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Processing and Utilization of Nuclear Reaction Data for Advanced Gas Cooled Reactor (AGCR) Applications

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Processing and Utilization of Nuclear Reaction Data for Advanced Gas Cooled Reactor (AGCR) Applications

Lecture 2 - Exercises on multi-group cross-section generation

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OUTLINE

- Introduction
  - Overview of the NJOY code
- Example
  - Fuel specification
  - Model
    - Coated Particle
    - Pebble (1D and 3D)
    - Prismatic assembly
- Execution command

Overview of the NJOY Code

- ✓ The NJOY code is a nuclear data processing system which produces pointwise and group wise cross sections from the Evaluated Nuclear Data File (ENDF).

- ✓ The code converts the evaluated nuclear data into libraries useful for application calculations in nuclear engineering problems.

- ✓ The data is converted from the ENDF format to the Pointwise Evaluated Nuclear Data File (PENDF) format and Groupwise Evaluated Nuclear Data File (GENDF) format.

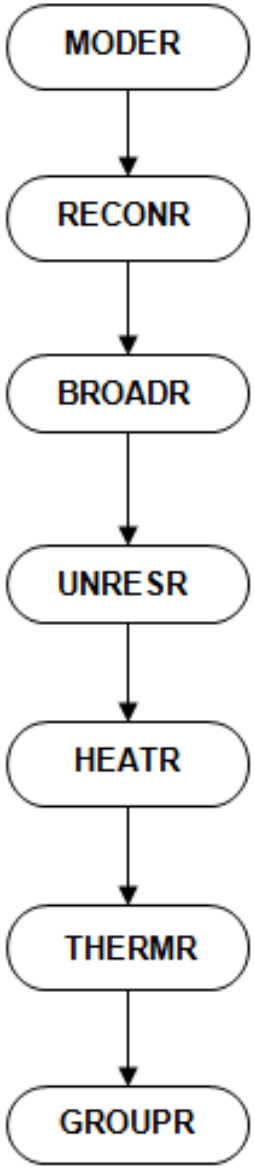
Overview of the NJOY Code

- ✓ The ENDF data is freely obtainable from various source such as national laboratories and data banks. In this work, the ENDF data was downloaded from the Los Alamos National Laboratory website.

- ✓ The NJOY code consists of a number of modules. Each module operates as a separate computer program, processing a well-defined task.

- ✓ This feature makes it possible to choose only the modules that are relevant to a specific problem. The modules are linked by input and output files.

NJOY methodology for multi-group xs



RECONR

- ✓ **The RECONR module reconstructs resonance cross sections from ENDF resonance parameters.**
- ✓ **It also reconstructs the cross sections from nonlinear interpolation schemes.**
- ✓ **It reads the ENDF-format tape and produces a common energy grid for all neutron reactions such that all cross sections can be obtained (within a specified tolerance) by interpolation.**
- ✓ **The output is written onto a PENDF tape.**

RECONR

```
*---INPUT SPECIFICATIONS (FREE FORMAT)-----------------------------*
*                                                                  *
* CARD 1                                                          *
*    NENDF     UNIT FOR ENDF/B TAPE                               *
*    NPEND     UNIT FOR PENDF TAPE                                *
* CARD 2                                                          *
*    LABEL     66 CHARACTER LABEL FOR NEW PENDF TAPE              *
*              DELIMITED WITH *, ENDED WITH /.                    *
* CARD 3                                                          *
*    MAT       MATERIAL TO BE RECONSTRUCTED                       *
*    NCARDS    NUMBER OF CARDS OF DESCRIPTIVE DATA FOR NEW MF1    *
*              (DEFAULT=0.)                                       *
*    NGRID     NUMBER OF USER ENERGY GRID POINTS TO BE ADDED.     *
*              (DEFAULT=0.)                                       *
* CARD 4                                                          *
*    ERR       FRACTIONAL RECONSTRUCTION TOLERANCE USED WHEN      *
*              RESONANCE-INTEGRAL ERROR CRITERION (SEE ERRINT)    *
*              IS NOT SATISFIED.                                  *
*    TEMPR     RECONSTRUCTION TEMPERATURE (DEG KELVIN)            *
*              (DEFAULT=0.)                                       *
*    NDIGIT    NO. SIGNIFICANT DIGITS (DEFAULT=7)                 *
*    ERRMAX    FRACTIONAL RECONSTRUCTION TOLERANCE USED WHEN      *
*              RESONANCE-INTEGRAL ERROR CRITERION IS SATISFIED    *
*              (ERRMAX.GE.ERR, DEFAULT=20.*ERR)                   *
*    ERRINT    MAXIMUM RESONANCE-INTEGRAL ERROR (IN BARNS)        *
*              PER GRID POINT (DEFAULT=ERR/10000)                 *
*              (NOTE: THE MAX CROSS SECTION DIFFERENCE FOR        *
*               LINEARIZATION, ERRLIM, AND FOR RECONSTRUCTION,    *
*               ERRMIN, ARE ALSO TIED TO ERRINT.  TO GET MAXIMUM  *
*               ACCURACY, SET ERRINT TO A VERY SMALL NUMBER.      *
*               FOR ECONOMICAL PRODUCTION, USE THE DEFAULTS.)     *
* CARD 5                                                          *
*    CARDS     NCARDS OF DESCRIPTIVE COMMENTS FOR MT451           *
*              EACH CARD DELIMITED WITH *, ENDED WITH /.          *
* CARD 6                                                          *
*    ENODE     USERS ENERGY GRID POINTS                           *
*       CARDS 3, 4, 5, 6 MUST BE INPUT FOR EACH MATERIAL DESIRED  *
*       MAT=0/ TERMINATES EXECUTION OF RECONR.                    *
*                                                                  *
********************************************************************
```

