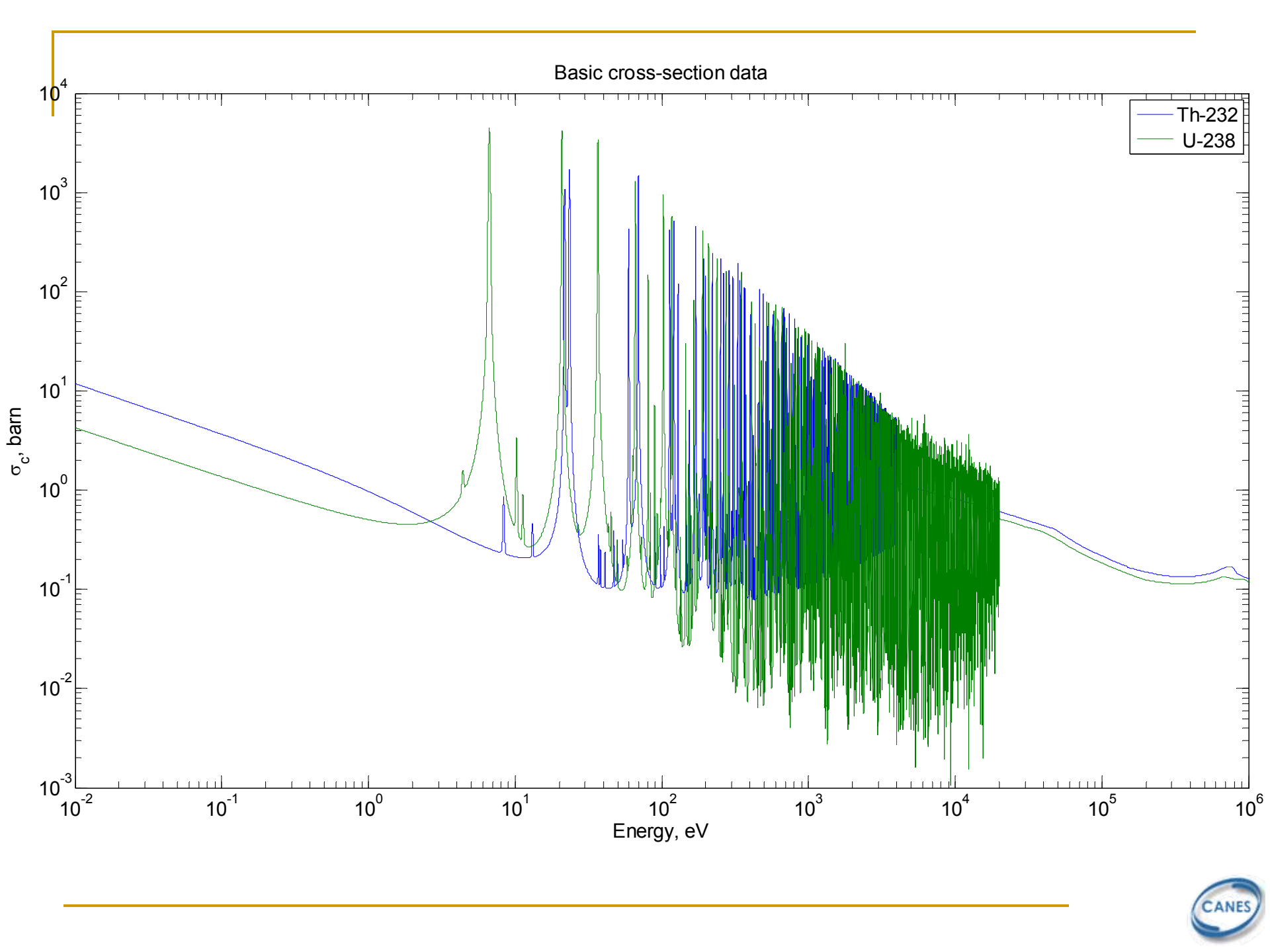
* Many different versions of these codes are in use today

