Monte Carlo Burnup Interactive Tutorial

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Overview

- Introduction
- A simple criticality calculation
- Depletion theory
- Setup sample burn cases
- Fixed passive source calculation
- Further considerations

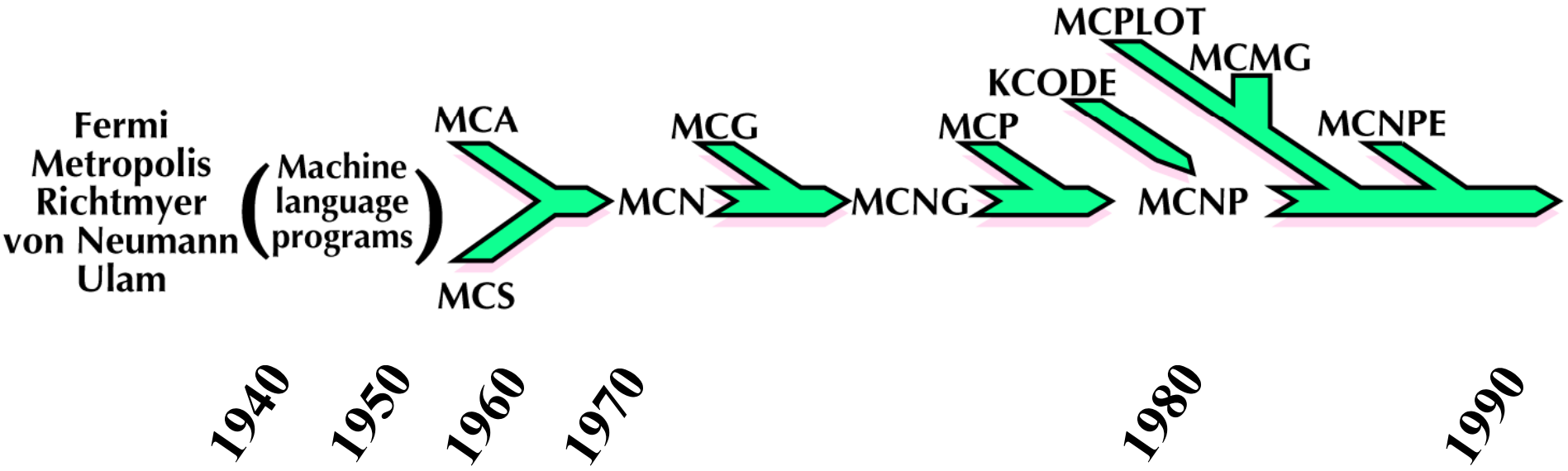
User Base

- **~2500 users world wide**
  - **Provide 6-8 workshops per year (4-6 US, ~2 international)**
  - **150 workshop participants per year**
  - **Access to RSICC/NEA released versions only**
    - http://www-rsicc.ornl.gov/ (C00730) 2.5.0
    - http://www.nea.fr/html/dbprog/ (CCC-0730) 2.5.0
  - **Limited access to MCNPX web site**
    - http://mcnpx.lanl.gov (some documentation)
- **~2000 registered Beta Testers**
  - **Full access to MCNPX web site**
  - **Access to intermediate versions**
  - **Increased user support**