RECONR

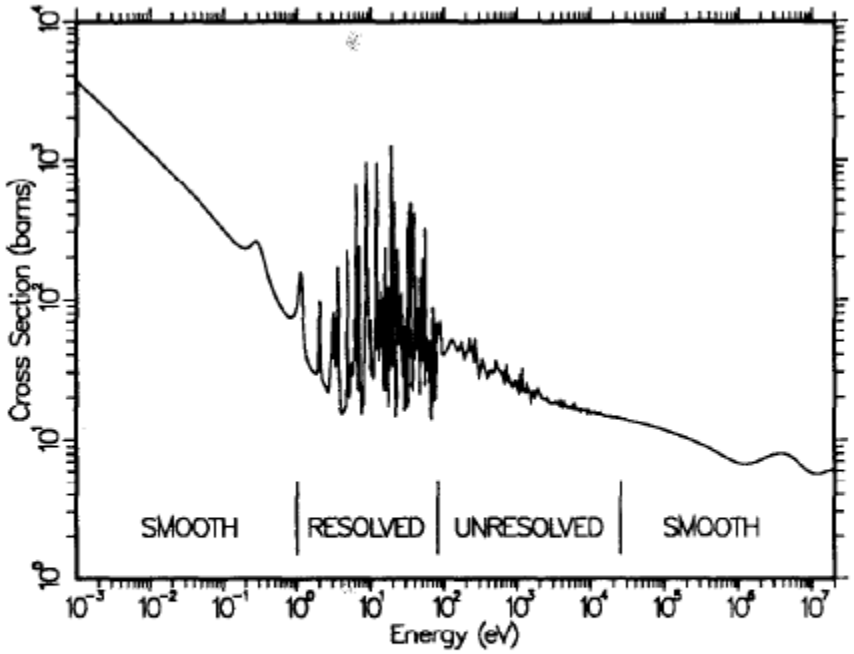


Figure 1: A typical cross section reconstructed from an ENDF/B evaluation using RECONR. The smooth, resolved, and unresolved energy regions use different representations of the cross sections. This is the total cross section for ^{235}U from ENDF/B-V.

BROADR

- ✓ **The BROADR module reads the PENDF tape from RECONR, and Doppler-broadens the thin pointwise resonance cross sections.**
- ✓ **This module uses the kernel broadening method, also known as the SIGMA1 method, but modified for better behavior at high temperatures and low energies.**
- ✓ **The output is written onto a new PENDF tape.**

BROADR

```
*---INPUT SPECIFICATIONS (FREE FORMAT)--------------------------*
*                                                               *
* CARD 1                                                        *
*    NIN       INPUT PENDF TAPE                                 *
*    NOUT      OUTPUT PENDF TAPE                                *
* CARD 2                                                        *
*    MAT1      MATERIAL TO BE PROCESSED                         *
*    NTEMP2    NUMBER OF FINAL TEMPERATURES (MAXIMUM=10)        *
*    ISTART    RESTART (0 NO, 1 YES, DEFAULT 0)                 *
*    ISTRAP    BOOTSTRAP (0 NO, 1 YES, DEFAULT 0)               *
*    TEMP1     STARTING TEMPERATURE FROM NIN (DEFAULT=0.K)       *
* CARD 3                                                        *
*    ERRTHN    FRACTIONAL TOLERANCE FOR THINNING                *
*    THNMAX    MAX. ENERGY FOR BROADENING AND THINNING          *
*              (DEFAULT=1 MEV)                                  *
*    ERRMAX    FRACTIONAL TOLERANCE USED WHEN INTEGRAL CRITERION *
*              IS SATISFIED (SAME USAGE AS IN RECONR)           *
*              (ERRMAX.GE.ERRTHN, DEFAULT=20*ERRTHN)            *
*    ERRINT    PARAMETER TO CONTROL INTEGRAL THINNING           *
*              (USAGE AS IN RECONR) (DEFAULT=ERRTHN/10000)      *
*              SET VERY SMALL TO TURN OFF INTEGRAL THINNING.    *
*      (A GOOD CHOICE FOR THE CONVERGENCE PARAMETERS           *
*       ERRTHN, ERRMAX, AND ERRINT IS THE SAME SET OF          *
*       VALUES USED IN RECONR)                                 *
* CARD 4                                                        *
*    TEMP2     FINAL TEMPERATURES (DEG KELVIN)                  *
* CARD 5                                                        *
*    MAT1      NEXT MAT NUMBER TO BE PROCESSED WITH THESE       *
*              PARAMETERS.  TERMINATE WITH MAT1=0.              *
*                                                               *
```

UNRESR

- ✓ The UNRESR module computes the effective self-shielded pointwise cross sections for resonance reactions in the unresolved resonance region.
- ✓ The unresolved range begins at the energy where it is difficult to measure individual resonances. It extends to the energy where the effects of fluctuations in the resonance cross sections become unimportant.
- ✓ The UNRESR module averages the values of resonance widths and spacings together with distribution functions for the widths and spacings.
- ✓ This representation is converted into effective cross sections. The module uses the ENDF tape and the PENDF tape from BROADR as input. The computed effective cross sections are written onto a new PENDF tape.