** Codes developed by Studsvik of America

*** Scanpower has merged with Studsvik

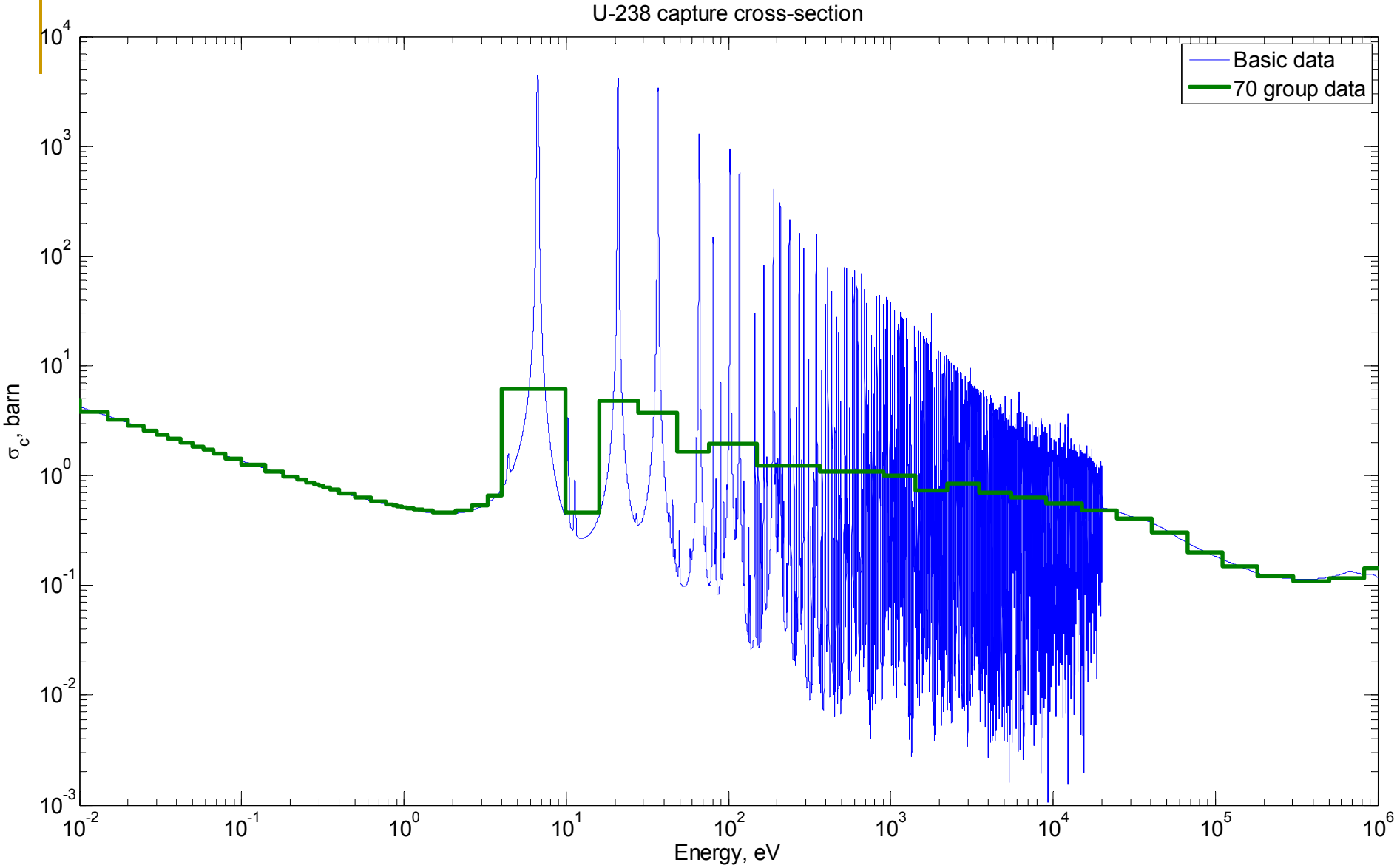
Basic data libraries

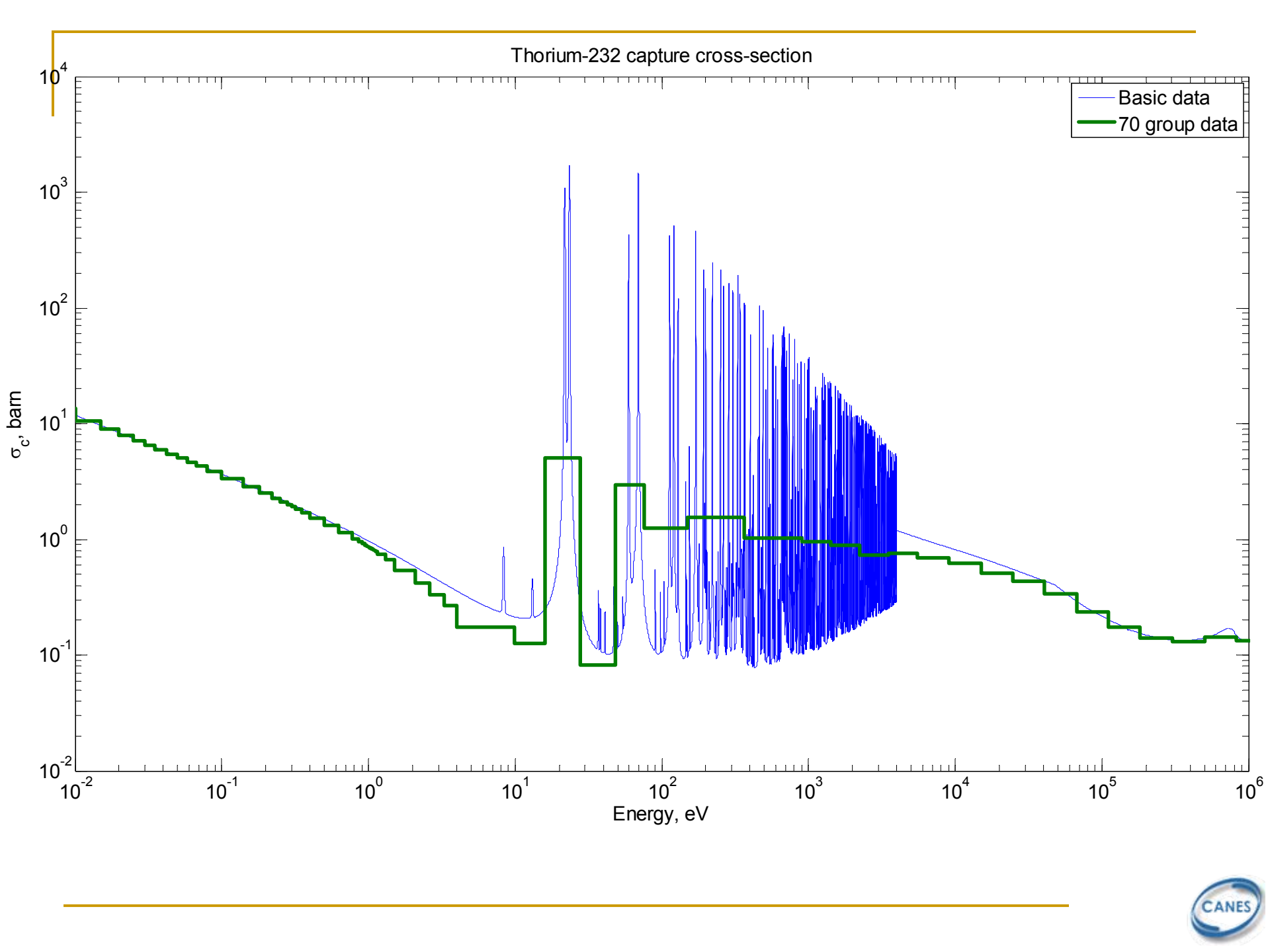
- Core simulation requires nuclear data for all isotopes relevant to nuclear reactor design
  - Actinides, fission products, structural and control materials.
- Basic data includes:
  - Decay data: decay constants, decay modes, branching ratios, etc
  - XS for neutron reactions: **(n, n), (n, n'), (n, 2n), (n, c), (n, f),** etc
- Basic XS data libraries:
  - Contain microscopic XS data,
  - Cover wide neutron energy range (0 – 15 MeV).
  - Include thousands of energy points and interpolation schemes.
  - Resonance XS treated by special mathematical models.
  - Most use ENDF-6 format
  - Examples:
    - Evaluated Nuclear Data Files (ENDF) – Latest: ENDF VII
    - Joint European Data Files (JEFF) – Latest: JEFF-3.1
  - The data is collected from a large amount of experimentally measured points, analyzed, and evaluated with additional theoretical models.
  - The libraries are available in public domain


