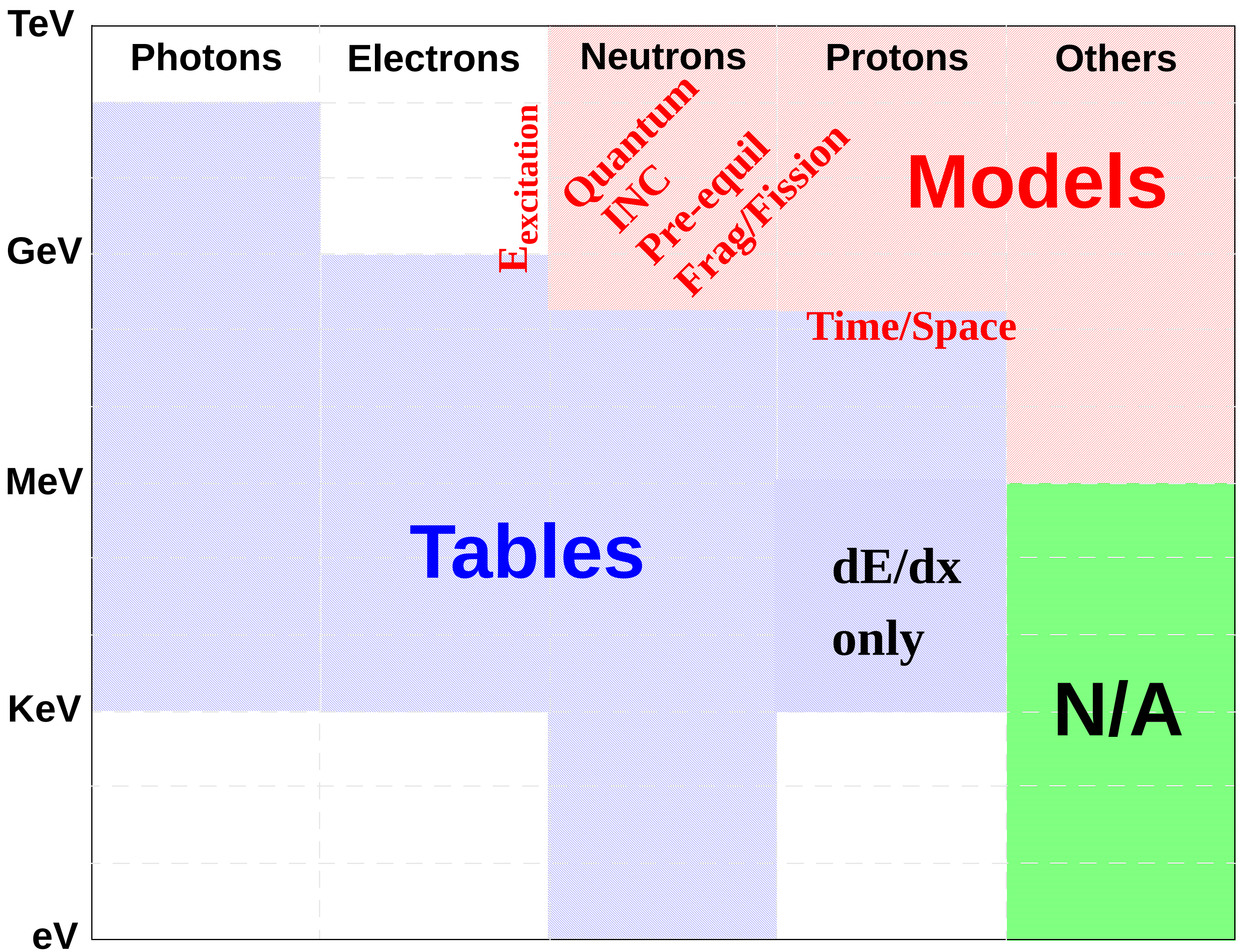
TABLE PHYSICS

- Neutron Physics (0 - 150 MeV)
- Photon Physics (1KeV - 10^5 MeV)
- Electron Physics (1KeV - 1000 MeV)
- Proton Physics (1KeV - 150 MeV)
- Summary (Details in MCNP Manual Ch. 2)


TeV
GeV
MeV
KeV
eV
Photons
Electrons
Neutrons
Protons
Others
Excitation
Quantum
INC
Pre-equil
Frag/Fission
Models
Time/Space
Tables
dE/dx
only
N/A

MCNPX Input "Cards" - Cross Sections and Physics

Type	Card				
Problem Type	***MODE***				
Material	***M***	DRXS	***TOTNU***	***NONU***	AWTAB
	XS	VOID	PIKMT	MGOPT	***MX***
Variance Reduction	PWT	***FCL***	BBREM	SPABI	***PHYS***
Tally	***FM***				
Energy	***PHYS***	TMP	***THTME***	***MT***	
Cutoff	***CUT***	ELPT			
Peripheral	***PERT***				

Mn CARDS

Mn $ZAID_1$ $fraction_1$ $ZAID_2$ $fraction_2$ ...

For example:

M1	**1001 2 8016 1**
M75	**92235.60c -.95 92238.60 -.05**
M10	**82000.02p 1**
M4	**5010 .8 5011 3.2 6000.50c 1.0 nlib=.60c plib=.02p hlib=.24h elib=.01e gas=0 estep=20 cond=0 pnlib=.24u**

Mix and Match

The MX Card

Form: MXn:p   zzaaa$_1$ zzaaa$_2$ ....

where

n = material number (material card <u>must</u> <u>precede</u> MX card in input file)

p = particle type (*n, p, h*)

***p* is for photonuclear, not photoatomic**

zzaaa$_n$ = replacement nuclide for the nth nuclide on the material card, *OR* "MODEL"

Mix and Match

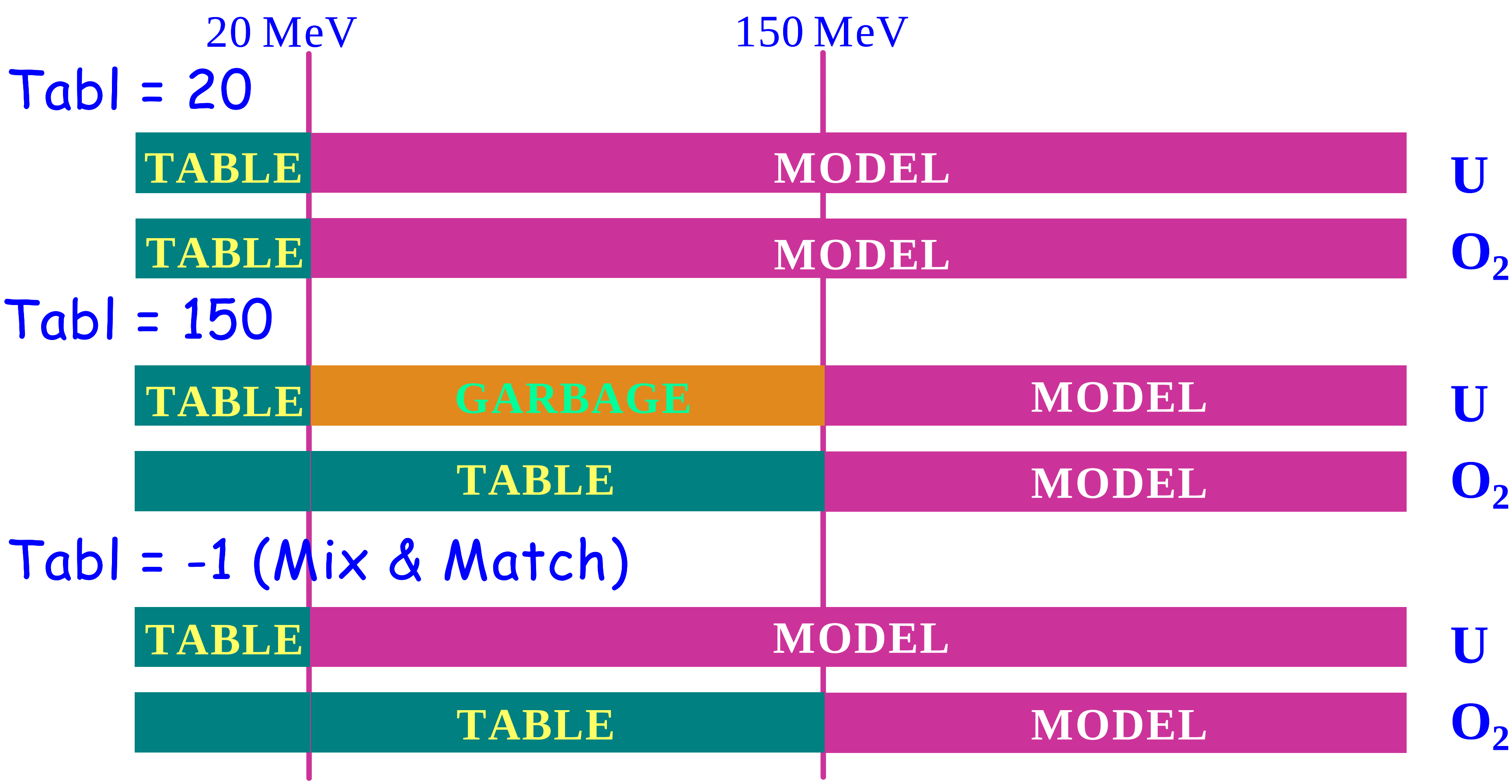
Makes the interface between table physics and model physics seamless.

- **Cross-section Tables are used when available for a particular nuclide, particle, and energy.**
  - < 20 MeV N, P, & H Tables exist for <u>many</u> nuclides (<u>but not all</u>)
  - < 150 MeV N, P, & H tables exist for <u>some</u> nuclides
  - Tables for most particle types are <u>non-existent</u>, regardless of energy or nuclide.

- **Physics Models are used when tabular data are not available**
  - outside tabular data energy range
  - nuclide not represented in data tables
  - particle type not represented in data tables for selected nuclide

From Table to Model Physics

Mix and Match



Mix and Match

Example

mode	**n h p**				
phys:p	**3j 1**				
m1	**1002 1**	**1003.6 1**	**6012 1**	**20040 1**	**nlib .24c**
mx1:n	**j**	**model**	**6000**	**20000**	
mx1:h	**model**	**1001**	**j**	**j**	
mpn1	**6012**	**0**	**j**	**j**	

Models will be used for neutron tritium and proton deuterium.

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Mix and Match

1particles and energy limits print table 101

Particle type			particle cutoff energy	maximum particle energy	smallest table maximum	largest table maximum	always use table below	always use model above
1	n	neutron	0.0000E+00	1.0000E+37	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02
2	p	Photon	1.0000E-03	1.0000E+02	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05
9	h	proton	1.0000E+00	1.0000E+02	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02

CLASSES OF MCNPX DATA

(10th character of ZAID)

C - Continuous-energy neutron
D - Discrete-reaction neutron
M - Multigroup neutron
Y - Neutron dosimetry
T - Neutron S(α,β) thermal

P - Continuous-energy photon
G - Multigroup photon
U - Continuous-energy photonuclear

H - Continuous-energy proton

E - Continuous-energy electron

Default Cross Sections

e.g., ZAID = 74000

- Based on other cards (MODE, DRXS, MGOPT) and options, MCNPX knows which class of data is required.
- MCNPX will "read" the cross-section directory file, XSDIR, starting at the beginning. The first valid match will define which cross-section table to use.
- Therefore, defaults depend upon the configuration of the XSDIR file that you happen to be using.