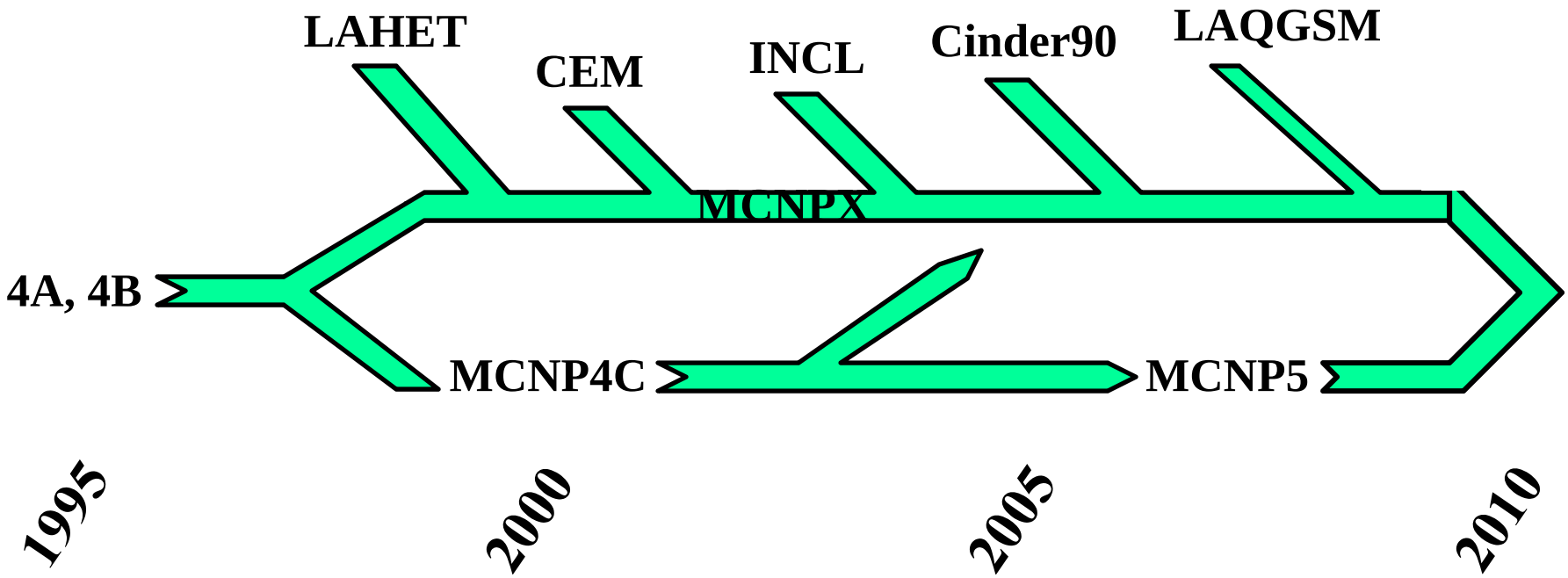
History of MCNPX

- Monte Carlo radiation transport code
  - Extends MCNP4C to virtually all particles and energies
  - 35 particles (n,p,e, 5 leptons, 11 baryons, 11 mesons, 5 ions)
  - Continuous energy (roughly 0-100 GeV)
  - Data libraries below ~ 150 MeV (n,p,e,h) & models otherwise
- General 3-D geometry
  - 1st & 2nd degree surfaces, tori, 10 macrobodies, lattices
- General sources and tallies
  - Interdependent source variables, 7 tally types, many modifiers
- Supported on virtually all computer platforms
  - Unix, Linux, Windows, OS X (parallel with MPI)

History of MCNPX



History of MCNPX



Set up to run MCNPX

- Right click on dos icon
  - Click properties
    - In the “Start In” box type the path of where you would like the prompt to start i.e. C:\MCNPX or C:\MCNPX\class
- Open dos window
  - Type **PATH**
    - Look to see if a path exists to the MCNPX.exe executable
    - If not, type SET PATH=%PATH%;C:\MCNPX\BIN
  - Type **DATAPATH**
    - Look to see if the variable datapath exists and points to the directory containing MCNPX/MCNP5 cross sections
    - If not, type SET datapath=C:\MCNPX\data