Basic cross-section data
Th-232
U-238
σ_c, barn
Energy, eV
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}

Multi-group XS library

- Routine reactor calculations:
  - Do not use directly the basic data libraries
  - Based on pre-preprocessed multi-group (MG) libraries of microscopic XS
- MG library
  - Extends over the energy range of **0.001** eV – **10 M**eV
  - The range is divided into **~ 100 energy groups**
  - Each cross section comes with **one value for each group**
- MG XS must:
  - Conserve the **reaction rates**
  - Be tabulated as function of temperature
  - Include special scattering laws for moderators – S(α,β)


U-238 capture cross-section
Basic data
70 group data
σc, barn
Energy, eV
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-2
10^-1
10^0
10^1
10^2
10^3
10^4
10^5
10^6

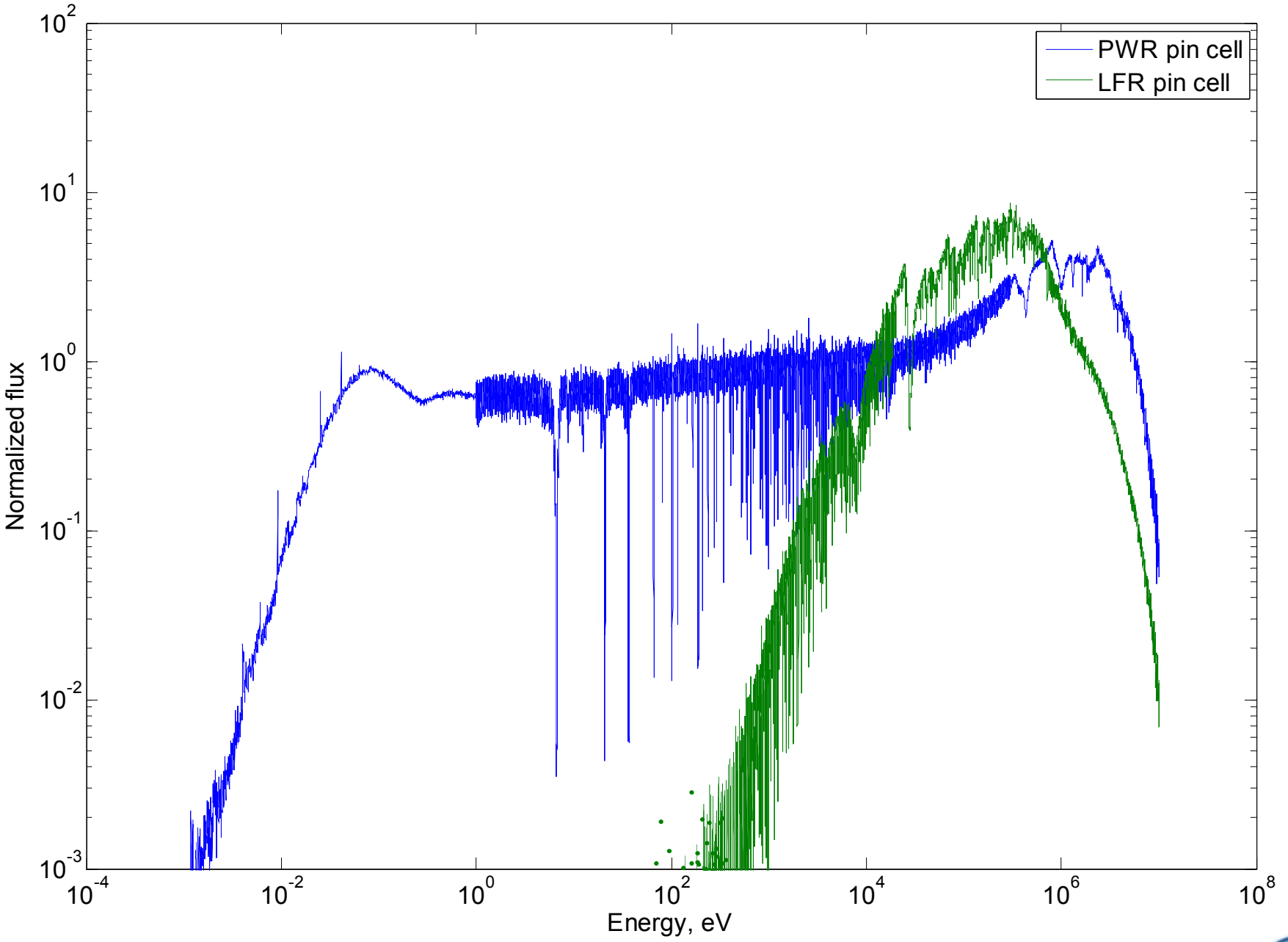

Thorium-232 capture cross-section
Basic data
70 group data
σ_c, barn
Energy, eV
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}