UNRESR

```
*---INPUT SPECIFICATIONS (FREE FORMAT)-------------------------*
*                                                             *
* CARD 1                                                      *
*   NENDF    UNIT FOR ENDF/B TAPE                             *
*   NIN      UNIT FOR INPUT PENDF TAPE                        *
*   NOUT     UNIT FOR OUTPUT PENDF TAPE                       *
* CARD 2                                                      *
*   MATD     MATERIAL TO BE PROCESSED                         *
*   NTEMP    NO. OF TEMPERATURES (MAX. NO. ALLOWED=9)         *
*   NSIGZ    NO. OF SIGMA ZEROES (MAX. NO. ALLOWED=8)         *
*   IPRINT   PRINT OPTION (0=MIN, 1=MAX) (DEFAULT=0)          *
* CARD 3                                                      *
*   TEMP     TEMPERATURES IN KELVIN (INCLUDING ZERO)          *
* CARD 4                                                      *
*   SIGZ     SIGMA ZERO VALUES (INCLUDING INFINITY)           *
*        CARDS 2, 3, 4 MUST BE INPUT FOR EACH MATERIAL DESIRED *
*        MATD=0/ TERMINATES EXECUTION OF UNRESR.              *
*                                                             *
***************************************************************
```

HEATR

- ✓ The HEATR module generates pointwise heat production cross sections for specified reactions.
- ✓ Neutron heating arises from the kinetic energy of the charged products of a neutron-induced reaction. It is proportional to the local neutron flux.
- ✓ The module uses the ENDF tape and the PENDF tape from UNRESR as input. The output is written onto a new PENDF tape.

HEATR

```
*---INPUT SPECIFICATIONS (FREE FORMAT)-----------------------------*
*                                                                  *
* CARD 1                                                           *
*    NENDF     UNIT FOR ENDF/B TAPE                                *
*    NIN       UNIT FOR INPUT PENDF TAPE                           *
*    NOUT      UNIT FOR OUTPUT PENDF TAPE                          *
* CARD 2                                                           *
*    MATD      MATERIAL TO BE PROCESSED                            *
*    NPK       NUMBER OF PARTIAL KERMAS DESIRED (DEFAULT=0)        *
*    NQA       NUMBER OF USER Q VALUES (DEFAULT=0)                 *
*    NTEMP     NUMBER OF TEMPERATURES TO PROCESS                   *
*              (DEFAULT=0, MEANING ALL ON PENDF)                   *
*    LOCAL     0/1=GAMMA RAYS TRANSPORTED/DEPOSITED LOCALLY        *
*              (DEFAULT=0)                                         *
*    IPRINT    PRINT (0 MIN, 1 MAX, 2 CHECK) (DEFAULT=0)           *
```

THERMR

- ✓ **The THERMR module generates pointwise neutron scattering cross sections in the thermal energy range.**
- ✓ **It produces inelastic cross sections and energy-to-energy matrices for free atoms or bound scatterers.**
- ✓ **THERMR module uses the ENDF tape and the PENDF tape from UNRESR as input. The output is written onto a new PENDF tape.**

THERMR

```
*---INPUT SPECIFICATIONS (FREE FORMAT)-------------------------*
*                                                              *
*  CARD 1                                                      *
*     NENDF       ENDF/B TAPE FOR MF7 DATA                     *
*     NIN         OLD PENDF TAPE                               *
*     NOUT        NEW PENDF TAPE                               *
*  CARD 2                                                      *
*     MATDE       MATERIAL DESIRED ON ENDF TAPE                *
*     MATDP       MATERIAL DESIRED ON PENDF TAPE               *
*     NBIN        NUMBER OF EQUI-PROBABLE ANGLES               *
*     NTEMP       NUMBER OF TEMPERATURES                       *
*     IINC        INELASTIC OPTIONS                            *
*                    0      NONE                               *
*                    1      COMPUTE AS FREE GAS                *
*                    2      RESERVED                           *
*                    3      RESERVED                           *
*                    4      READ S(A,B) AND COMPUTE MATRIX     *
*     ICOH        ELASTIC OPTIONS                              *
*                    0      NONE                               *
*                    1      GRAPHITE                           *
*                    2      BERYLLIUM                          *
*                    3      BERYLLIUM OXIDE                    *
*                   11      POLYETHYLENE                       *
*                   12      H(ZRH)                             *
*                   13      ZR(ZRH)                            *
*     NATOM       NUMBER OF PRINCIPAL ATOMS                    *
*     MTREF       MT FOR INELASTIC REACTION (201-250 ONLY)     *
*     IPRINT      PRINT OPTION (0=MINIMUM, 1=MAXIMUM,          *
*                 2=MAX. NORMAL + INTERMEDIATE RESULTS)        *
*                 (DEFAULT=0)                                  *
*  CARD 3                                                      *
*     TEMPR       TEMPERATURES (KELVIN)                        *
*  CARD 4                                                      *
*     TOL         TOLERANCE                                    *
*     EMAX        MAXIMUM ENERGY FOR THERMAL TREATMENT         *
*                 (FOR TEMPERATURES GREATER THAN 3000,         *
*                 EMAX AND THE ENERGY GRID ARE SCALED BY       *
*                 TEMP/300.  FREE GAS ONLY.)                   *
*                                                              *
****************************************************************
```