XSDIR File

directory
1001.60c 0.999170 endf60 0 1 1 3484 0 0 2.5300E-08
1002.60c 1.996800 endf60 0 1 884 2704 0 0 2.5300E-08
1003.60c 2.990140 endf60 0 1 1572 3338 0 0 2.5300E-08
2003.60c 2.989032 endf60 0 1 2419 2834 0 0 2.5300E-08
2004.60c 4.001500 endf60 0 1 3140 2971 0 0 2.5300E-08
3006.60c 5.963400 endf60 0 1 3895 12385 0 0 2.5300E-08
3007.60c 6.955732 endf60 0 1 7004 14567 0 0 2.5300E-08
4009.60c 8.934780 endf60 0 1 10658 64410 0 0 2.5300E-08
5010.60c 9.926921 endf60 0 1 26773 27957 0 0 2.5300E-08
5011.60c 10.914700 endf60 0 1 33775 108351 0 0 2.5300E-08
6000.60c 11.898000 endf60 0 1 60875 22422 0 0 2.5300E-08

MCNPX Cross-Section Plotting

- Use "MCNPX IXZ" options to enable
- Plots cross sections as actually used in MCNPX
- Neutron, photon, protons and electron data can be displayed
- Can plot individual isotope / element or combined material
- Some plots require an FM card to omit expunging (MT>4)
- Most regular MCPLOT commands apply (e.g., coplot)
- Can dump an ASCII listing of points (printpts)
- Cannot currently plot secondary distributions

MCNPX Cross-Section Plotting Commands

xs = material or ZAID

- xs = m5
- xs = 8016.60c (complete ZAID required)
- xs = ? will give brief help package

mt = reaction number

- mt = 102
- mt = -5
- mt = 999 (or some other unavailable value) will give list of available mt's

par = particle type

- par = n
- par = p
- par = e
- par = h

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Periodic Table of the Elements

Group**

Period	1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 vIIIA 8A
1	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.47	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	57 La* 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 190.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.5	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (210)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra (226)	89 Ac~ (227)	104 Rf (257)	105 Db (260)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 --- ()	111 --- ()	112 --- ()		114 --- ()		116 --- ()		118 --- ()

Lanthanide Series*	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (147)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
Actinide Series~	90 Th 232.0	91 Pa (231)	92 U (238)	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lr (257)

Some Neutron MT's (Reaction Identifiers)

MT	FM	Description
1	-1	Total
2	-3	Elastic
16		(n,2n)
17		(n,3n)
18	-6	Fission
51		(n,n') to 1st excited state
90		(n,n') to 40th excited state
91		(n,n') to continuum
101	-2	Total absorption (i.e., neutron disappearance)
102		Radiative capture (n,γ)
103		(n,p)
107		(n,α)
202	-5	Total photon production
301	-4	Average heating numbers (MeV/collision)

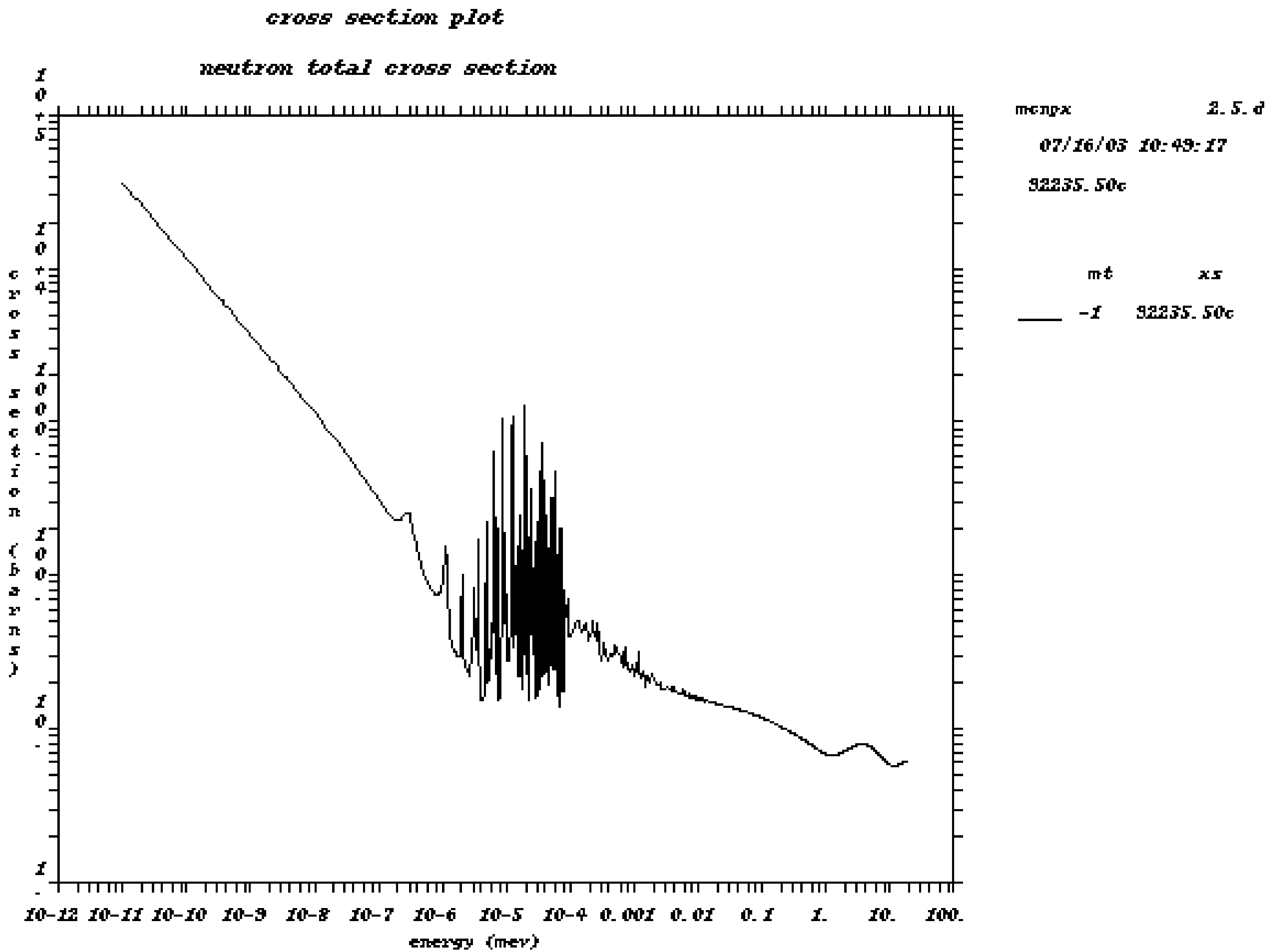
Exercise #1 - Plotting Neutron Cross Sections in MCNPX

- **Input file: copy %inputs%\physics\intxs3**

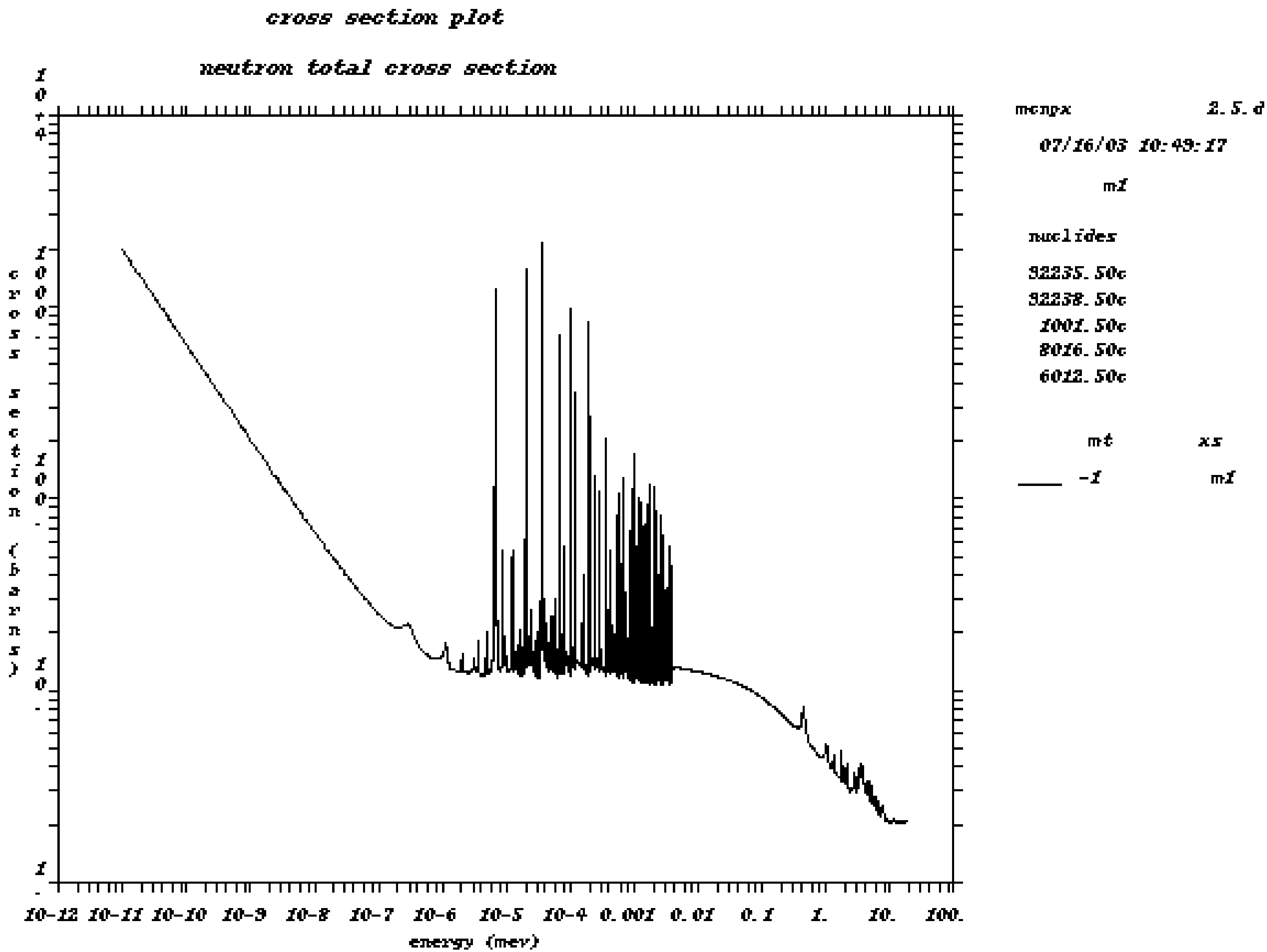
```
basic xs plotting
1    1 -1 -1
2    0 1

1    so 5

mode n
sdef
imp:n 1 0
m1   92235.50c .2 92238.50c .8 1001.50c 2 8016.50c 1 6012.50c 1
m2   92235.60c 1
mt1 grph.01t
f4:n 1
fm4  (1 1 (102) (-6)) (1 2 -6)
nps 100
```