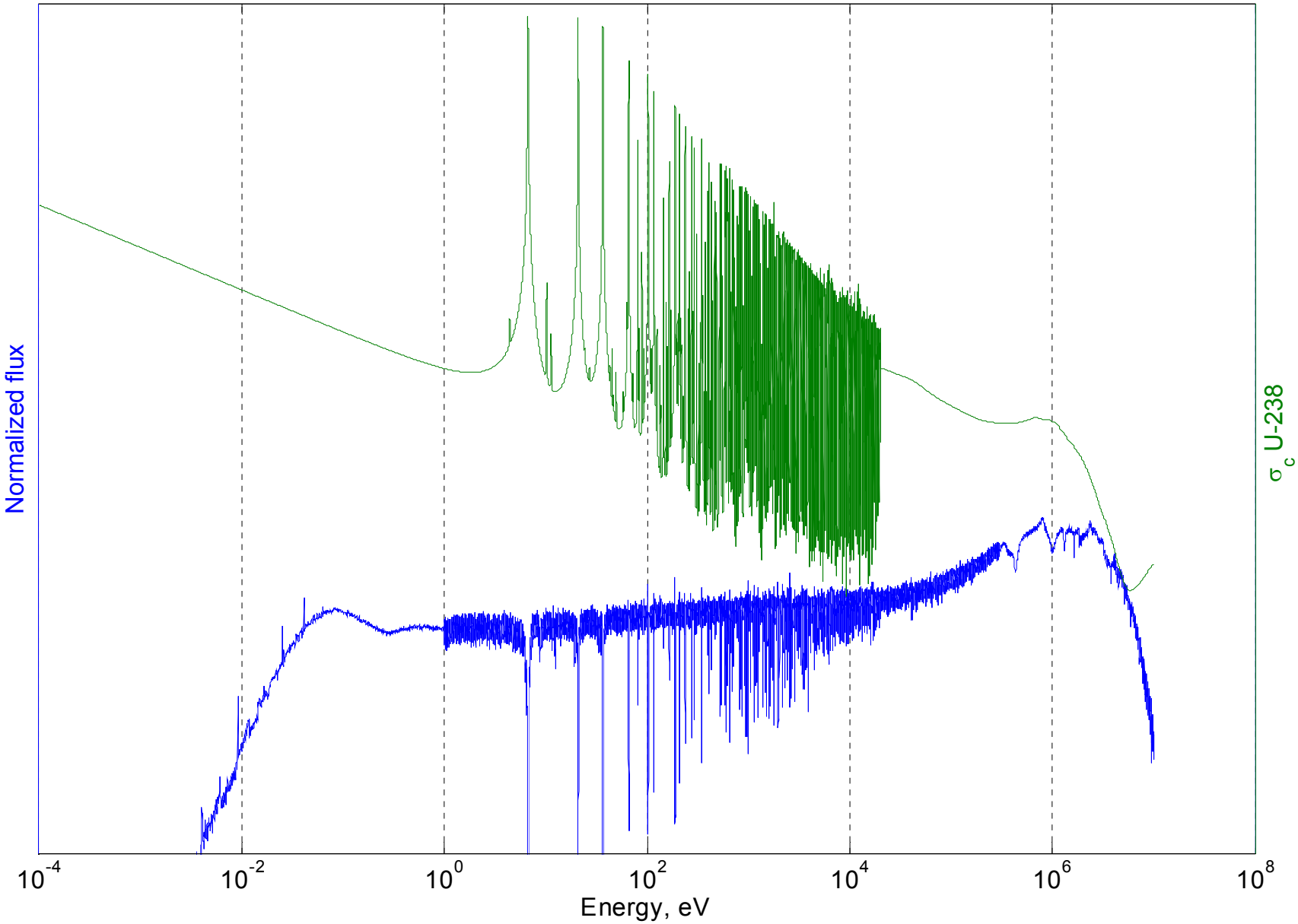
Unit cell calculations

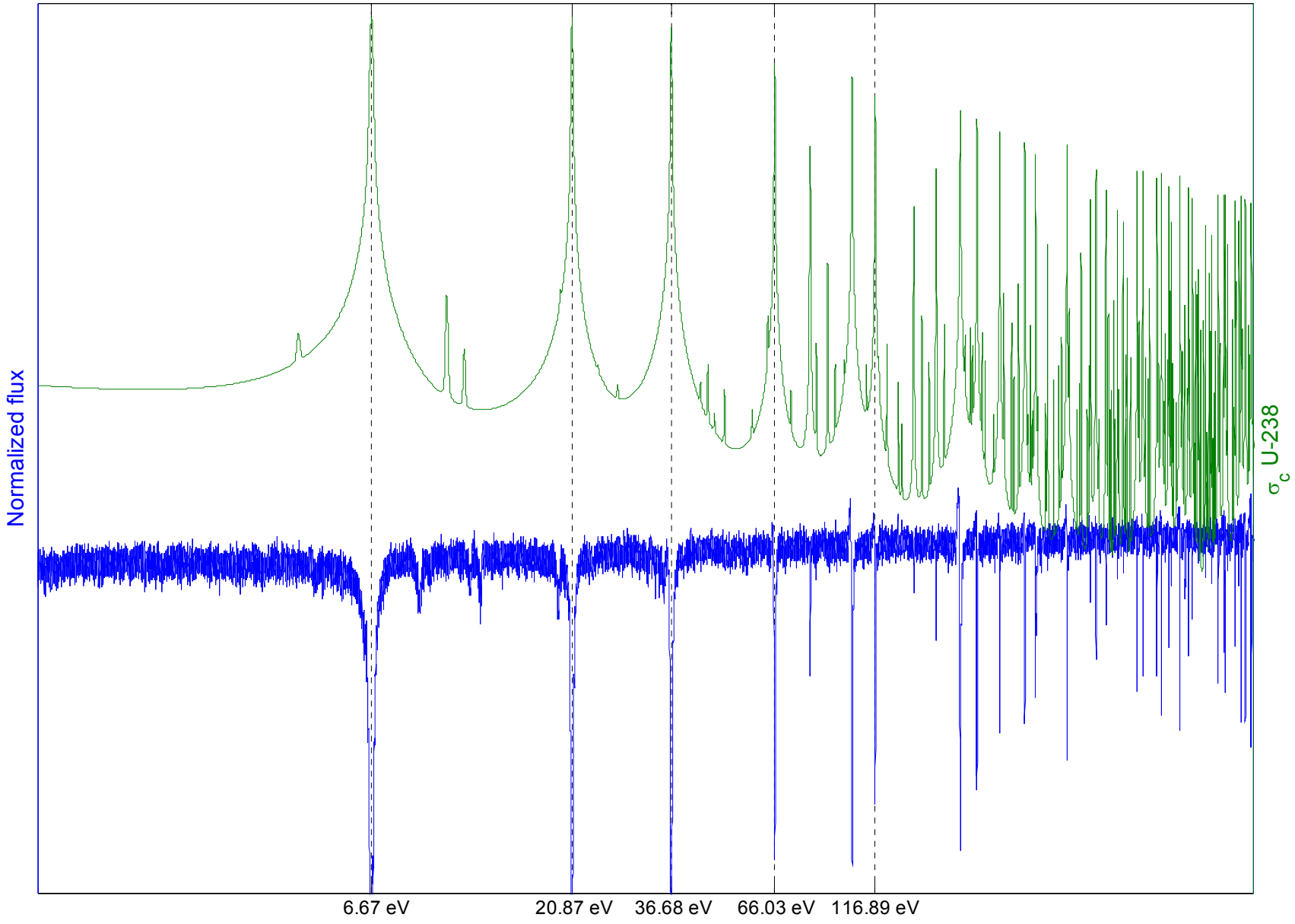
- Unit-cell calculation precede those of the lattice
- Basic assumption:
  - The fuel is arranged in an infinite lattice of identical cells
  - This results in zero currents on the cell boundaries
  - Never the case in reality
    - Example: PWR assembly – 264 fuel rods, 25 guide tubes