Changing XSDIR

- If you would like to use your own XSDIR you will need the updated atomic weight ratio data
  - Temporarily copy your XSDIR file to XSDIROLD
  - Rename your XSDIR to XSDIR1
  - Download the distributed XSDIR file and open it
  - Highlight all information from the top till you reach “directory” and copy it into XSDIR1
  - DELETE XSDIR
  - RENAME XSDIR1 to XSDIR

```
atomic weight ratios
 0001  1.000000    0001  1.000000
 1000  0.99931697   1001  0.99916732   1002  1.99679966   1003  2.99013994
 2000  3.96821760   2003  2.99012015   2004  3.96821894
 3000  6.88131188   3006  5.96344945   3007  6.95573316
 4000  8.93476310   4007  6.95665041   4009  8.93476310
...
...
 96000  244.878000   96241  238.986844   96242  239.979426   96243  240.973367
               96244  241.966128   96245  242.960254   96246  243.953380
               96247  244.947892   96248  245.941280
 97000  244.878000   97245  242.961116   97246  243.954817   97247  244.947844
               97248  245.942011   97249  246.935305
 98000  248.844000   98249  246.935173   98250  247.928122   98251  248.922684
               98252  249.916116
 99000  251.818000   99240  238.006611   99241  238.997765   99242  239.990202
               99243  240.981544   99244  241.974280   99245  242.966035
               99246  243.959078   99247  244.951167   99248  245.944369
               99249  246.936717   99250  247.930357   99251  248.923084
               99252  249.917457   99253  250.910696   99254  251.905276
               99255  252.898917   99256  253.893623   99257  254.887399
 100000  254.792000
03/10/2003
directory
```

Problem Execution

- mcnpx i=filename n=output_family options
- output_family:
  - OUTP, RUNTPE, MCTAL, …
  - or NAMEo, NAMEr, NAMEm , …
- Options:
  - opxrz
  - p = geometry plot
  - ixz = cross section plot
  - z = tally plot
  - ixr = run

Input File

Title Card
Cell cards
    cell# mat den --- surfaces --- data
Blank
Surface cards
    sur# type --- parameters ---
Blank
Data cards
    everything else (source, tally, physics, variance, …)
Blank

Input File Formatting

- Comments
  - C_ in column 1
  - $ starts (*after input stuff)*
- Capitalization irrelevant
- 80-column limit
- Continuation
  - 1st 5 columns blank
  - or, following card with &

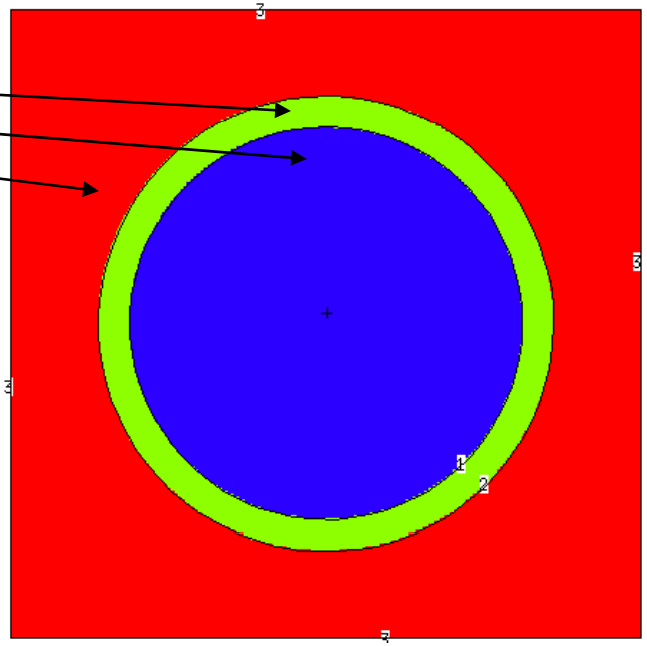
Ex1 Input File

Open by typing: notepad Ex1

```
Infinitely Reflected PWR Fuel Pin
C  Cell Cards
1  1  6.87812e-2    -1  imp:n=1 vol=192.29 $ Fuel
3  2  4.5854e-2    1 -2 imp:n=1 vol=66.53 $ Clad
4  3  7.1594e-2    2 -3 imp:n=1 vol=374.27 $ Water
5  0               3    imp:n=0 $ Outside Universe

C  Surface Cards
C Fuel Pin
1 RCC 0 0 0 0 0 365.0 0.4095
C Cladding
2 RCC 0 0 -0.0655 0 0 365.131 0.4750
C Water Box
*3 BOX -0.65665 -0.65665 -0.1 1.3133 0 0 0 1.3133 0 0 0
367.0

C KCODE Cards
C  Material Cards
m1
      8016.60c   4.5854e-2
      92235.60c  1.4456e-4
      92238.60c  1.9939e-2
      94238.60c  1.1467e-4
      94239.60c  1.0285e-3
      94240.60c  7.9657e-4
      94241.60c  3.3997e-4
      94242.60c  5.6388e-4       $ Fuel Material
m2    40000.60c -1.0             $ Clad Material
m3     1001.60c  4.7716e-2
       8016.60c  2.3858e-2
       5010.60c  3.6346e-6
       5011.60c  1.6226e-5       $ Water Material
mt3 lwtr.01t                     $ S(alpha,beta) treatment
print
```