GROUPR

- ✓ **The GROUPR module generates self-shielded multi-group cross sections and group-to-group neutron scattering matrices.**

- ✓ **This module uses the ENDF tape and the PENDF tape from THERMR as input. The output is written onto a GENDF tape.**

GROUPR

```
*---INPUT SPECIFICATIONS (FREE FORMAT)-------------------------*
*                                                              *
* CARD1                                                        *
*    NENDF   UNIT FOR ENDF/B TAPE                              *
*    NPEND   UNIT FOR PENDF TAPE                               *
*    NGOUT1  UNIT FOR INPUT GOUT TAPE (DEFAULT=0)              *
*    NGOUT2  UNIT FOR OUTPUT GOUT TAPE (DEFAULT=0)             *
* CARD2                                                        *
*    MATB    MATERIAL TO BE PROCESSED                          *
*            MATB LT 0 IS A FLAG TO ADD MTS TO AND/OR REPLACE  *
*            INDIVIDUAL MTS ON NGOUT1.                         *
*    IGN     NEUTRON GROUP STRUCTURE OPTION                    *
*    IGG     GAMMA GROUP STRUCTURE OPTION                      *
*    IWT     WEIGHT FUNCTION OPTION                            *
*    LORD    LEGENDRE ORDER                                    *
*    NTEMP   NUMBER OF TEMPERATURES                            *
*    NSIGZ   NUMBER OF SIGMA ZEROES                            *
*    IPRINT  LONG PRINT OPTION (0/1=MINIMUM/MAXIMUM)           *
*            (DEFAULT=1)                                       *
* CARD3                                                        *
*    TITLE   RUN LABEL (UP TO 80 CHARACTERS DELIMITED BY *,    *
*            ENDED WITH /)  (DEFAULT=BLANK)                    *
* CARD4                                                        *
*    TEMP    TEMPERATURES IN KELVIN                            *
* CARD5                                                        *
*    SIGZ    SIGMA ZERO VALUES (INCLUDING INFINITY)            *
*                                                              *
*          IF IGN=1, READ NEUTRON GROUP STRUCTURE (6A AND 6B)  *
* CARD6A                                                       *
*    NGN     NUMBER OF GROUPS                                  *
```

MODER

- ✓ The MODER module converts the data from formatted mode (e.g. ASCII) to blocked-binary mode, and vice versa (from blocked-binary to formatted mode).

- ✓ A formatted file has a positive unit number, while a binary file has a negative unit number.

- ✓ MODER was used in this study, however it is not a requirement. Users may prefer to work with binary data since the execution time is faster and the size of files are relatively smaller.

MODER

```
*---INPUT SPECIFICATIONS (FREE FORMAT)--------------------------*
*                                                               *
* CARD 1       UNIT NUMBERS                                     *
*      NIN     INPUT UNIT                                       *
*      NOUT    OUTPUT UNIT                                      *
*                                                               *
*  A POSITIVE UNIT IS CODED (MODE 3).                           *
*  A NEGATIVE UNIT IS BLOCKED BINARY (NJOY MODE).               *
*                                                               *
*  NOTE: ABS(NIN) GE 1 AND LE 19 IS A FLAG TO SELECT VARIOUS    *
*        MATERIALS FROM ONE OR MORE INPUT TAPES, WITH OR        *
*        WITHOUT MODE CONVERSION.  THE KIND OF DATA TO BE       *
*        PROCESSED IS KEYED TO NIN AS FOLLOWS:                  *
*             NIN=1, FOR ENDF OR PENDF INPUT AND OUTPUT,        *
*                 2, FOR GENDF INPUT AND OUTPUT,                *
*                 3, FOR ERRORR-FORMAT INPUT AND OUTPUT.        *
*                                                               *
*      CARDS 2 AND 3 FOR ABS (NIN) GE 1 AND LE 19 ONLY.         *
*                                                               *
* CARD 2                                                        *
*      TPID    TAPEID FOR NOUT.  66 CHARACTERS ALLOWED          *
*              (DELIMITED WITH *, ENDED WITH /)                 *
* CARD 3                                                        *
*      NIN     INPUT UNIT                                       *
*              TERMINATE MODER BY SETTING NIN=0                 *
*      MATD    MATERIAL ON THIS TAPE TO ADD TO NOUT             *
*****************************************************************
```