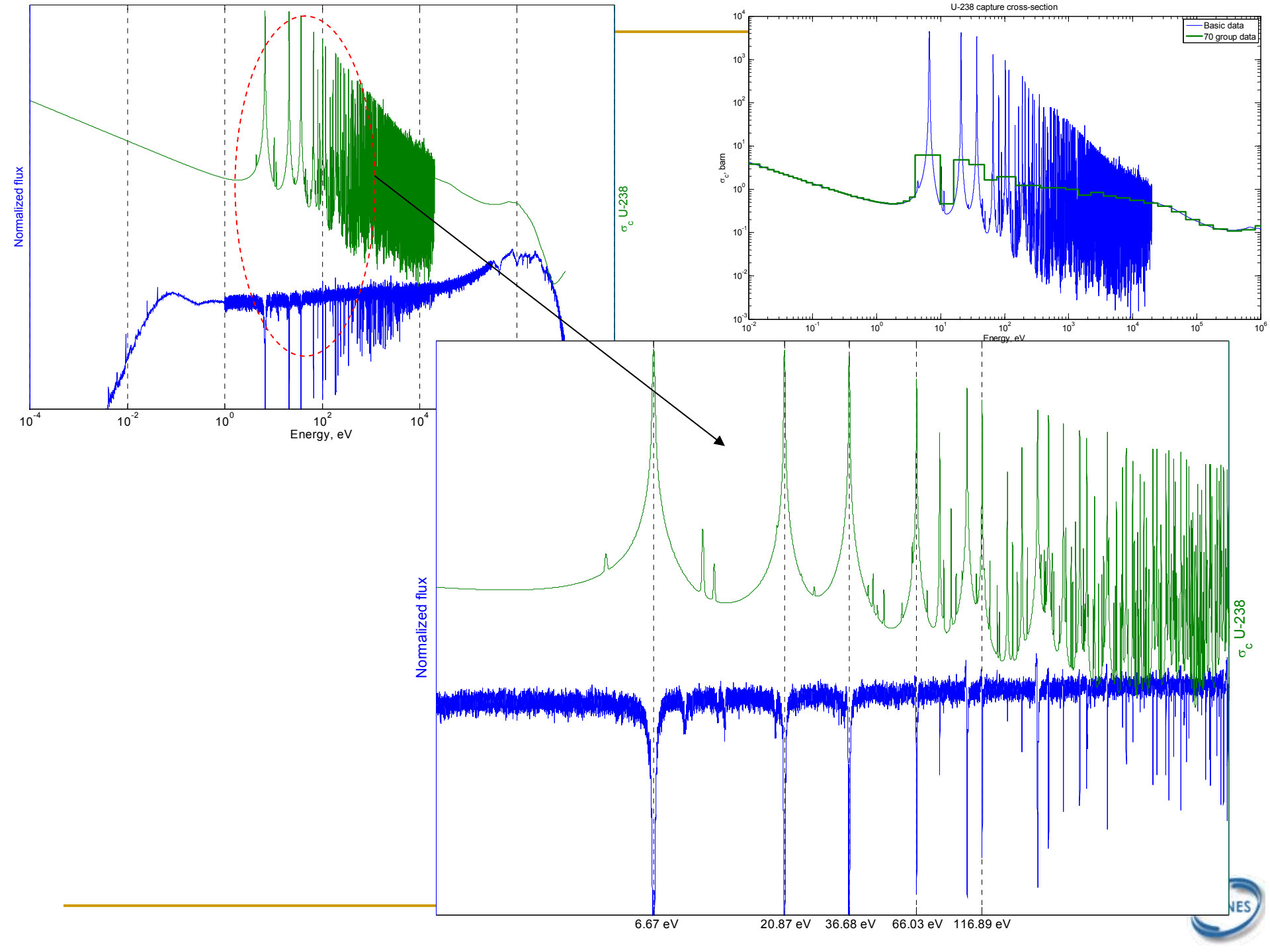
but

  - Unit cell approach will suffice in obtaining the main physics characteristics of an average fuel rod.


PWR pin cell
LFR pin cell
Normalized flux
Energy, eV
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
10^{8}


Normalized flux
σ_c U-238
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
10^{8}
Energy, eV


Normalized flux
σ_c U-238
6.67 eV
20.87 eV
36.68 eV
66.03 eV
116.89 eV


Normalized flux
Energy, eV
σc U-238
U-238 capture cross-section
Basic data
70 group data
σc, barn
Energy, eV
Normalized flux
σc U-238
6.67 eV
20.87 eV
36.68 eV
66.03 eV
116.89 eV

Fuel depletion

- The rate at which the amount of nuclide N changes as function of time is given by a system of linear, homogeneous, first-order differential equations with constant coefficients:

$$
\begin{cases}
\dfrac{dN_1(t)}{dt} = -\lambda_1 N_1(t) - \phi\sigma_1 N_1(t) + \lambda_2 BR_{2\to 1} N_2(t) + \ldots \\
\qquad\qquad \lambda_n BR_{n\to 1} N_n(t) + \phi\left(\sigma_{2\to 1} N_2(t) + \ldots \sigma_{n\to 1} N_n(t)\right) \\
\dfrac{dN_2(t)}{dt} = -\lambda_2 N_2(t) - \phi\sigma_2 N_2(t) + \lambda_1 BR_{1\to 2} N_1(t) + \ldots \\
\qquad\qquad \lambda_n BR_{n\to 1} N_n(t) + \phi\left(\sigma_{2\to 1} N_2(t) + \ldots \sigma_{n\to 1} N_n(t)\right) \\
\vdots \\
\dfrac{dN_n(t)}{dt} = -\lambda_n N_n(t) - \phi\sigma_n N_n(t) + \lambda_1 BR_{1\to n} N_1(t) + \ldots \\
\qquad\qquad \lambda_{n-1} BR_{n-1\to n} N_{n-1}(t) + \phi\left(\sigma_{1\to n} N_1(t) + \ldots \sigma_{n-1\to n} N_{n-1}(t)\right)
\end{cases}
$$

Nomenclature is on the next slide

Fuel depletion

$$\frac{dN_j(t)}{dt} = -\lambda_j N_j(t) - \phi\sigma_j N_1(t) + \sum_{k=1}^{k=n} \lambda_k BR_{k\to j} N_k(t) + \phi\left(\sigma_{k\to j} N_k(t)\right)$$

$N_i(t)$	-	Atoms of nuclide **i** at time **t**,
$\frac{dN_i(t)}{dt}$	-	Rate of amount change of nuclide **i**,
n	-	Number of nuclides,
λ_i	-	Radioactive decay constant of nuclide **i** (sec^{-1})
$BR_{k\to j}$	-	Branching ratio per decay of nuclide **j** to nuclide **i**.
σ_i	-	Single group Absorption cross section of isotope **i**.
$\sigma_{i\to j}$	-	Single group cross section leading from isotope **i** to isotope **j**.
ϕ	-	Flux.