- **mcnpx i=intxs3 ixz**

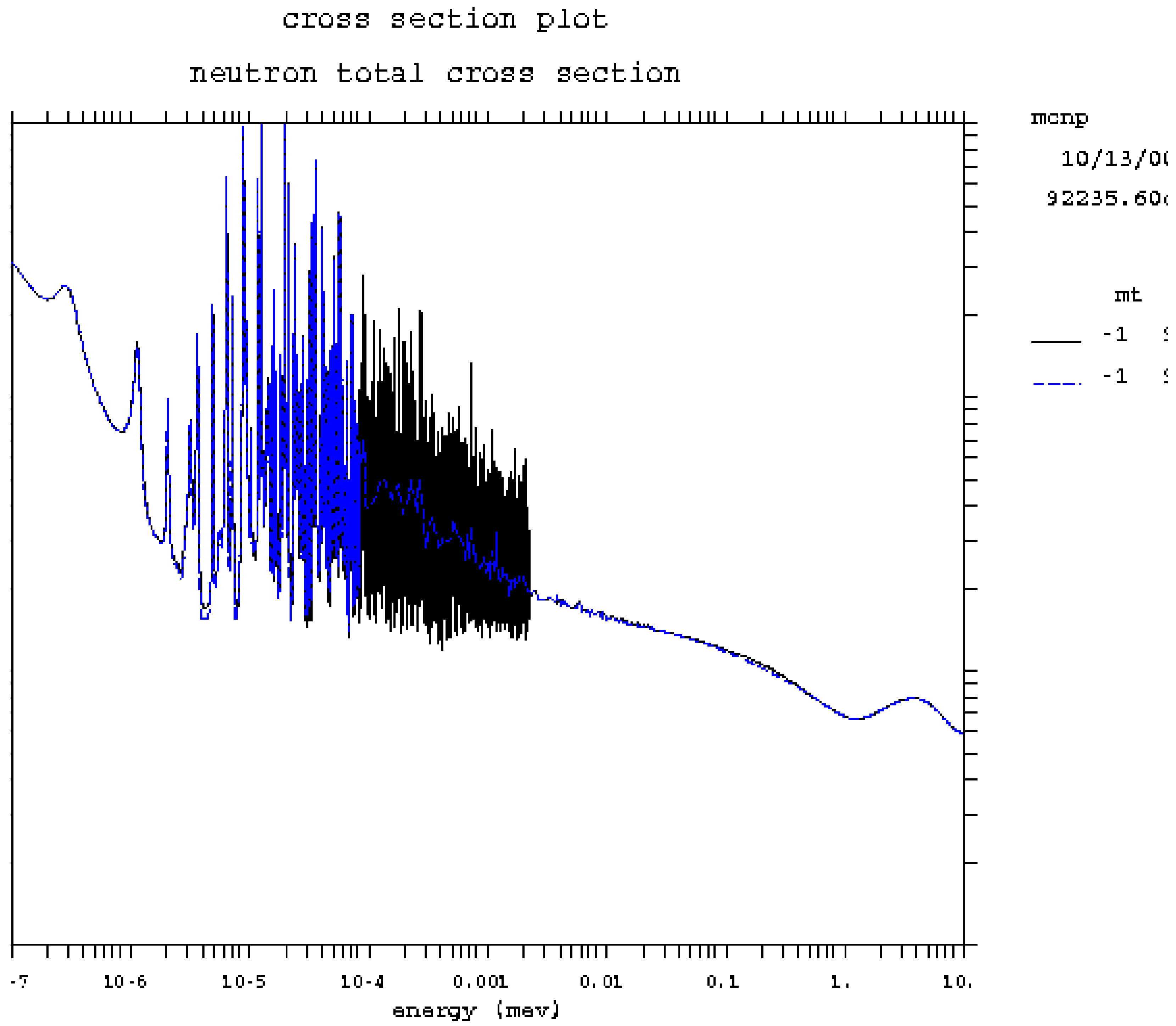
1. Plot the total cross section for ZAID=92235.50c
2. Plot the total cross section for Material M1.
3. Compare the fission cross sections for ENDF/B-V U^{235} (ZAID=92235.50c) with ENDF/B-VI U^{235} (ZAID=92235.60c).



cross section plot
neutron total cross section
mcnpx 2.5.d
07/16/03 10:49:17
92235.50c
mt xs
-1 92235.50c
cross section (barns)
energy (mev)
10-12 10-11 10-10 10-9 10-8 10-7 10-6 10-5 10-4 0.001 0.01 0.1 1. 10. 100.



cross section plot
neutron total cross section
mcnpx 2.5.d
07/16/03 10:49:17
m1
nuclides
92235.50c
92238.50c
1001.50c
8016.50c
6012.50c
mt xs
-1 m1
cross section (barns)
10+4
1000.
100.
10.
1.
10-12 10-11 10-10 10-9 10-8 10-7 10-6 10-5 10-4 0.001 0.01 0.1 1. 10. 100.
energy (mev)



cross section plot
neutron total cross section
mcnp
10/13/0(
92235.60(
mt
-1
-1
-7
10-6
10-5
10-4
0.001
0.01
0.1
1.
10.
energy (mev)

THERMAL ISSUES

FREE GAS THERMAL TREATMENT

- **Target nuclei are in motion as a result of non-zero temperature of the material. We assume an isotropic Maxwellian distribution of target velocities.**
- **Cross sections are a function of relative velocity between the neutron and the target. In a Maxwellian "sea" of targets, monoenergetic neutrons "see" targets with a spectrum of relative velocities. This leads to Doppler broadening of the cross sections.**
- **Temperature also impacts kinematics of neutron collisions. Neutrons tend to be "thermalized" to energies consistent with the material temperature.**

MCNPX Input - Temperature

- TMPn card
  - enter the temperature for each cell (in MeV) at time n
  - default - room temperature (2.53e-08 MeV)
- THTME card
  - enter the times (in shakes) that correspond to the n's on the TMPn cards
  - default - no entry (temperatures are time-independent)
- MCNPX knows the temperature at which a particular ZAID was processed from a value on the appropriate entry of the XSDIR file.
- If ZAID temperature is equal to cell temperatures containing that ZAID, MCNPX does nothing.
- If ZAID temperature is not equal to cell temperatures containing that ZAID, MCNPX adjusts cross sections based on a rather simple model.

THERMAL EFFECTS

MOLECULAR BINDING THERMAL TREATMENT
S(α,β)

- **Low energy-wavelength neutrons can interact with the lattice spacing of solids**
- **Cross sections show very jagged behavior. Each peak corresponds to a particular set of crystal planes.**
- **Coherent scattering (interference of scattered waves) add constructively in some directions and add destructively in other directions. Thus angular distributions change (Bragg scattering).**
- **Molecular energy levels of liquids and solids can be important**
- **Vibrational and rotational levels (~0.1 eV spacing below a few eV).**
- **Neutron loses or gains energy in discrete amounts which modifies the double-differential cross section (thermal inelastic scatter).**

Thermal S(α,β) Tables (Class T)

- designed to model neutron scattering as impacted by the binding of the scattering nucleus in the solid, liquid, or gas moderator
- data are provided at very low energies (< 4 eV) for several moderators
- temperature-dependent data based on ENDF/B-V are provided for MCNPX (ENDF/B-VI in Sab2002.60t)
- can be very important for LWR, criticality safety, and ultra-cold applications
- to invoke in MCNPX, use appropriate MT card(s)

```
Mn 1001 2 8016 1
MTn LWTR.01T
```

- when invoked, will override isotopic scattering data if in S(α,β) energy range

ZAID	Date of Processing	Material Description	Nuclides[a]	Temp (°K)
THERXS1 (Source: LANL)				
smeth.01t	04/10/88	Solid methane	1001	22
lmeth.01t	04/10/88	Liquid methane	1001	100
hpara.01t	03/03/89	Para H	1001	20
hortho.01t	03/03/89	Ortho H	1001	20
dpara.01t	05/30/89	Para D	1002	20
dortho.01t	05/30/89	Ortho D	1002	20
TMCCS1 (Source: ENDF)				
lwtr.01t	10/22/85	H in light water	1001	300
lwtr.02t	10/22/85	H in light water	1001	400
lwtr.03t	10/22/85	H in light water	1001	500
lwtr.04t	10/22/85	H in light water	1001	600
lwtr.05t	10/22/85	H in light water	1001	800
poly.01t	10/22/85	H in polyethylene	1001	300
h/zr.01t	10/22/85	H in Zr-hydride	1001	300
h/zr.02t	10/22/85	H in Zr-hydride	1001	400
h/zr.04t	10/22/85	H in Zr-hydride	1001	600
h/zr.05t	10/22/85	H in Zr-hydride	1001	800
h/zr.06t	10/22/85	H in Zr-hydride	1001	1200
benz.01t	09/08/86	Benzene	1001, 6000, 6012	300
benz.02t	09/08/86	Benzene	1001, 6000, 6012	400
benz.03t	09/08/86	Benzene	1001, 6000, 6012	500
benz.04t	09/08/86	Benzene	1001, 6000, 6012	600
benz.05t	09/08/86	Benzene	1001, 6000, 6012	800
hwtr.01t	10/22/85	D in heavy water	1002	300
hwtr.02t	10/22/85	D in heavy water	1002	400
hwtr.03t	10/22/85	D in heavy water	1002	500
hwtr.04t	10/22/85	D in heavy water	1002	600
hwtr.05t	10/22/85	D in heavy water	1002	800
be.01t	10/24/85	Be metal	4009	300
be.04t	10/24/85	Be metal	4009	600
be.05t	10/24/85	Be metal	4009	800
be.06t	10/24/85	Be metal	4009	1200
beo.01t	09/08/86	Be oxide	4009, 8016	300
beo.04t	09/08/86	Be oxide	4009, 8016	600
beo.05t	09/08/86	Be oxide	4009, 8016	800
beo.06t	09/08/86	Be oxide	4009, 8016	1200
grph.01t	09/08/86	Graphite	6000, 6012	300
grph.04t	09/08/86	Graphite	6000, 6012	600
grph.05t	09/08/86	Graphite	6000, 6012	800
grph.06t	09/08/86	Graphite	6000, 6012	1200
grph.07t	09/08/86	Graphite	6000, 6012	1600
grph.08t	09/08/86	Graphite	6000, 6012	2000
zr/h.01t	09/08/86	Zr in Zr-hydride	40000	300
zr/h.02t	09/08/86	Zr in Zr-hydride	40000	400
zr/h.04t	09/08/86	Zr in Zr-hydride	40000	600
zr/h.05t	09/08/86	Zr in Zr-hydride	40000	800
zr/h.06t	09/08/86	Zr in Zr-hydride	40000	1200

a. Nuclides for which the $S(\alpha,\beta)$ data are valid. For example, lwtr.01t provides scattering data only for 1H; 16O would still be represented by the default free-gas treatment.

Exercise #2 - Plotting Neutron S(α,β) Cross Sections

• Input file: intxs3

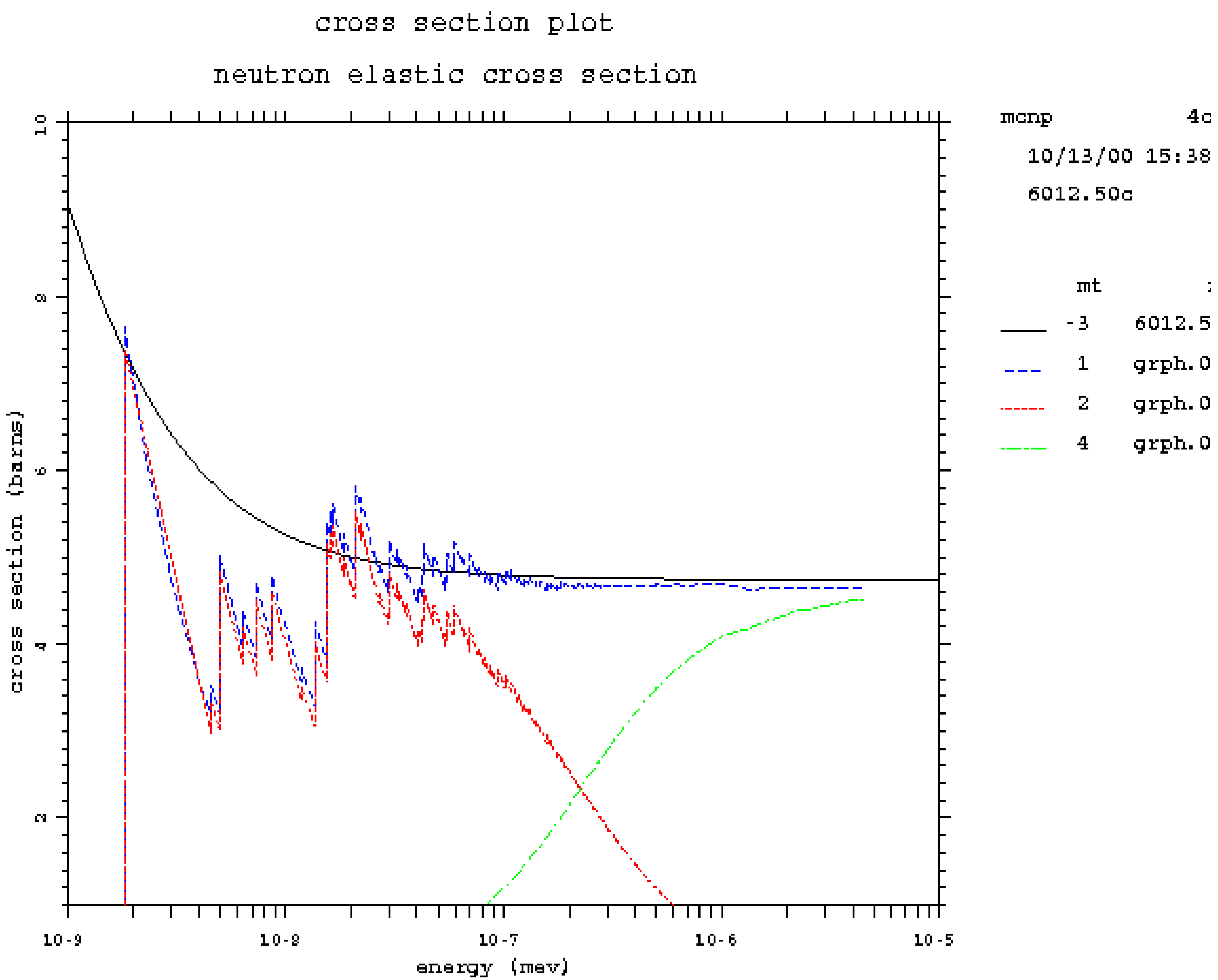
```
basic xs plotting
1    1 -1 -1
2    0 1

1    so 5

mode n
sdef
imp:n 1 0
m1   92235.50c .2 92238.50c .8 1001.50c 2 8016.50c 1 6012.50c 1
m2   92235.60c 1
mt1 grph.01t
f4:n 1
fm4  (1 1 (102) (-6)) (1 2 -6)
nps 100
```