KCODE (Source) Card

KCODE A B C D E F G

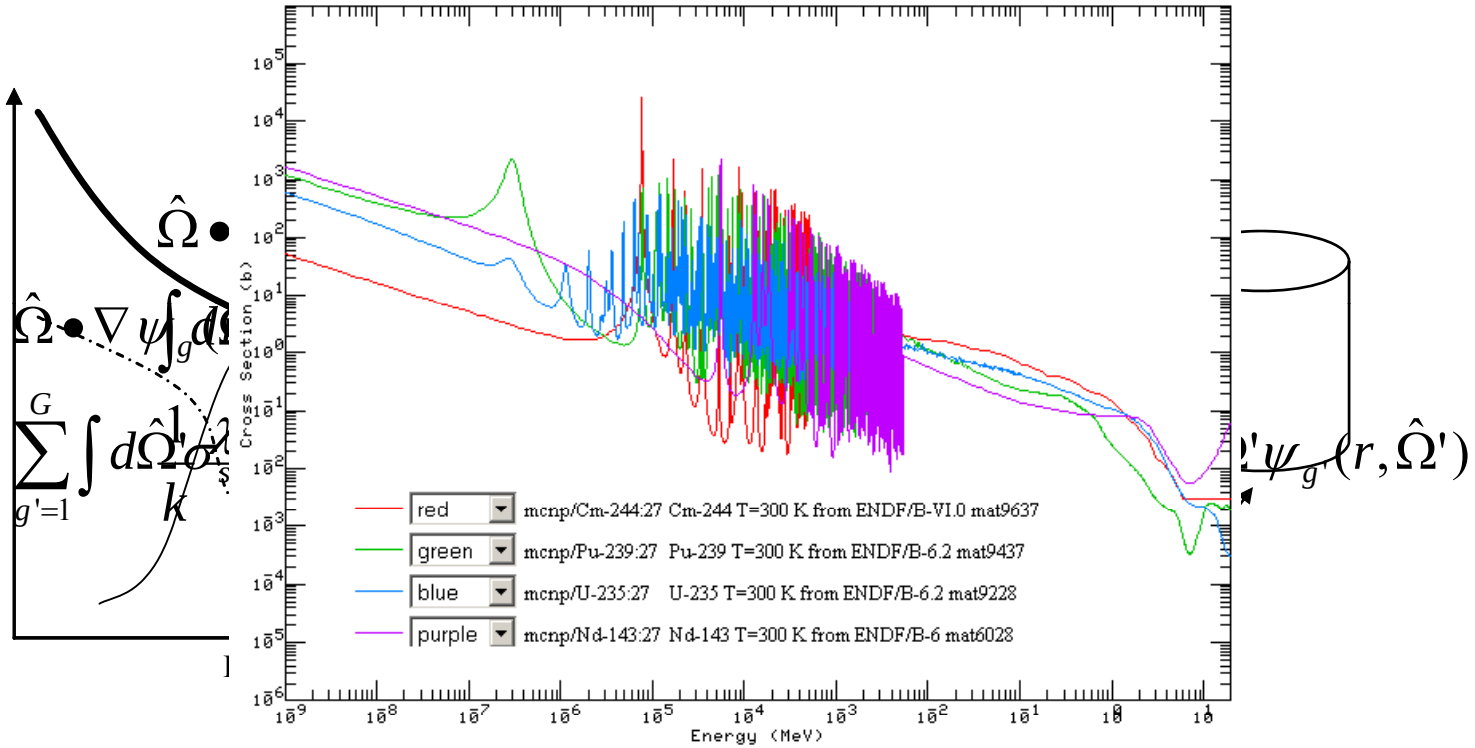
- **A = Source size per cycle** — **1000**
- **B = initial guess for k_{eff}** — **1.0**
- **C = # settle cycles** — **15**
- **D = total cycles to run** — **50**
- **E = storage for new source points (use default)**
- **F = tally normalization method (use default)**
  - ***0 = by weight (default)*** ***1 = by number of particles***
- **G = storage for plotting k_{eff} values (use default)**