Fuel depletion

Rate of change of nuclide **i**

Disappear due to decay

Disappear due to neutron absorption

$$\frac{dN_j(t)}{dt} = -\lambda_j N_j(t) - \phi\sigma_j N_1(t) +$$

Buildup due to decay of other nuclides

Buildup due to absorption in other nuclides

$$+ \sum_{k=1}^{k=n} \lambda_k BR_{k\to j} N_k(t) + \phi\left(\sigma_{k\to j} N_k(t)\right)$$

Introduction to CASMO-4

- 2D, multi-group, neutron transport code for simulation of BWR/PWR assemblies or pin cells
- Uses metric units
  - densities in g/cm^3, temperatures in Kelvin, dimensions in cm, burnup in MWd/kgIHM
- Automatic thermal expansion of dimensions and densities
- Input file is the problem description and consists of different *cards* (three character identifier). Default values are recommended.
- Comments begin with an asterisk (*)

Computer Running Information

- CASMO-4 is located in UNIX machine:
- Class account is 251 (username: 251, password: xxx)
- Use ssh for remote access, on athena* e.g.,
- After login, create your own directory, e.g., mkdir xxx
- Running command for CASMO-4 is cas4. Suppose your input file is `a.inp`, the running command would be

```
cas4  -J  a.inp
```

  Important note: include option `-J` to use JEF-2.2 library

  Three files will be generated upon successful completion:

  `a.log` (log file), `a.out` (output), `a.cax` (card image)

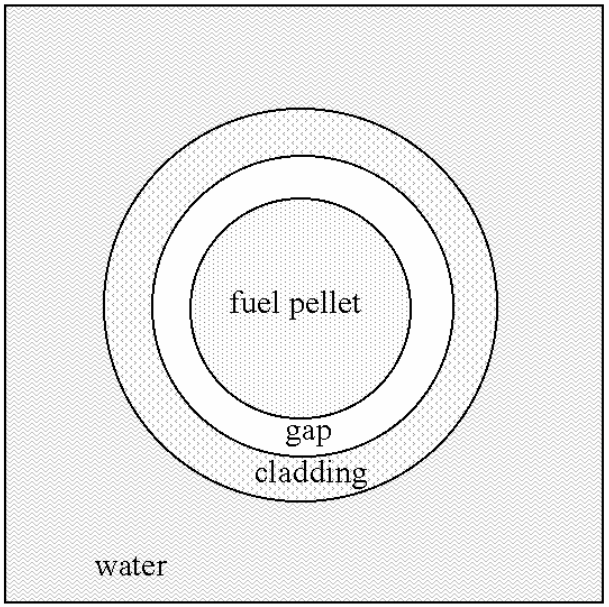
- For a complete reference of how to use `cas4`, type

```
cas4  -h
```

*Athena is MIT's UNIX-based computing environment. OCW does not provide access to it.

Sample PWR unit cell input (2528.inp)

```
TTL * U235/U238, PWR PIN CELL
TFU=900 TMO=583.1
FUE 1 /1.16321E21 92234=0.0 92238=2.18219E22 8000=4.59686E22
PIN 1 0.4096 0.4178 0.4750/'1' 'AIR' 'CAN'
PWR 2 1.26
PDE 104.5 'KWL'
DEP -80
STA
END
```



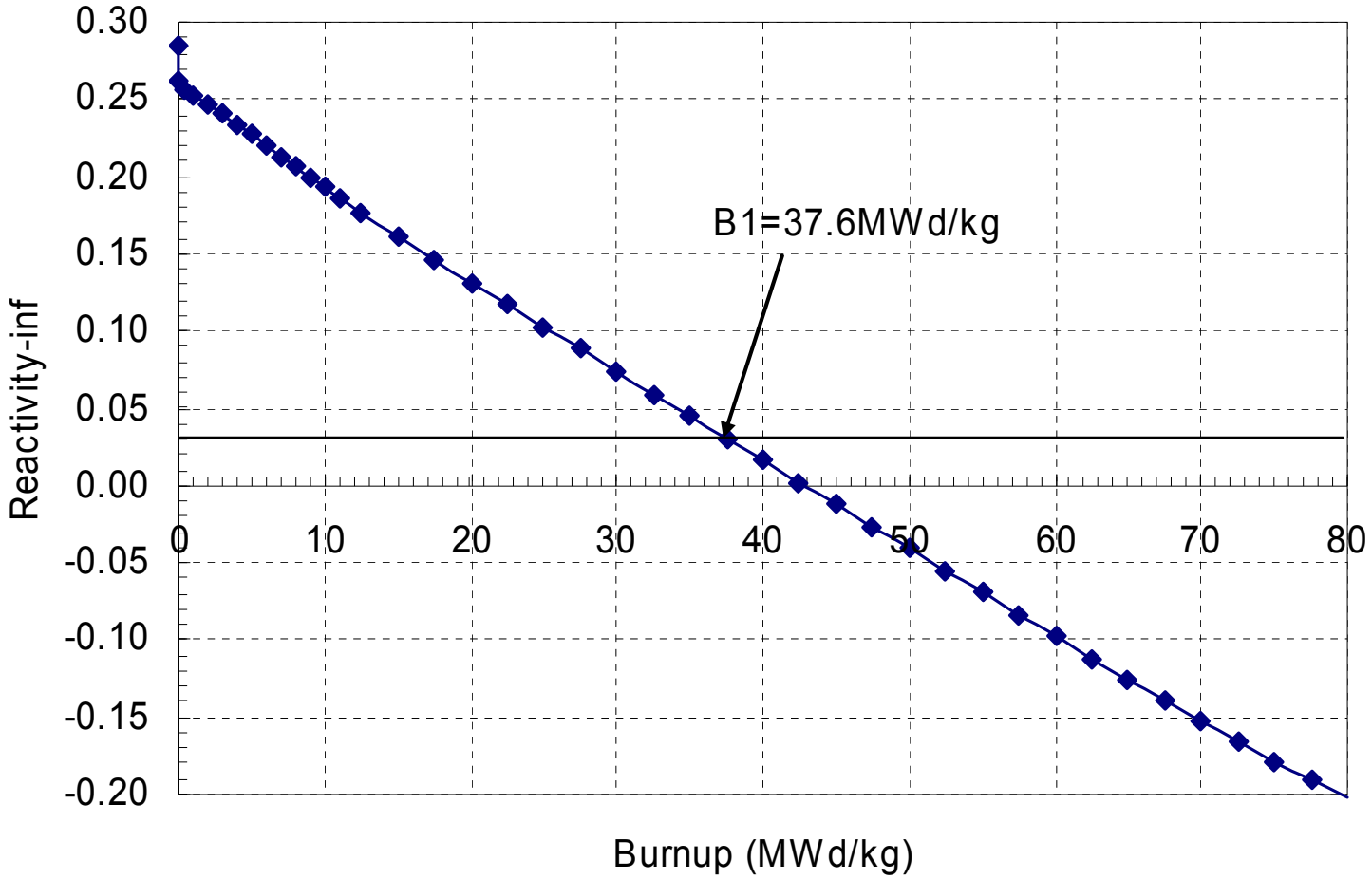
UO2 fuel with 5 w/o U-235 (in total U)