- mcnpx i=intxs3 ixz

mcplot> xs=6012.50c xlim 1e-9 1e-5 &

mcplot> ylim=.1 10   loglin

mcplot> cop xs=grph.01t mt=1 cop mt=2 cop mt=4



cross section plot
neutron elastic cross section
mcnp 4c
10/13/00 15:38
6012.50c
mt :
-3 6012.5
1 grph.0
2 grph.0
4 grph.0
cross section (barns)
10
8
6
4
2
10-9
10-8
10-7
10-6
10-5
energy (mev)

Thermal Effects

MCNPX calculation of k_{eff} for ORNL-2 benchmark (unreflected sphere of uranyl nitrate in water plus B-10)

	k_{eff}
no S(α,β) treatment for light water	0.980 (.001)
with S(α,β) treatment for light water	0.996 (.001)

PHYS:N EMAX EAN IUNR DNB TABL FISM RECL

- Neutron data above EMAX are expunged

  Default: 100MeV

Note: Neutron data below EMIN is also expunged (EMIN is second entry on CUT:N card - *Default: 0*)

- EAN = Analog energy limit (MeV) E>EAN=implicit capture; E<EAN = analog capture. *Default: 0*
- IUNR = 0/1 = on/off unresolved resonance range probability tables.

  Default: 0
- DNB = -1/0/n = analog/off/produce up to *n<10* delayed neut./fission

  Default: -1
- TABL = Maximum energy for use of table-based data

  Default: -1 = Mix & Match
- FISM = -1/0/>0 = isotopic/average/FWHM nu Gaussian dist.

  2-5 fission neutrons for FISM=0; otherwise 0-10 neutrons

  Default: FISM=0
- RECL = 0/n = off/produces n recoils per collision

  Default: 0

CUT Card

Form: **CUT:*pl*** ***T E WC1 WC2 SWTM***

Neutron default:T=very large, E=0.0 MeV, *WC1* =–.50 , *WC2* = –.25
***SWTM* = minimum source weight if the general source is used.**

***pl* = particle type/designator**

***T* = time cutoff in shakes (10^{-8} sec).**

***E* = lower energy cutoff in MeV.**

***WC1* = weight cutoff survival weight**

***WC2*= weight cutoff. If weight goes below WC2 roulette is played to restore weight to WC1. Negative values make WC1 and WC2 relative to importances.**

Setting WC1 = 0 invokes analog capture.

TOTNU Card

Criticality (k_{eff} or alpha) Problems

- default is total nubar

  TOTNU

- can get prompt nubar with

  TOTNU NO

Fixed-Source Problems

- default is prompt nubar

  TOTNU NO

- can get total nubar with

  TOTNU

- can turn off fission neutrons with

  NONU

Exercise #3 - See Physics Options

• Input file: COPY %inputs%\physics\inpw14

```
testprob32 -- simple neutron problem to test delayed treatment
c     Simple sphere representation
1     1 -18.6    -1
2     0          +1

1      so 4.7407

mode   n a
imp:n  1 0
sdef pos= 0 0 0 erg=d10
sp10 -3 .968 2.29
phys:n j j j 15.0 j -1 $multiplicity turned on
c phys:n j j j 15.0       $ multiplicity off
cut:n 180.+8 j j j
totnu
f4:n 1
T4   0 100i 1 200i 200 1+8 180i 180.+8
fq4 t f
print
c      Materials specified with atom densities
m1     94239.61 0.95   2004.05  .05
prdmp j j -1
nps 1000
```

	by number			by weight			
	fissions	fission neutrons	multiplicity fraction	fissions	fission neutrons	multiplicity fraction	error
nu = 2	219	438	2.11799E-02	1.66291E-01	3.32581E-01	2.10476E-02	0.0619
nu = 3	8496	25488	8.21663E-01	6.48963E+00	1.94689E+01	8.21402E-01	0.0000
nu = 4	1595	6380	1.54255E-01	1.22335E+00	4.89339E+00	1.54841E-01	0.0000
nu = 5	30	150	2.90135E-03	2.14072E-02	1.07036E-01	2.70954E-03	0.1892
total	10340	32456	1.00000E+00	7.90068E+00	2.48019E+01	1.00000E+00	0.0000

factorial moments	by number		by weight	
nu	3.13888E+00	0.0013	3.13921E+00	0.0013
nu(nu-1)/2!	3.44072E+00	0.0034	3.44139E+00	0.0035
nu(nu-1)(nu-2)/3!	1.46770E+00	0.0080	1.46786E+00	0.0082
nu(nu-1) .... (nu-3)/4!	1.68762E-01	0.0259	1.68389E-01	0.0264
nu(nu-1) .... (nu-4)/5!	2.90135E-03	0.1823	2.70954E-03	0.1915

	by number fissions	by number fission neutrons	by number multiplicity fraction	by weight fissions	by weight fission neutrons	by weight multiplicity fraction	error
nu = 0	175	0	1.58586E-02	1.37436E-01	0.00000E+00	1.65909E-02	0.0713
nu = 1	807	807	7.31309E-02	5.98239E-01	5.98239E-01	7.22177E-02	0.0185
nu = 2	2302	4604	2.08609E-01	1.71929E+00	3.43858E+00	2.07548E-01	0.0000
nu = 3	3517	10551	3.18713E-01	2.64214E+00	7.92643E+00	3.18952E-01	0.0000
nu = 4	2846	11384	2.57907E-01	2.15490E+00	8.61959E+00	2.60133E-01	0.0000
nu = 5	1114	5570	1.00952E-01	8.27356E-01	4.13678E+00	9.98760E-02	0.0000
nu = 6	250	1500	2.26552E-02	1.87198E-01	1.12319E+00	2.25980E-02	0.0575
nu = 7	24	168	2.17490E-03	1.72629E-02	1.20840E-01	2.08393E-03	0.2115
total	11035	34584	1.00000E+00	8.28383E+00	2.59637E+01	1.00000E+00	0.0000

factorial moments	by number		by weight	
nu	3.13403E+00	0.0038	3.13426E+00	0.0039
nu(nu-1)/2!	4.10720E+00	0.0079	4.10670E+00	0.0082
nu(nu-1)(nu-2)/3!	2.88908E+00	0.0139	2.88314E+00	0.0144
nu(nu-1) .... (nu-3)/4!	1.17861E+00	0.0244	1.17142E+00	0.0252
nu(nu-1) .... (nu-4)/5!	2.82556E-01	0.0451	2.79227E-01	0.0465
nu(nu-1) .... (nu-5)/6!	3.78795E-02	0.0898	3.71855E-02	0.0924
nu(nu-1) .... (nu-6)/7!	2.17490E-03	0.2039	2.08393E-03	0.2136

SECONDARY PARTICLE PRODUCTION IN LA150

Table 0-1. Charged Particle Production Thresholds for Low Energy Neutron Libraries (MeV)

Isotope	ZAID	Proton	Deuteron	Triton	Alpha
H-1	1001.24c		1.0E-11		
H-2	1002.24c	3.339		1.0E-11	
Be-9	4009.24c	14.266	16.301	11.709	0.667
C	6000.24c	20.0	20.0		20.0
N-14	7014.24c	20.0	20.00		20.0
O-16	8016.24c	20.0	20.0		20.0
Al-27	13027.24c	1.897	6.274	11.29	3.25
Si-28	14028.24c	4.0	20.0	20.0	2.746
Si-29	14029.24c	3.0	20.0	20.0	1.3
Si-30	14030.24c	8.012	20.0	20.0	4.345
P-31	15031.24c	20.0	20.0		20.0
Ca	20000.24c	20.0	20.0	20.0	20.0
Cr-50	24050.24c	1.0	20.0	20.0	2.25
Cr-52	24052.24c	3.256	20.0	20.0	1.233
Cr-53	24053.24c	2.69	20.0	20.0	1.0
Cr-54	24054.24c	6.33	20.0	20.0	1.581
Fe-54	26054.24c	0.7	20.0	20.0	3.0
Fe-56	26056.24c	2.966	20.0	20.0	0.862
Fe-57	26057.24c	1.943	20.0	20.0	0.8
Ni-58	28058.24c	0.5	20.0	20.0	0.5
Ni-60	28060.24c	2.076	20.0	20.0	2.021E-8
Ni-61	28061.24c	0.549	20.0	20.0	0.07
Ni-62	28062.24c	4.532	20.0	20.0	0.445
Ni-64	28064.24c	6.627	20.0	20.0	2.481
Cu-63	29063.24c	0.9	20.0	20.0	1.742
Cu-65	29065.24c	1.375	20.0	20.0	0.112
Ni-93	41093.24c	20.0	20.0	20.0	20.0
W-182	74182.24c	20.0	20.0	20.0	20.0
W-183	74183.24c	20.0	20.0	20.0	20.0

Table 0-1. Charged Particle Production Thresholds for Low Energy Neutron Libraries (MeV)

W-184	74184.24c	20.0	20.0	20.0	20.0
W-186	74186.24c	20.0	20.0	20.0	20.0
Hg-196	80196.24c	20.0	20.0	20.0	20.0
Hg-198	80198.24c	20.0	20.0	20.0	20.0
Hg-199	80199.24c	20.0	20.0	20.0	20.0
Hg-200	80200.24c	20.0	20.0	20.0	20.0
Hg-201	80201.24c	20.0	20.0	20.0	20.0
Hg-202	80202.24c	20.0	20.0	20.0	20.0
Hg-204	80204.24c	20.0	20.0	20.0	20.0
Pb-206	82206.24c	20.0	20.0	20.0	20.0
Pb-207	82207.24c	20.0	20.0	20.0	20.0
Pb-208	82208.24c	4.236	5.816	6.403	1.0e-11
Bi-209	83209.24c	20.0	20.0	20.0	20.0

Major Neutron Physics Approximations

- each secondary particle from a neutron collision is sampled independently
- neutron reaction and photon-production reaction are not correlated
- no consideration of delayed photon production (e.g., about half of the steady-state fission gamma energy is not modeled)
- charged-particle production (& recoils) with LA-150 libraries only
- treatment of temperature effects is limited in its range of validity
- neutron heating (energy-deposition) tallies are the same whether or not secondary photons are transported

Useful Web Sites at LANL for Nuclear Data

http://www-xdiv.lanl.gov/XCI/PROJECTS/DATA/nuclear/dataweb.html (X-5)

- Currently supported MCNPX cross-section libraries.
- Documentation for certain topics related to nuclear data.
- Answers to frequently-asked questions.

http://t2.lanl.gov/data/data.html (T-16)

- Maintained by Bob MacFarlane (Group T-16; Nuclear Theory and Applications).
- Includes a nuclear data viewer.
- Extensive information on ENDF/B-VI neutron data.
- Also provides information about other evaluated neutron data (e.g., JENDL-3.2 and JEF-2.2).