KSRC $x_1\ y_1\ z_1\ \ x_2\ y_2\ z_2\ \ldots$ **or,**

Run KCODE Calculation

- Rename Ex1 to Ex1a
- Add KCODE card
  - 1000 particles per cycle
  - k_{eff} =1 for the initial guess
  - 15 settle cycles
  - 50 total cycles
- Add KSRC card
  - Place a KSRC in the middle of the fuel pin
- Run the case → mcnpx i=ex1a n=ex1a.

Deterministic Method



$$\sigma(r)_g = \frac{\int \sigma(r,E)\psi(r,\Omega,E)dE}{\int \psi(r,\Omega,E)dE}$$

The Monte Carlo Method

- The Monte Carlo method uses probability theory to model a system stochastically
  - Random sampling of events

$e^{-\Sigma_t x}dx =$ Probability that a neutron moves a distance dx without any interaction

$\Sigma_t e^{-\Sigma_t x}dx =$ Probability that a neutron has its first interaction in dx = p(x)dx

- Probability density function (PDF)→ A real-valued function whose integral over any set gives the probability that a random variable has values in the set

$$PDF = f(x) \rightarrow \Sigma_t e^{-\Sigma_t(E)x}dx = p(x)dx \rightarrow \int_a^b f(x)dx = P(a \le x \le b)$$

- Cumulative distribution function (CDF) →The probability that the variable takes a value less than or equal to x'

$$CDF = \int_0^{x'} p(x)dx = 1 - e^{-\Sigma_t(E)x} = \xi \rightarrow x = -\frac{\ln(1-\xi)}{\Sigma_t(E)} \Rightarrow -\frac{\ln(\xi)}{\Sigma_t(E)} \Rightarrow -\frac{\ln(\xi)}{\sum_i N_i \sigma_{i,t}(E)}$$

What is Depletion Analysis?

- During reactor operation the isotopic concentration of the reactor material (fuel/coolant/clad/shielding) will change as isotopes consume neutrons and undergo various nuclear reactions
  - (n,f), (n,alpha), (n,beta), (n,p), etc.

- Changes in the isotopic concentration over time will result in changes in reactor parameters
  - Flux/ Core Reactivity/ Power Distribution/ SDM/ Poison Concentration
  - These reactor parameters limit reactor operation characteristics therefore it is necessary to accurately calculate these values at many time steps

- The study of the interaction of these reactor parameters with the time-dependant production/depletion of nuclei is know as depletion analysis (J. J. Duderstadt and L. J. Hamilton, *Nuclear Reactor Analysis*, (1976).)

Depletion Equation

$$\frac{dN_m(r,t)}{dt} = -N_m(r,t)\beta_m + \overline{Y}_m + \sum_{k \neq m} N_k(r,t)\gamma_{k \to m}$$

$$\beta_m = \lambda_m + \sum_j \int \sigma_{m,j}(E)\Phi(r,E,t)dE$$

$$\gamma_{k \to m} = \sum_{m \neq k} L_{km}\lambda_k + \sum_{m \neq k}\sum_j \int Y_{km,j}(E)\sigma_{k,j}(E)\Phi(r,E,t)dE$$

Matrix Exponential Method

- Formulas for solving normal systems of equations are identical to solving first order differential equations with constant coefficients
  - Large amount of memory required to store the matrix of coefficients
    - User must choose an acceptable subset of nuclides to follow exactly
  - Very large and very small eigenvalues depending upon the half-lives
    - Short half-life isotopes must be decayed analytically
      - Relative to time step size
  - Numerical precision depends upon the size of time step

$$\frac{d}{dt} n_m(r,t) = \sum_k B_{mk}(r,t) n_k(r,t) \qquad B_{mk}(r,t) = \begin{cases} L_{km}\lambda_k + \sum_r Y_{km,r}\sigma_{k,r}\Phi(r,t) & m \neq k \\ -\lambda_m - \sum_r \sigma_{m,r}\Phi(r,t) & m = k \end{cases}$$

$$N(t) = N(t_0)\exp(Bt) \qquad \exp(Bt) = \sum_{m=0}^{\infty} \frac{(Bt)^m}{m!}$$