Fuel Specifications

Table 1: Coated particle specification

Item	Units	Value
UO_2 fuel density	g/cm^3	10.4
Uranium enrichment (by mass $^{235}U/(^{235}U+^{238}U)$	%	8.2
Fuel natural boron impurity by mass	ppm	1
Outer coated particle radius	mm	0.455
Fuel kernel radius	mm	0.25
Coated material	-	C/C/SiC/C
Coated thickness	mm	0.09/0.04/0.035/0.04
Coated densities	g/cm^3	1.05/1.9/3.18/1.9

Fuel specifications

Table 2: Material specification

Material	Nuclide	Atoms per barn cm
UO_2 fuel	U-238	2.12877e-02
	U-235	1.92585e-03
	O	4.64272e-02
	B-10	1.14694e-07
	B-11	4.64570e-07
Inner low density carbon kernel coating	C (natural)	5.26449e-02
Pyro carbon kernel coating (inner and outer)	C (natural)	9.52621e-02
Silicon carbide kernel coating	C (natural)	4.77240e-02
	S (natural)	4.77240e-02
Pebble/Compact carbon matrix	C (natural)	8.77414e-02
	B-10	9.64977e-09
	B-11	3.90864e-08
Pebble outer coating/Prismatic block (note: fuel grain has the same packing)	C (natural)	8.77414e-02
	B-10	9.64977e-09
	B-11	3.90864e-08
Helium Coolant	He-3	3.71220e-11
	He-4	2.65156e-05

Fuel Specifications

Table 3: Fuel Grain Lattice Data

Item	Units	Value
Unit cell grain square array pitch (cubical outer boundary)	cm	0.16341
Unit cell grain outer radius (spherical outer boundary	cm	0.10137
Grain outer radius	cm	0.0455
Packing fraction of coated particles	%	9.043
Graphite matrix density	g/cm^3	1.75
Graphite matrix natural boron impurity by mass	ppm	0.5
UO_2 fuel mass	g	6.806e-04

Fuel Specifications

Table 4: Pebble Bed Fuel Lattice Data

Item	Units	Value
Unit cell pebble square array pitch (cubical outer boundary)	cm	6.0
Unit cell coolant outer radius (spherical outer boundary	cm	3.53735
Pebble radius	cm	3.0
Radius of fuel zone	cm	2.5
Pebble outer coating thickness	cm	0.5
Pebble outer carbon natural boron impurity by mass	ppm	0.5
Number of coated particles	-	15,000
Packing fraction of coated particles	%	9.043
Graphite matrix density	g/cm^3	1.75
Graphite matrix natural boron impurity by mass	ppm	0.5
Pebble outer carbon coating density	g/cm^3	1.75
UO_2 fuel mass per pebble	g	10.210

Fuel Specifications

Table 5: Prismatic fuel lattice data

Item	Units	Value
Triangular pitch (coolant channel-rod channel and rod channel-rod channel	cm	1.880
Fuel channel diameter	cm	1.270
Coolant channel diameter	cm	1.588
Fuel compact (centered in fuel channel) diameter	cm	1.245
Compact height	cm	4.93
Number of coated particles per compact	-	3,000
Packing fraction of coated particles	%	19.723
Graphite matrix density	g/cm^3	1.75
Graphite matrix natural boron impurity by mass	ppm	0.5
UO_2 fuel mass per pebble	g	2.042