TABLE PHYSICS

- Neutron Physics (0 - 150 MeV)
- Photon Physics (1KeV - 10^5 MeV)
- Electron Physics (1 KeV- 1000 MeV)
- Proton Physics (1 KeV - 150 MeV)
- Summary

PHOTON PHYSICS

- Storm and Israel - ENDF, EPDL
- Coherent (Thomson) Scattering + Form Factors
- Incoherent (Compton) Scattering + Form Factors
- Pair Production
- Photoelectric Absorption and Fluorescence
- Thick-Target Bremsstrahlung

PHYS:P EMCPF IDES NOCOH PNB PDB

- **EMCPF = simple physics if E>EMCPF**
  Default: 100 MeV
- **IDES = 0/1 = TTB or electron transport per mode/turn off electron production**
  Default: 0
- **NOCOH = 0/1 = on/off coherent scatter (for detector convergence)**
  Default: 0
- **PNB = -1/0/1 = analog/none/biased photonuclear particle production 0<PNB≤15**
  Default: 0
- **PDB = 0/1 = on/off Photon Doppler broadening**
  Default: 1

NOTE: There is photonuclear modeling for all nuclides in MCNPX

Simple vs. Detailed Photon Physics

Simple (E>100 MeV)	Detailed
Ignores coherent scattering	Coherent scattering with form factors
Compton scattering on free electron	Compton scattering with incoherent form factors
Photoelectric effect is pure absorption modeled by implicit capture	Photoelectric effect is analog absorption plus possible K and L-shell fluorescence
Pair production	Pair production

Detailed physics is recommended for most applications, particularly for high Z nuclides, low energy photons, and deep penetration problems.

Results for Simple/Detailed Photon Physics

	simple	detailed
SIMP1 (high energy, low Z, thin material)	1.129 (.003)	1.129 (.003)
SIMP2 (low energy, high Z, thick material)	1.904-6 (8%)	1.799-6 (8%)
SIMP2 (longer run)	1.849-6 (2%)	1.678-6 (2%)

Thick-Target Bremsstrahlung

- Electrons generated in direction of incident photon and immediately annihilated after generating bremsstrahlung photons
- Eliminates expensive electron transport
- Slows photon-only problems considerably
- Is default, but should not be used! Turn off TTB if bremsstrahlung unimportant; transport electrons if bremsstrahlung is important

Electron Production At Photon Collisions

	MODE P E	MODE P (w/ TTB)	MODE P (w/o TTB)
Coherent	No electrons	No electrons	No electrons
Incoherent	Electron produced and transported	Electron produced; TTB photon(s) transported	Electron energy deposited
Photoelectric	Electron(s) produced and transported	Electron(s) produced; TTB photon(s) transported	Electron energy deposited
Pair Prod.	Electron and positron produced and transported	Electron and positron produced; TTB photon(s) transported	Electron energy deposited; two 0.511 MeV photons created and transported

Results for Photon/Electron Physics

	tally	particles / minute
MODE P w/ TTB	0.132 (.013)	1.04+5
MODE P w/o TTB	0.097 (.014)	2.31+5
MODE P E	0.115 (.029)	84

PHOTONUCLEAR CAPABILITY

- **Data in LA150U library (.24u ZAID)**

  note: IAEA has a large collection of PhotoNuclear library data

- **May use PNLIB keyword on the material card**

  m1   plib=02p elib=03e nlib=49c pnlib=24u 74184 1 6000.24c 3

- **Use photonuclear material card (MPNm or MXm:p) - 0 entry omits PN for that nuclide**

  mx1:p 74184 6012

- **Make the 4th entry on PHYS:p card nonzero**

  phys:p .05 2j -1

- **Models used if library data is not available**

Exercise #5 - Photonuclear Effects

- Input file: inpw04

```
testprob04 -- photoneutrons
1     1  .02  -1
2     2  .1 -2 1 3 4
3     0         2
4     2 .1 -3 5
5     2 .1 -4 6
6     2 .1 -5
7     2 .1 -6

1     so 10
2     so 20
3     s -10 2r 2.1
4     s 10 2r 1.1
5     s -10 2r 1.9
6     s 10 2r .9

mode n p
imp:n,p 1 1 0 1 1 1 1
m1    plib=02p elib=03e nlib=49c 74184 1  6000.24c 3
mpn1 74184 6012
m2    plib=02p elib=03e nlib=49c 74184 1  8016.24c 3
c    monoenergetic isotropic photon point source at (0,0,0)
sdef  erg=d1   cel=1  par=2
sp1 -4
f4:p  1 2 4 5 6 7    $ flux tally
f14:n  1 2 4 5 6 7
nps   10000
prdmp 2j -1
phys:p .05 2j -1
```

- mcnpx i=inpw04

Photon MT's (Reaction Identifiers)

MT	FM	Description
501	-5	Total
504	-1	Incoherent (Compton)
502	-2	Coherent (Thomson)
522	-3	Photoelectric
516	-4	Pair Production
301	-6	Heating

PHOTONUCLEAR MT's

1	Total
2	Non-elastic
3	Elastic
4	Heating
5	Other (fission)
2005	Yield of Particle 2 from reaction 5

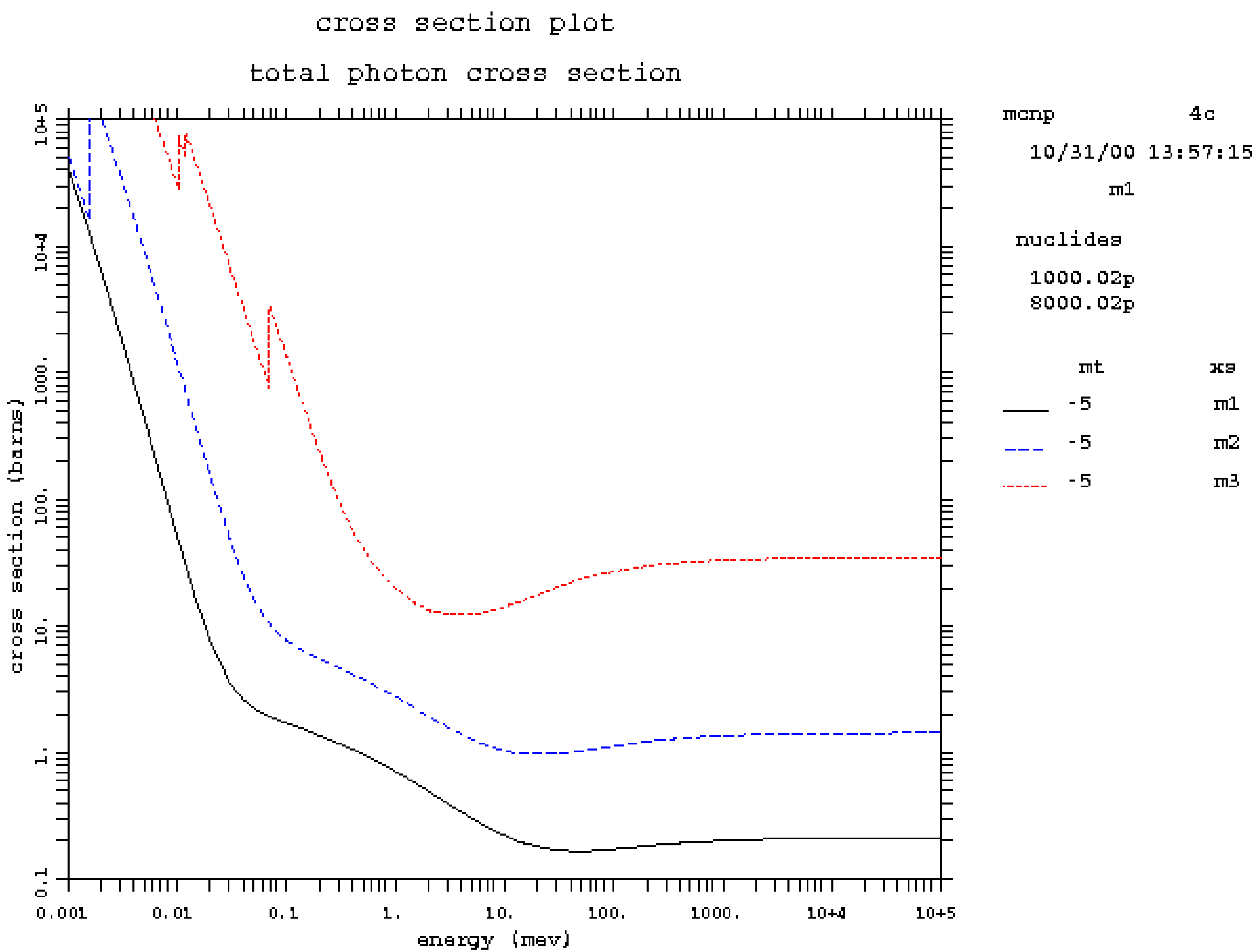
Exercise #6 - Plotting Photon Data in MCNPX

• Input file: intxs4

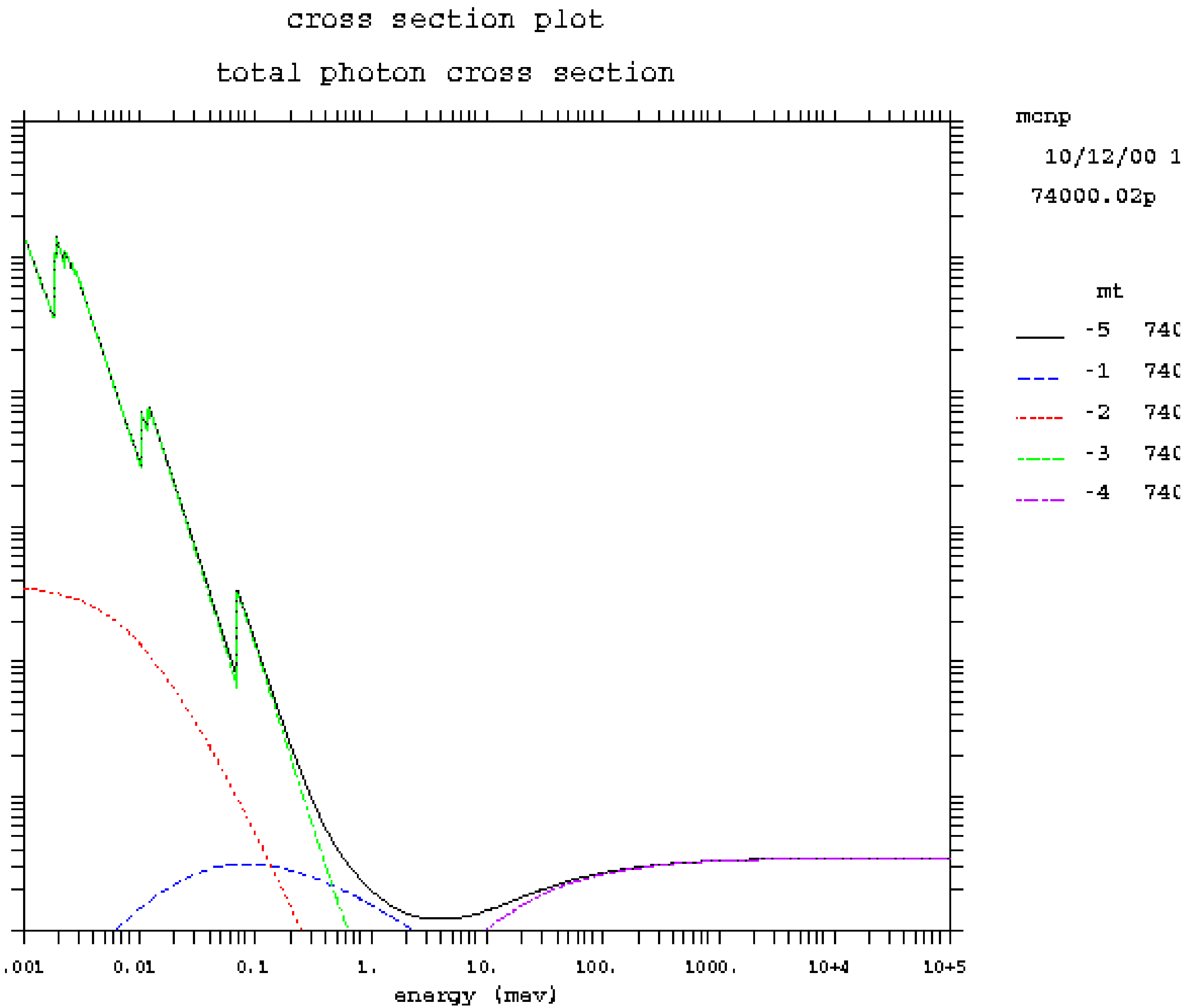
```
xs and physics ---- gamma, electron plotting
1    1 -1 -1
2    2 -2.7 1 -2
3 3 -19.2 2 -3
4           0 3

1    so 1
2          so 2
3          so 3

mode p e
sdef
m1   1001 2 8016 1
m2   13027 1
m3   74000 1
mpn1 0 8016
imp:p 1 2r 0
prdmp 2j -1
phys:p 3j -1
```