CINDER90 Method

- The set of coupled differential equations is reduced to a set of linear differential equations
  - Markov Chains (Andrei Markov) → given the present state, future states are independent of the past states
  - Linear chains are created for each isotope transmutation path

$$\frac{d\mathrm{N}_i}{dt} = \bar{Y}_i + \mathrm{N}_{i-1}(t)\gamma_{i-1} - \mathrm{N}_i(t)\beta_i$$

  - The solutions of each linear chain determines a partial nuclide density

$$\mathrm{N}_n(t) = \sum_{m=1}^{n}\prod_{k=m}^{n-1}\gamma_k\left\{\bar{Y}_m\left[\frac{1}{\prod_{l=m}^{n}\beta_l} - \sum_{j=m}^{n}\frac{e^{-\beta_{jt}}}{\prod_{i=m,\neq j}^{n}\left(\beta_i-\beta_j\right)}\right] + \mathrm{N}_m^0\sum_{j=m}^{n}\frac{e^{-\beta_{jt}}}{\prod_{i=m,\neq j}^{n}\left(\beta_i-\beta_j\right)}\right\}$$

CINDER90 Method

– Partial nuclide densities are then summed to determine the total nuclide density

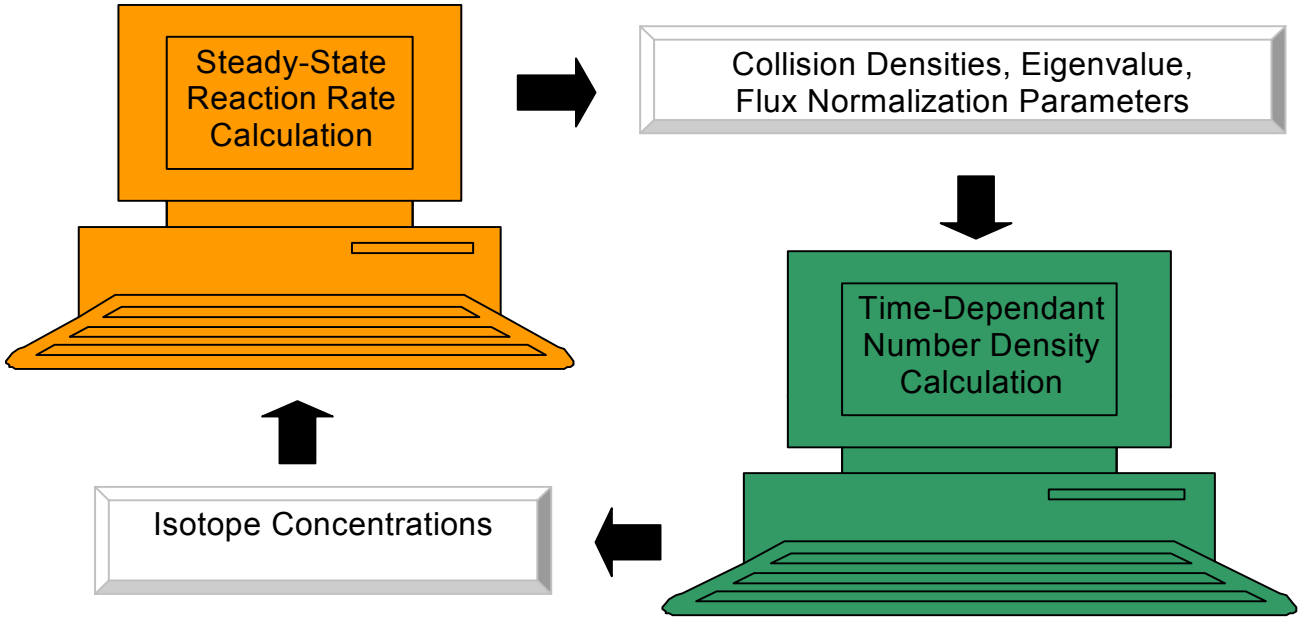
$$N_m = \sum_{j=1}^{M} \mathrm{N}_{i,j}$$