Models

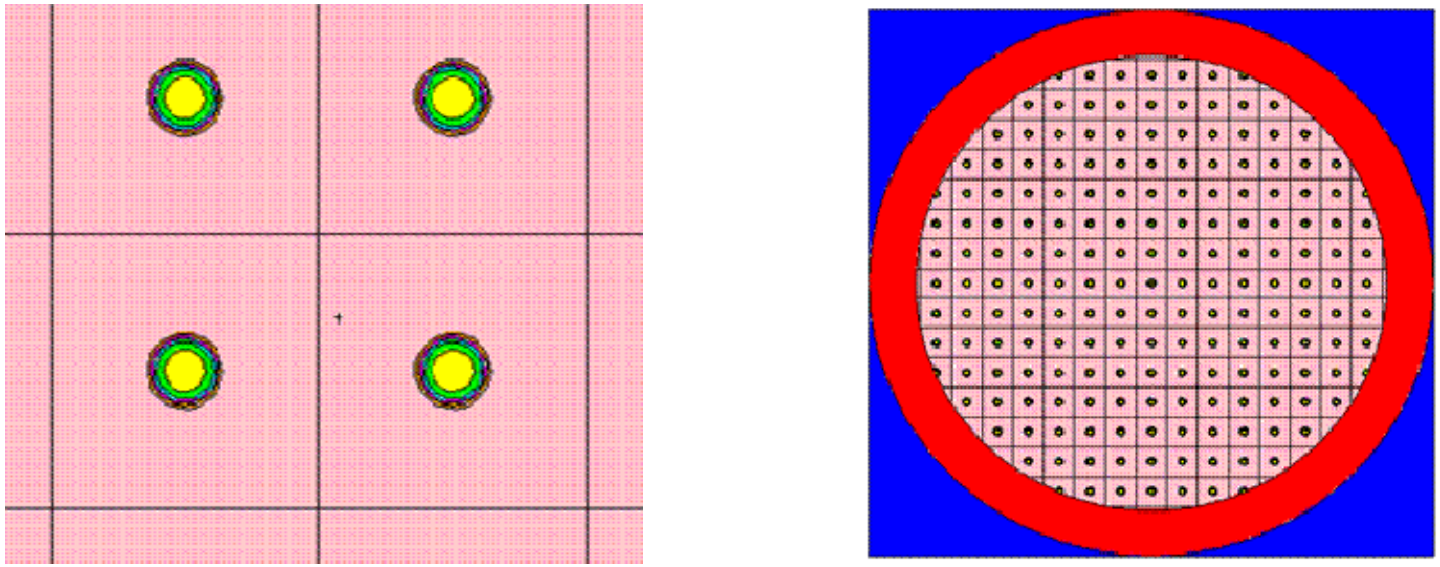


Figure 1 Pebble 3D

Models

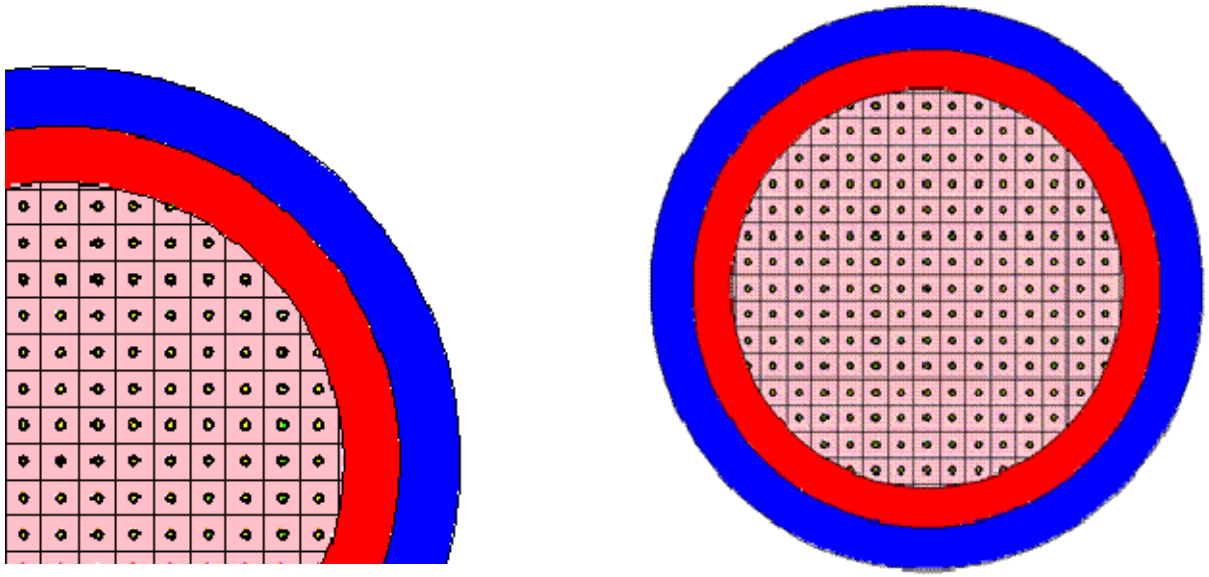


Figure 2: Pebble 1D

Models

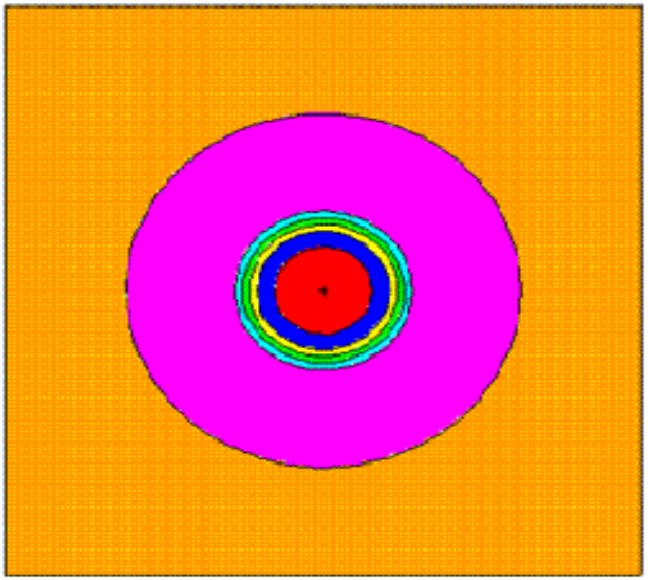