• mcnpx i=intxs4 ixz

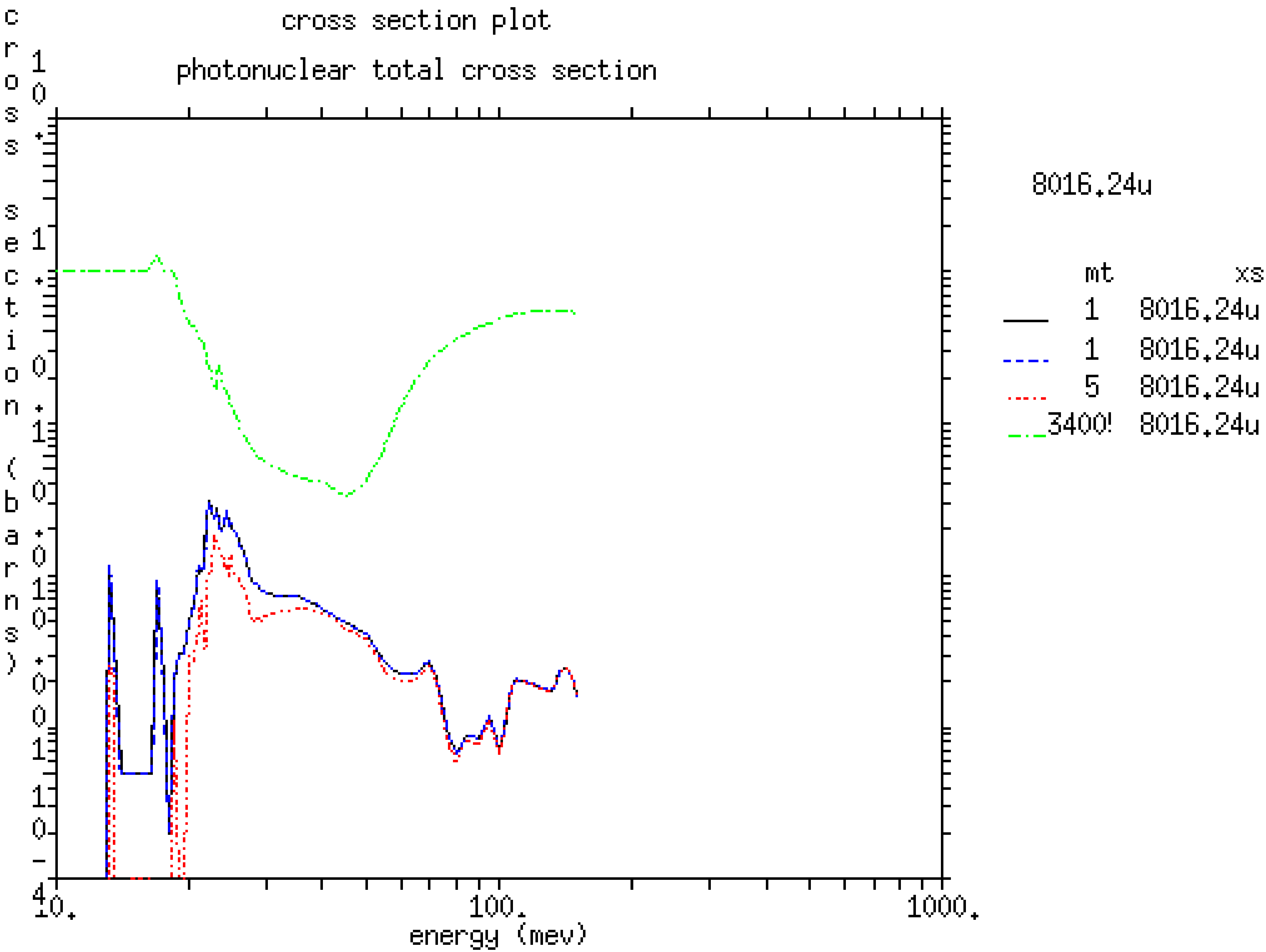
1. Plot the total photon cross sections for M1, M2 and M3.
2. Plot the total and four partial photon cross sections for Tungsten.
3. Plot photonuclear cross sections



cross section plot
total photon cross section
mcnp 4c
10/31/00 13:57:15
m1
nuclides
1000.02p
8000.02p
mt xs
-5 m1
-5 m2
-5 m3
cross section (barns)
10+5
10+4
1000.
100.
10.
1.
0.1
0.001
0.01
0.1
1.
10.
100.
1000.
10+4
10+5
energy (mev)



cross section plot
total photon cross section
mcnp
10/12/00 1
74000.02p
mt
-5 74(
-1 74(
-2 74(
-3 74(
-4 74(
.001
0.01
0.1
1.
10.
100.
1000.
10+4
10+5
energy (mev)



cross section plot
photonuclear total cross section
cross section (barns)
energy (mev)
10.
100.
1000.
8016.24u
mt
xs
1
8016.24u
1
8016.24u
5
8016.24u
3400!
8016.24u

Major Photon Physics Approximations in MCNPX

- Only K,L edges treated for photoelectric absorption
- Thick-target bremsstrahlung is the default
- No distinction between pair and triplet production
- No anomalous scattering factors

TABLE PHYSICS

- Neutron Physics (0 - 150 MeV)
- Photon Physics (1KeV - 10^5 MeV)
- Electron Physics (1KeV - 1000 MeV)
- Proton Physics (1MeV - 150 MeV)
- Summary

Electron Physics in MCNPX

- Foundation is the condensed history method of Berger.
- Angular deflections from Goudsmit and Saunderson.
- Energy straggling from Landau, Blunck and Leisegang, Blunck and Westphal, and Seltzer. Equivalent to ITS 3.0.
- Density effect correction from prescription of Sternheimer, Berger, and Seltzer.
- Occupation numbers and atomic binding energies from Carlson.
- Bremsstrahlung cross sections from Berger and Seltzer.
- Riley cross sections and Mott / Rutherford cross sections.
- Moller cross sections for knock-on electrons.

(References provided in the MCNP4C manual, LA-13709-M)

Condensed History Algorithm

An electron passing through matter will interact with each atom along its trajectory

- Energy loss from the electron to the media or to radiation
- Small deflections or scatterings along its path
- Production of secondary electrons or photons

This algorithm attempts to average the effect of all these interactions into aggregate quantities. Thus

- The effect of many small deflections is a single scattering deflection in a substep due to the multiple-scattering theory of Goudsmit and Saunderson.
- The effect of energy loss is accounted for by a single energy loss modified for straggling in each step.
- A step is related to the average distance an electron traverses to lose a specified amount of energy.
- Number of substeps per step is material dependent (ESTEP on M card)

Electron Options

- Bremsstrahlung angular distribution options:
  - detailed
  - simple (always used for next-event estimators; can be used for transport)
- Bremsstrahlung energy biasing (BBREM card)
- Production biasing for:
  - Bremsstrahlung photons (2 methods)
  - Knock-on electrons
  - Electron generated x-rays
  - Photon generated electrons
- ESTEP, GAS, and COND entries on material cards
- Energy indexing option:
  - DBCN(18)=0 bin-centered treatment (MCNP style) default
  - DBCN(18)=1 nearest group boundary treatment (ITS style)

Electron Data for MCNPX

On libraries:

- energies
    - radiative stopping power parameters
    - bremsstrahlung production cross sections
- bremsstrahlung energy distributions (EL03 only)
    - K-edge energies
- Auger electron production energies
- parameters for the evaluation of the Goudsmit-Saunderson theory for angular deflections
- atomic data of Carlson for density effect calculations (EL03 only)

Internally calculated:

- electron stopping powers and ranges
    - K x-ray production probabilities
- knock-on probabilities

PHYS:E EMAX IDES IPHOT IBAD ISTRG BNUM XNUM RNOK ENUM NUMB

- EMAX = upper limit for electron energy *(100 MeV)*
- IDES = *0*/1 = *on*/off electron production from photons
- IPHOT = *0*/1 = *on*/off photon production from electrons
- IBAD = *0*/1 = *detailed*/simple bremsstrahlung prod.
- ISTRG = *0*/1 = *straggling*/expected-value e energy loss
- BNUM ≥ 0; scaling of bremsstrahlung photons *(1.0)*
- XNUM ≥ 0; scaling of electron-induced x-rays *(1.0)*
- RNOK ≥ 0; scaling of knock-on electrons *(1.0)*
- ENUM ≥ 0; scaling of photon-induced electrons *(1.0)*
- NUMB = *0*/1 = *on*/off substep bremsstrahlung prod.

photon creation	tracks	weight (per source particle)	energy (per source particle)
source	0	0.	0.
nucl. interaction	0	0.	0.
particle decay	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	0.	0.
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
from neutrons	0	0.	0.
bremsstrahlung	1631	1.6310E+00	3.3926E+00
p-annihilation	156	1.5600E-01	7.9717E-02
photonuclear	0	0.	0.
electron x-rays	0	0.	0.
1st fluorescence	0	0.	0.
2nd fluorescence	0	0.	0.
(gamma,xgamma)	0	0.	0.
tabular sampling	0	0.	0.
total	1787	1.7870E+00	3.4723E+00

photon loss	tracks	weight (per source particle)	energy (per source particle)
escape	668	6.6800E-01	1.2374E+00
energy cutoff	625	6.2500E-01	8.4539E-01
time cutoff	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	0.	0.
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
compton scatter	0	0.	7.4540E-01
capture	412	4.1200E-01	3.2646E-01
pair production	82	8.2000E-02	3.1764E-01
photonuclear abs	0	0.	0.
total	1787	1.7870E+00	3.4723E+00

number of photons banked	1783
photon tracks per source particle	1.7870E+00
photon collisions per source particle	1.7140E+00
total photon collisions	1714

average time of (shakes)	
escape	7.8822E-02
capture	6.9011E-02
capture or escape	7.5079E-02
any termination	7.1563E-02

cutoffs	
tco	1.0000E+34
eco	5.0000E-01
wc1	0.0000E+00
wc2	0.0000E+00

electron creation	tracks	weight (per source particle)	energy (per source particle)
source	1000	1.0000E+00	1.0000E+01
nucl. interaction	0	0.	0.
particle decay	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	0.	0.
energy importance	0	0.	0.
pair production	153	1.5300E-01	2.3251E-01
compton recoil	771	7.7100E-01	6.9749E-01
photo-electric	412	4.1200E-01	3.0407E-01
photon auger	0	0.	0.