– Each path for each nuclide defined by available data is followed until tests of significance are failed

$$P_m(t) = \int_0^t N_m(t')\beta_m dt'$$

– 3400 Isotopes, 1325 Fission Products, Yield sets for over 30 actinides
  - ORIGEN2 1700 isotopes, 850 Fission Products, 8 yields
  - ORIGEN-S 1946 isotopes, 1119 Fission Products, 30 yield sets

Necessity for Linked Approach



- Reaction rates are spatially dependent
- Spectrum changes evolve due to buildup/depletion of highly absorbing isotope
- Since it is assumed that considerable changes in the isotope concentration are required in order to significantly alter the neutron energy spectrum, the depletion equation may be considered separable in time and space
- Steady-state reaction rate calculator linked to temporal nuclide inventory calculator

Simple Interface

BURN TIME=T1,T2,T3,...
PFRAC=F1,F2,F3,...
POWER=P
MAT=±M1,±M2,±M3,...
OMIT=J1,N1,I11,I12,...,
J2,N2,I21,I22,...
AFMIN=A1 A2
BOPT=B1, B2, B3
MATMOD=
MATVOL= V1, V2, V3

```
...
C  Control Cards
vol   192.287
kcode  5000 1.0 5 300
ksrc  0.65665 0.65665 150.0
BURN TIME=0.645,40,100,140,200,250
     MAT=1
     POWER=0.066956
     PFRAC=1.0,1.0,1.0,1.0,1.0,1.0
     OMIT=1,8,6014,7016,8018,9018,90234,91232,95240,95244
     BOPT=1.0, -14
C  Material Cards
m1
      8016.60c   4.5854e-2
      92235.60c  1.4456e-4
      92238.60c  1.9939e-2
      94238.60c  1.1467e-4
      94239.60c  1.0285e-3
      94240.60c  7.9657e-4
      94241.60c  3.3997e-4
      94242.60c  5.6388e-4
...
```

Total Depletion Input

Isotope Tracking

- CINDER90 contains transmutation path data for 3400 isotopes
- The current ENDF/B VII library only contains actual transport cross sections for 390 isotopes
- To save computation time and reduce the influx of memory-prohibitive information, MCNPX only tracks those isotopes accounted for from the following processes:
  - Listing the isotope on a material card
  - Selecting an isotope from a preset fission product tier
  - Producing the isotope from the Isotope Generator Algorithm
- CINDER90 still tracks transmutation path data for the other isotopes not containing ENDF transport data

Fission Product Tiers

- Certain Monte Carlo linked depletion codes force the user to input every fission product to be tracked during the depletion process
- MCNPX offers the user preset fission product “tier”s
- Eliminates the task of inputting every fission product to be tracked
- MCNPX offers three fission product tiers
  - Tier 1. (default) Zr-93, Mo-95, Tc-99, Ru-101, Xe-131, Cs-133, Cs-137, Ba-138, Pr-141, Nd-143, Nd-145
  - Tier 2. Isotopes contained in the fission product array that are included in the current cross section library file (XSDIR) for MCNPX version 2.6.0
  - Tier 3. All isotopes contained in the fission product array

BURN CARD

BURN TIME=T1,T2,T3,...
PFRAC=F1,F2,F3,...
POWER=P
MAT=M1,M2,M3,...
OMIT=J1,N1,I11,I12,...,J2,N2,I21,I22,...
AFMIN=A1 A2
BOPT=B1,B2,B3

Ti = Duration of burn step i (days). Default is one time step of one day.
Fi = Fraction of POWER. Default is 100% POWER (1.0)
P = Power level (MW). Default is 1.0 MW.
Mi = List of material numbers to include in the burn. If the BURN card is utilized then a burn material MUST be specified.
Ji = ith material for which to omit nuclides Ii1, Ii2, etc.
Ni = Number of omitted nuclides listed for the ith material.
Ii1, Ii2, ... = 1st, 2nd, etc. omitted nuclide for the ith material.