Figure 3: Fuel grain

Models

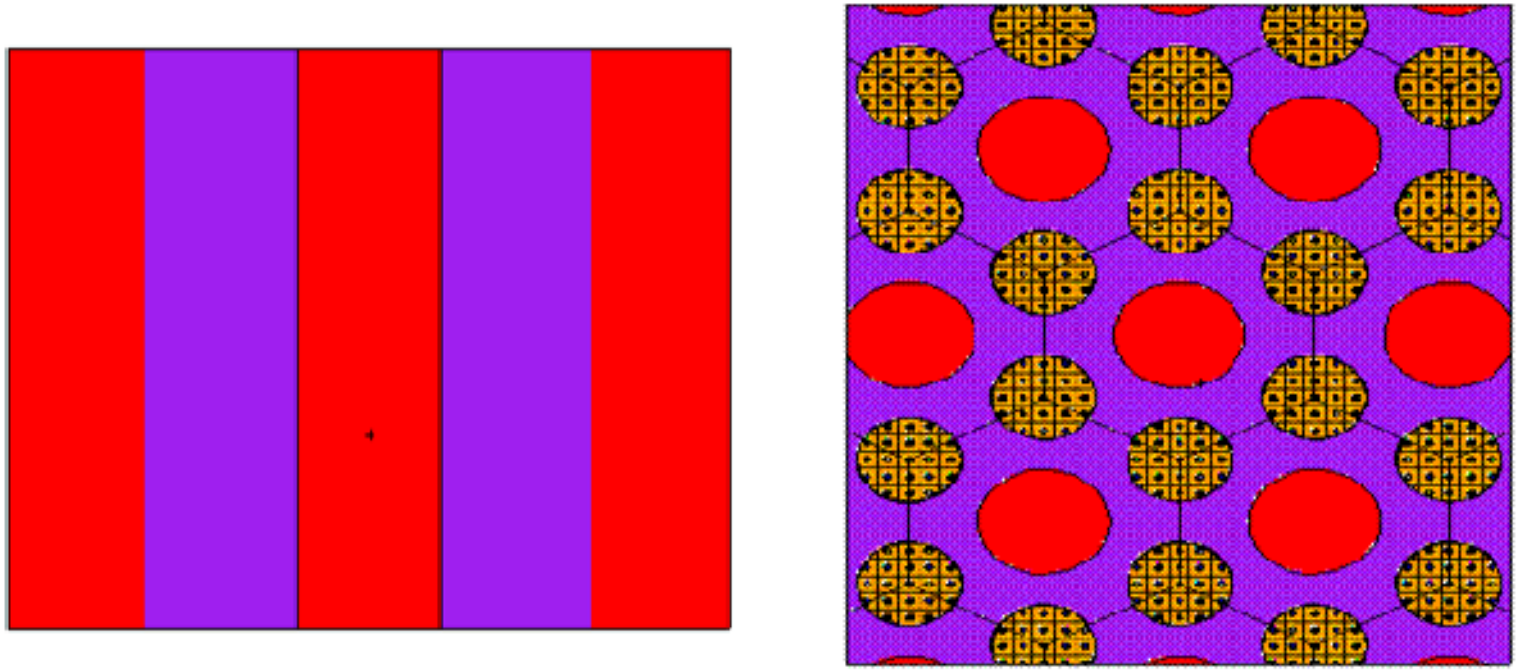


Figure 4: Prismatic assembly

Monte Carlo Results

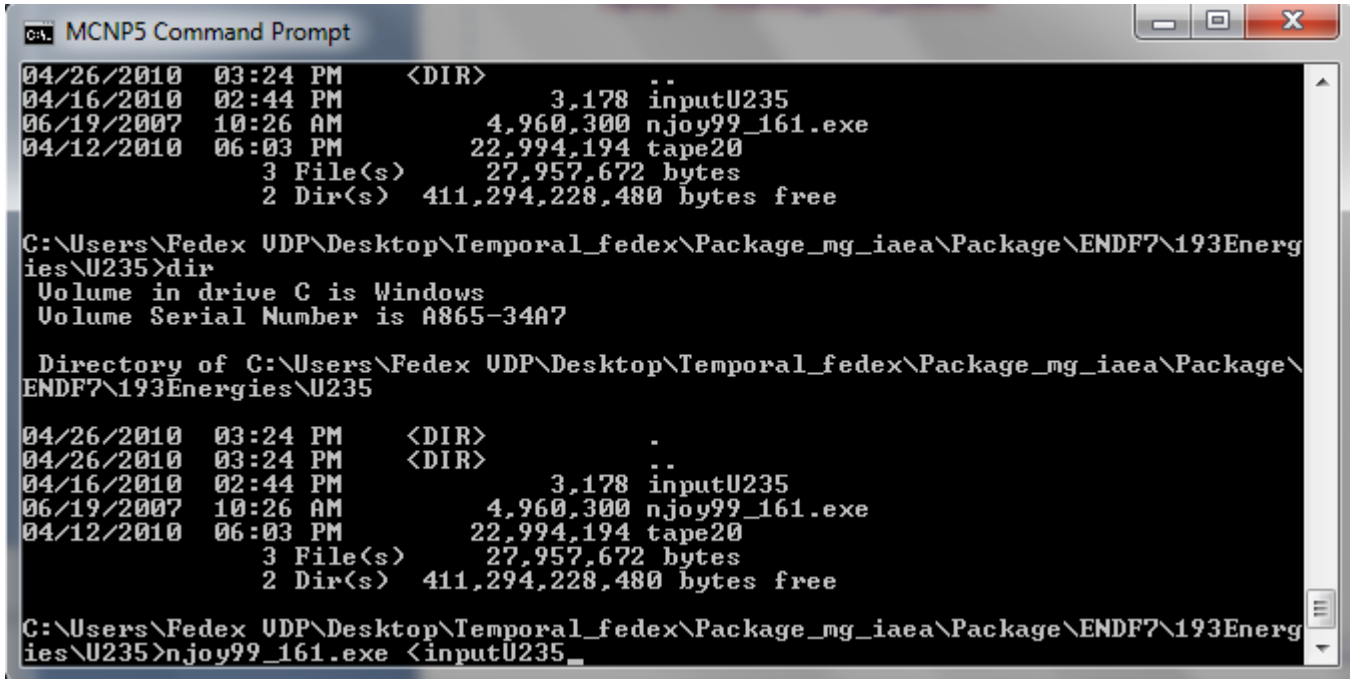
- ✓ **Monte Carlo continuous energy results**