electron loss	tracks	weight (per source particle)	energy (per source particle)
escape	9	9.0000E-03	1.2495E-02
energy cutoff	3832	3.8320E+00	9.3997E-01
time cutoff	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	0.	0.
energy importance	0	0.	0.
scattering	0	0.	7.8119E+00
bremsstrahlung	0	0.	3.4366E+00

Electron Plot Quantities

MT	Description
1	de/dx collision - collisional energy loss (MeV-cm2/g)
2	de/dx radiation - brem. energy loss (MeV-cm2/g)
3	de/dx total (MeV-cm2/g)
4	range - distance to energy cutoff (g/cm2)
5	radiation yield - fraction of energy to brem.
6	beta**2 - relativistic beta (v/c)
7	density correction - empirical correction (MeV-cm2/g)
8	radcol - ratio of de/dx radiation to de/dx collision
9	drange - major step size (log grid, g/cm2)
10	dyield - average radiative loss over energy step (MeV)
11	rng - range used in current calculation (g/cm2)
12	gav - average collisional energy loss (MeV)
13	ear - energy loss correction due to Landau straggling

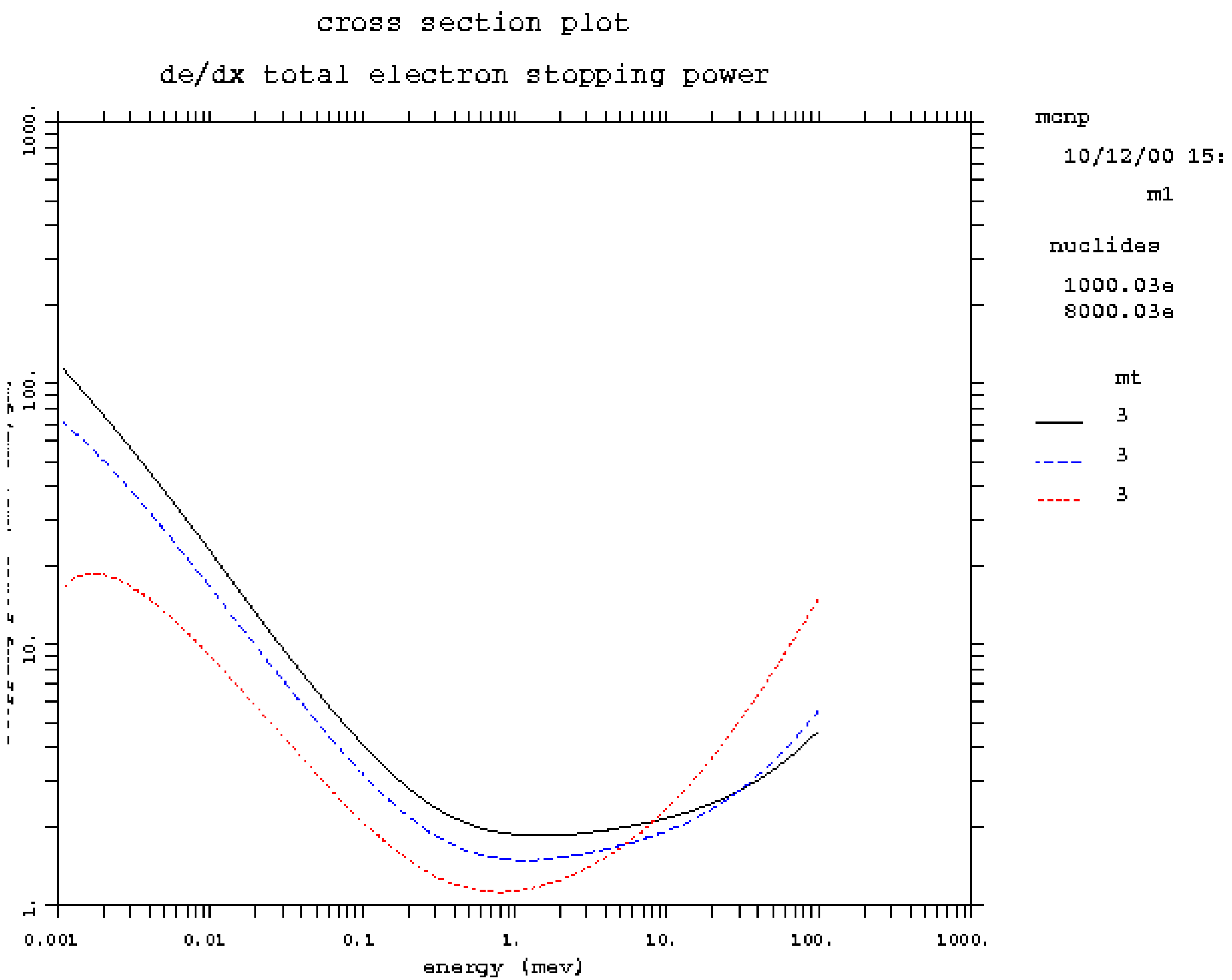
Exercise #7 - Plotting Electron Data in MCNPX

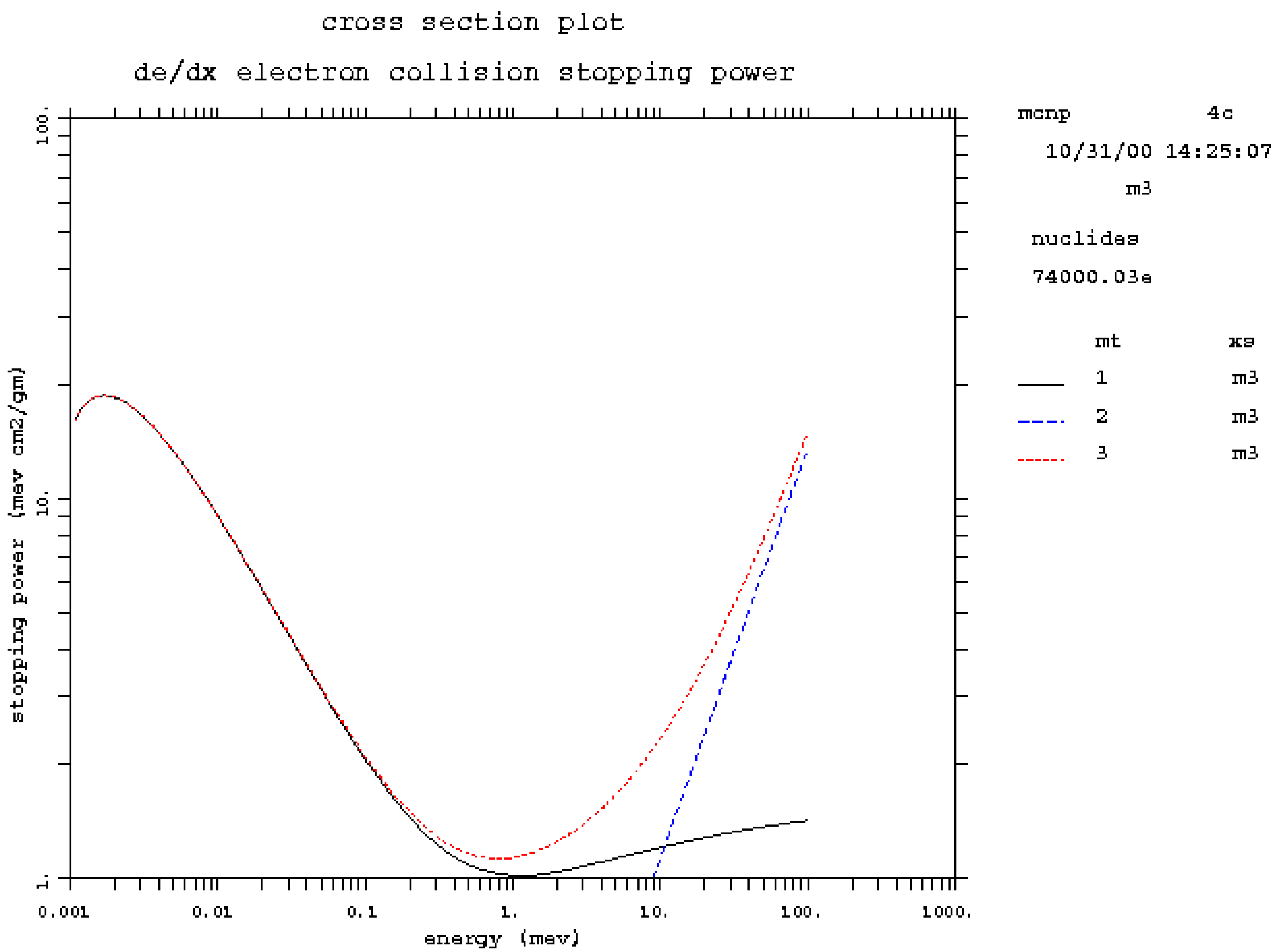
• Input file: intxs4

```
xs and physics ---- gamma, electron plotting
1    1 -1 -1
2    2 -2.7 1 -2
3 3 -19.2 2 -3
4           0 3

1    so 1
2          so 2
3          so 3

mode p e
sdef
m1   1001 2 8016 1
m2   13027 1
m3   74000 1
mpn1 0 8016
imp:p 1 2r 0
prdmp 2j -1
phys:p 3j -1
```

• mcnpx i=intxs4 ixz

1. Plot the total electron stopping powers for M1, M2 and M3.
2. Plot the collisional, radiative, and total stopping powers for Tungsten.


cross section plot
de/dx total electron stopping power
mcnp
10/12/00 15:
m1
nuclides
1000.03e
8000.03e
mt
3
3
3
1000.
100.
10.
1.
0.001
0.01
0.1
1.
10.
100.
1000.
energy (mev)


cross section plot
de/dx electron collision stopping power
mcnp 4c
10/31/00 14:25:07
m3
nuclides
74000.03e
mt xs
1 m3
2 m3
3 m3
stopping power (mev cm2/gm)
100.
10.
1.
energy (mev)
0.001
0.01
0.1
1.
10.
100.
1000.

POSITRONS

- Positron Sources are allowed: SDEF par = -e
- Positrons may be tallied separately: FTn ELC 3
- MCNPX uses ITS 3.0 physics:
    - Positron and electron physics are identical except when they stop (fall below energy cutoff). Electrons deposit energy whereas positrons generate annihilation photons.
    - At high energies positrons behave like electrons. At low energies (< 1 MeV), stopping powers, bremsstrahlung, knock-ons, and annihilations are increasingly poor.