Sample output (only summary is shown)

```
** C A S M O - 4   SUMMARY  **

  U235/U238, PWR PIN CELL

  HVOI=  0.0 HTFU=  900.0 HTMO=  583.1 HTCO=  583.1 HBOR=    0.0

  NO VOID    TFU    TMO    TCO    BOR ROD   BURNUP   K-INF   K-INF     M2     PIN   U-235 FISS PU  TOT PU
                                            MWD/KG             TWO-GROUP    PEAK    WT %    WT %    WT %

   1  0.0  900.0  583.1  583.1    0.0        0.000 1.39812 1.39751  62.33   1.000   5.000   0.000   0.000
   2                                        0.100 1.35589 1.35589  61.83   1.000   4.988   0.002   0.002
   3                                        0.500 1.34620 1.34630  61.71   1.000   4.940   0.019   0.019
   4                                        1.000 1.33867 1.33885  61.62   1.000   4.881   0.043   0.044
   5                                        2.000 1.32742 1.32769  61.49   1.000   4.765   0.089   0.092
   6                                        3.000 1.31627 1.31664  61.37   1.000   4.653   0.132   0.137
   7                                        4.000 1.30493 1.30539  61.24   1.000   4.542   0.173   0.182
   8                                        5.000 1.29355 1.29410  61.13   1.000   4.435   0.211   0.224
   9                                        6.000 1.28228 1.28291  61.01   1.000   4.330   0.248   0.266
  10                                        7.000 1.27122 1.27192  60.91   1.000   4.227   0.283   0.305
  11                                        8.000 1.26041 1.26118  60.80   1.000   4.126   0.316   0.344
  12                                        9.000 1.24990 1.25072  60.69   1.000   4.027   0.348   0.382
  13                                       10.000 1.23969 1.24054  60.60   1.000   3.931   0.378   0.418
  14                                       11.000 1.22976 1.23065  60.51   1.000   3.836   0.407   0.453
  15                                       12.500 1.21544 1.21638  60.38   1.000   3.697   0.448   0.504
  16                                       15.000 1.19293 1.19389  60.19   1.000   3.475   0.512   0.585
  17                                       17.500 1.17161 1.17258  60.01   1.000   3.264   0.569   0.660
  18                                       20.000 1.15145 1.15240  59.85   1.000   3.062   0.621   0.731
  19                                       22.500 1.13242 1.13331  59.71   1.000   2.870   0.667   0.797
  20                                       25.000 1.11418 1.11501  59.58   1.000   2.687   0.709   0.858
  21                                       27.500 1.09662 1.09737  59.46   1.000   2.513   0.746   0.916
  22                                       30.000 1.07965 1.08031  59.34   1.000   2.346   0.780   0.971
  23                                       32.500 1.06322 1.06377  59.23   1.000   2.188   0.810   1.022
  24                                       35.000 1.04737 1.04780  59.13   1.000   2.038   0.836   1.069
  25                                       37.500 1.03182 1.03212  59.02   1.000   1.895   0.860   1.114
  26                                       40.000 1.01674 1.01691  58.93   1.000   1.760   0.880   1.157
  27                                       42.500 1.00211 1.00213  58.85   1.000   1.632   0.898   1.196
  28                                       45.000 0.98789 0.98776  58.77   1.000   1.510   0.914   1.233
  29                                       47.500 0.97399 0.97370  58.69   1.000   1.396   0.927   1.269
  30                                       50.000 0.96045 0.95999  58.61   1.000   1.288   0.938   1.302
  31                                       52.500 0.94732 0.94670  58.54   1.000   1.186   0.948   1.333
```

Reactivity versus burnup

reference case 5 w/o U235 in U235 + U238



22.251 Systems Analysis of the Nuclear Fuel Cycle

Fall 2009