Model	No of histories	cycles	keff	std dev
CP/Grain	5000	500	1.63054	0.00032
Pebble1D	5000	500	1.53969	0.00026
Pebble3D	5000	500	1.53933	0.00025
Prismatic assembly	5000	500	1.66750	0.00031

Execution command

- ✓ **Write in the DOS prompt command:**

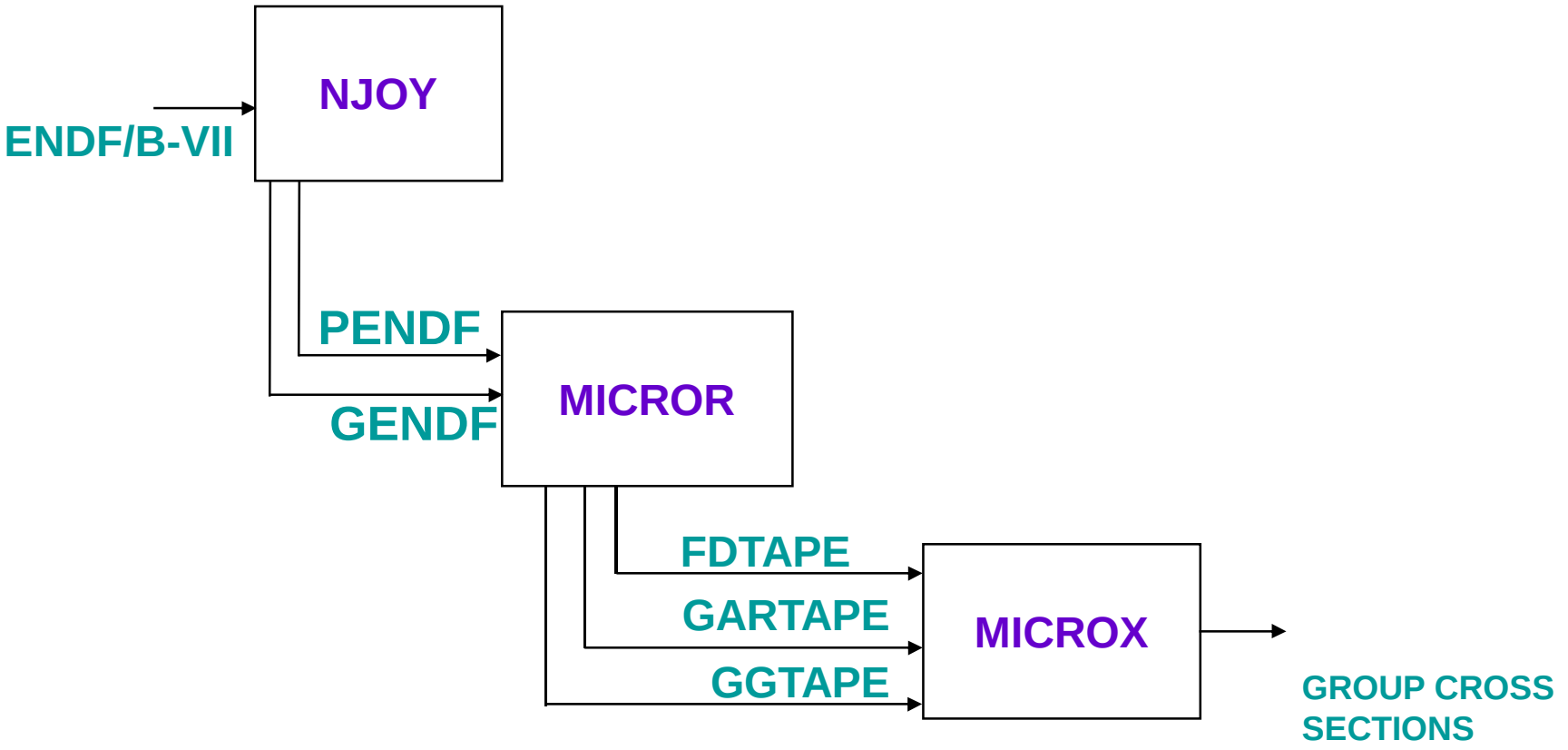
- ✓ **njoy < input_file_name**



Cross-Section Generation

- The cross sections are generated using a system of three codes:
  - NJOY
  - MICROR
  - MICROX-2
- The ENDF/B-VII (Evaluated Nuclear Data Files) are used

Cross-Section Generation



MICROX

To run MICROX type the following at the DOS prompt:

microx_<_ninp

(_ indicates the space)