TABLE PHYSICS

- Neutron Physics (0 - 150 MeV)
- Photon Physics (1KeV - 10^5 MeV)
- Electron Physics (1KeV - 1000 MeV)
- Proton Physics (1MeV - 150 MeV)
- Summary

PHYS:H EMAX U ECUT U ISTRG U RECL

- **EMAX = maximum proton energy**

  Default: Very large (100 MeV)
- **U = unused**
- **ECUT = use tables below ECUT and models above**

  Default: -1 (Tables when available, else models)
- **U = unused**
- **ISTRG = -1/0/1 = old Vavilov/new Vavilov/slowing down**

  Default: 0
- **U = unused**
- **RECL= 0/n = off/produce n recoil ions per elastic collision**

  Default: 0

Principal Proton Table Data Reactions

+/- 1 = total

+/- 2 = nonelastic

+/- 3 = elastic

+/- 4 = heating

> 4 = various reactions

In LA150H proton library, mt = 5 is all-inclusive

Proton Table Secondary Particle Yield

Reaction number + 1000∗p = multiplicity for particle type p

mt = 1005 is the number of neutrons produced from reaction 5

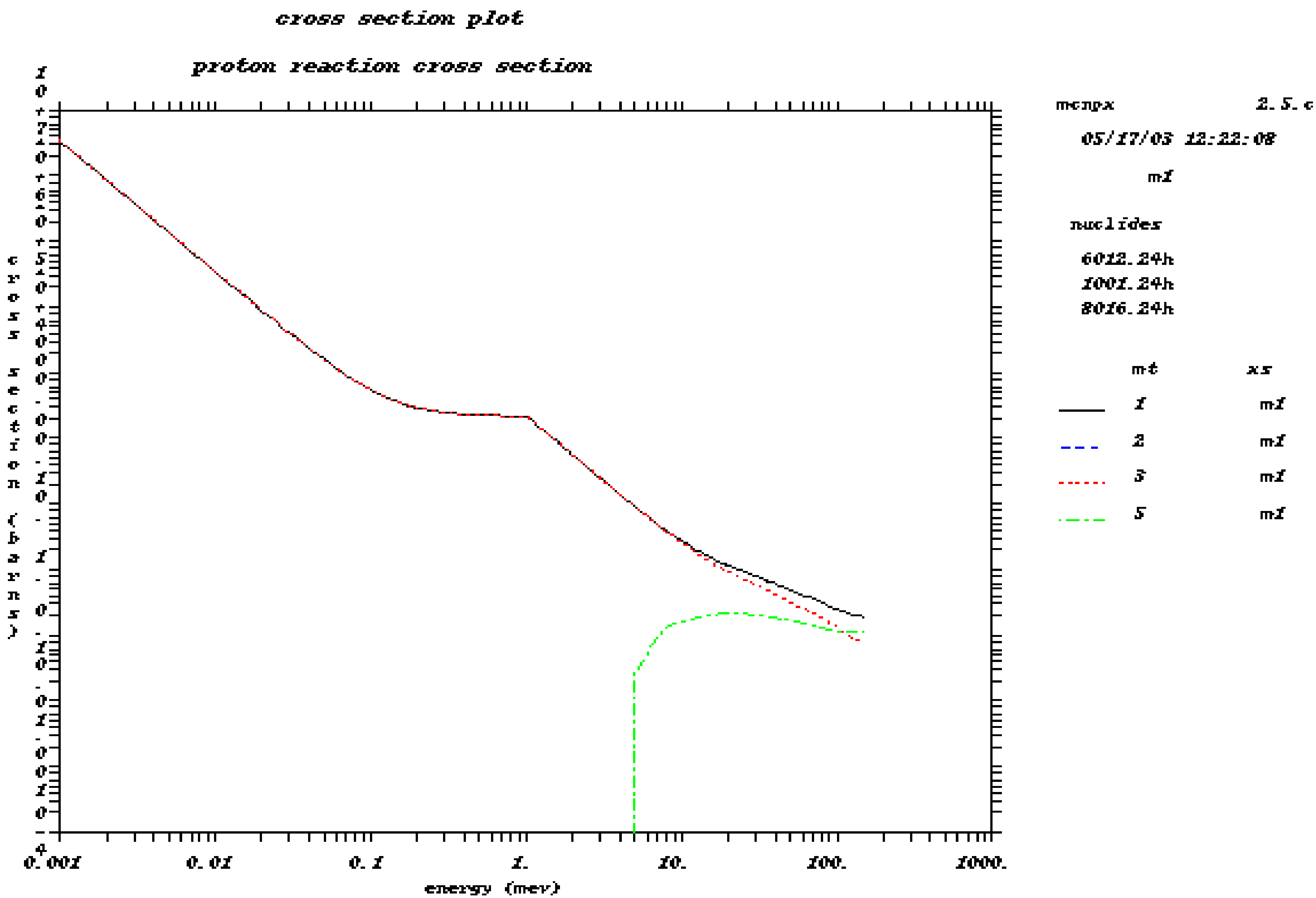
mt =34001 is the total number of alphas produced from h collisions

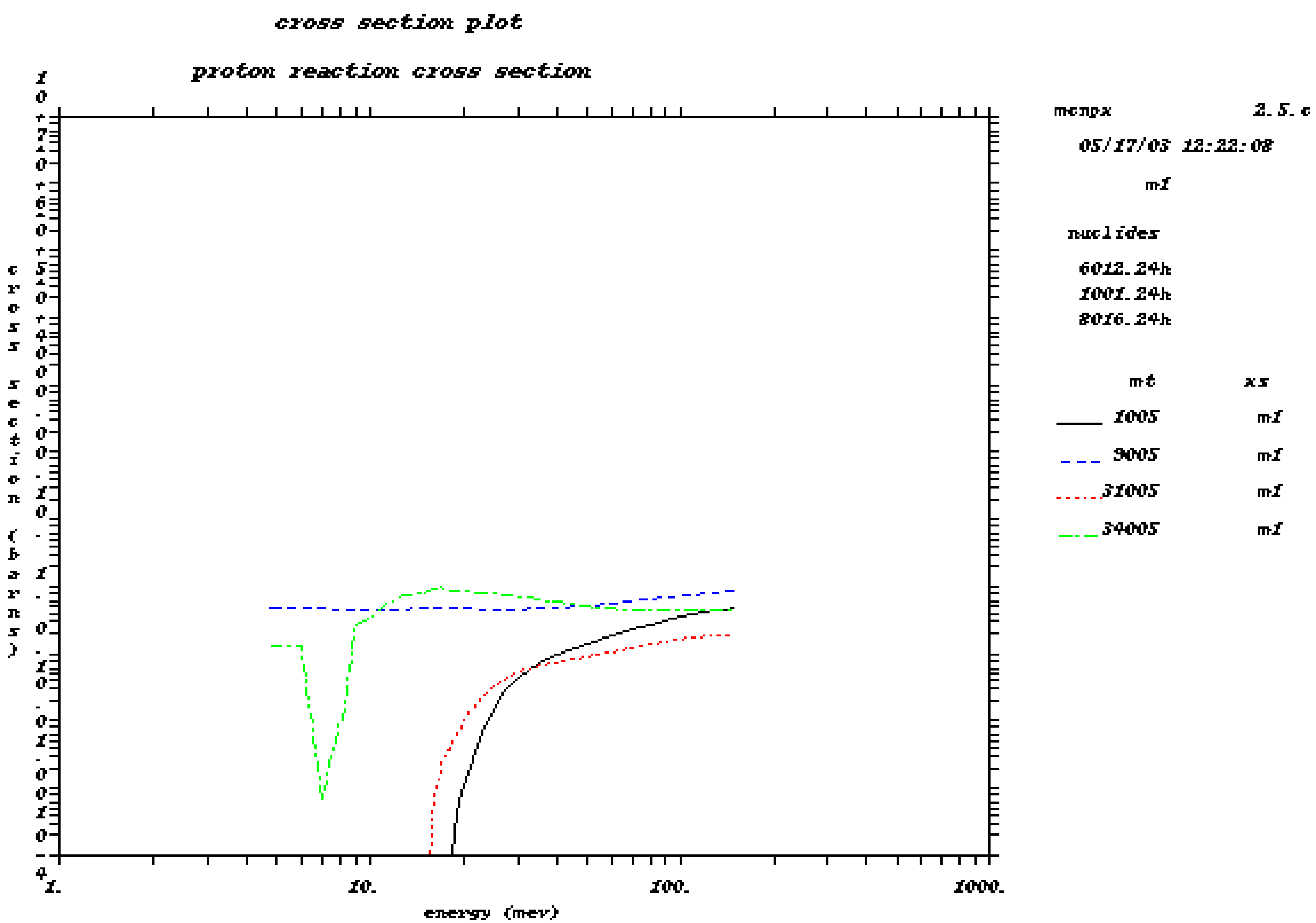
Exercise: Plot proton table data for inp = talmh*

* copy %inputs%\tally\talmh

for material 1, plot rxns 1, 2, 3, 5

MCNPX Workshops




cross section plot
proton reaction cross section
mcnpx 2.5.c
05/17/03 12:22:08
m1
nuclides
6012.24h
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cross section (barns)
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1.
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LA150 Neutron, Proton, Photonuclear Libraries

- Production cross sections for light particles
- Production cross sections for gammas
- Production cross sections for heavy recoil particles
- Energy-angle correlated spectra for secondary light particles (up to and including alphas)
- Energy spectra for gammas and heavy recoil nuclei

Isotopes in LA150 Libraries

Element	Neutrons	Protons	Photonuclear
Hydrogen	^{1}H, ^{2}H	^{1}H, ^{2}H	
Lithium		^{7}Li	
Beryllium	^{9}Be (100 MeV)		
Carbon	^{nat}C	^{12}C	^{12}C
Nitrogen	^{14}N	^{14}N	
Oxygen	^{16}O	^{16}O	^{16}O
Aluminum	^{27}Al	^{27}Al	^{27}Al
Silicon	^{28}Si, ^{29}Si, ^{30}Si	^{28}Si, ^{29}Si, ^{30}Si	^{28}Si
Phospho-rous	^{31}P	^{31}P	
Calcium	^{nat}Ca	^{40}Ca	^{40}Ca
Chromium	^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr	^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr	
Iron	^{54}Fe, ^{56}Fe, ^{57}Fe	^{54}Fe, ^{56}Fe, ^{57}Fe	^{56}Fe
Nickel	^{58}Ni,^{60}Ni,^{61}Ni,^{62}Ni,^{64}Ni	^{58}Ni,^{60}Ni,^{61}Ni,^{62}Ni,^{64}Ni	
Copper	^{63}Cu, ^{65}Cu	^{63}Cu, ^{65}Cu	^{63}Cu
Niobium	^{93}Nb	^{93}Nb	
Tantalum			^{181}Ta
Tungsten	^{182}W,^{183}W,^{184}W,^{186}W	^{182}W,^{183}W,^{184}W,^{186}W	^{184}W
Mercury	^{196}Hg, ^{198}Hg, ^{199}Hg, ^{200}Hg, ^{201}Hg, ^{202}Hg, ^{204}Hg	^{196}Hg, ^{198}Hg, ^{199}Hg, ^{200}Hg, ^{201}Hg, ^{202}Hg, ^{204}Hg	
Lead	^{206}Pb, ^{207}Pb, ^{208}Pb	^{206}Pb, ^{207}Pb, ^{208}Pb	^{206}Pb, ^{207} Pb, ^{208}Pb
Bismuth	^{209}Bi	^{209}Bi	

Getting the Data for MCNPX

From RSICC

- **MCNPX data distribution package is DLC-205.**
- **Contains the entire suite of currently-supported data libraries plus some documentation.**
- **CD-ROMs of DLC-205 are available from RSICC (pdc@ornl.gov, (865) 574-6176, or http://epicws.epm.ornl.gov/rsic.html).**

• DLC-165 JAERI (Japan)	JENDL-3	02/2000
• DLC-216 ENEA (Italy)	ENDF/B-VI Rel. 3	12/2003
• DLC-203 ENEA (Italy)	JEF22	11/2003
• DLC-205 LANL (MCNPX)	ENDF/B-VI rel. 2	09/2002
• CCC-710 LANL (MCNP5)	ENDF/B-VI rel. 6	11/2003
• DLC-211 UT (Texas)	High Temp.	04/2001
• DLC-183 IAEA (Austria)	FENDL-2.0	02/2000

Summary

MCNPX contains high-quality physics and has access to the most up-to-date cross-section data.

There are, however, approximations and assumptions that you should be aware of. It is important to know as much as possible about the cross-section libraries you are using and the physics models in the code, so that you can understand the strengths and weaknesses of the libraries and physics within the context of your application.

Questions: email to “nucldata@lanl.gov” (goes to Nuclear Data Team at LANL)