Practice

```
BURN  TIME=T1,T2,T3,...
      PFRAC=F1,F2,F3,...
      POWER=P
      MAT=M1,M2,M3,...
      OMIT=J1,N1,I11,I12,...,J2,N2,I21,I22,...
      AFMIN=A1 A2
      BOPT=B1,B2,B3
```

- **Burn material 1**
- **At 1 MW**
- **For 100 days and then 30 more days**
- **Burn at 30% power for the last 30 days**
- **And omit 92235 and 92238 from material 1**

Practice

```
BURN  TIME= 100,30
      PFRAC=1.0,0.3
      POWER=1
      MAT=1
      OMIT=1,2,92235,92238
```

BURN CARD cont.

A1 = atom fraction minimum below which the atom fraction is set to zero. Default is 1.0e-10.

A2 = decay chain convergence criteria. Default 1e-10.

B1 = Q value multiplier. Default is 1.0.

B2 = +/-mn

m = 0/1/2 = fission product tiers 1/2/3

n = 1/2/3/4 = print output by decreasing mass/decreasing activity/decreasing specific activity/increasing ZAID

If mn "+" only print output at the end of the entire run

If mn "-" print output at the end each kcode run

Example: B2 = 14 tier 2, print by increasing zaid printing output only at the end of the entire run

B3 = Models option

-1 Fatal error if models are used in the problem (DEFAULT)

1 Runs with models

Practice

```
BURN  TIME=T1,T2,T3,...
      PFRAC=F1,F2,F3,...
      POWER=P
      MAT=M1,M2,M3,...
      OMIT=J1,N1,I11,I12,...,J2,N2,I21,I22,...
      AFMIN=A
      BOPT=B1,B2,B3
```

- **Burn Material 1 At 1 MW**
- **For 100 Days and then 30 more days**
- **Burn at 30% power for the last 30 days**
- **Q value multiplier 1.1**
- **Fission Product tier 2 ordering by zaid**
- **Print output only at the end of the run**
- **Using Cross section models**

Practice

```
BURN  TIME= 100,30
      PFRAC=1.0,0.3
      POWER=1
      MAT=1
      BOPT=1.1 14 1.0
```

Stipulations for Each Burn Case

- For each case
  - Power level of 70 kW
  - 2 time steps (time durations 50, 500 days)
  - Q value multiplier = 1.0
  - AFMIN =1e-10 1e-4
  - Run all cases using only 100 particles per cycle
  - Place BURN card below KCODE cards and above material card

```
KCODE 100  1.0  15  50
KSRC   0 0 182.5
BURN   TIME= 50 500
       MAT=
       POWER= 0.07
       PFRAC=1.0 1.0
       AFMIN= 1e-10 1e-4
       BOPT= 1.0 B2 B3
```

Cross Section Models

- The following examples address the options available for identifying, and eliminating isotopes that do not posses continuous energy cross section data for steady state transport

- Example 2A
  - Rename this case ex2a.
  - Burn only the fuel region (m1)
  - Use fission product Tier 1
  - Ordering the output by zaid
  - Retrieving burnup output only at the end of the of run
  - Using the **DEFAULT** cross section option

Example 2A

```
E:\MCNPX\Documentation\conferences\ICRS\answers>mcnpx i=ex2a n=ex2a.
 mcnpx    ver=2.6.0 ld=Mon Apr 07 08:00:00 MST 2008   04/10/08
     14:02:47

 ************************************************************
 *                                                          *
 *                     MCNPX                                *
 *                                                          *
 * Copyright 2007. Los Alamos National Security, LLC.       *
 * All rights reserved.                                     *
 *                                                          *
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 *                                                          *
...

...
 total fission nubar data are being used.

 fatal error.  table data required for kcode, zaid =  6014.  c
 fatal error.  table data required for kcode, zaid =  7016.  c
 fatal error.  table data required for kcode, zaid =  8018.  c
 fatal error.  table data required for kcode, zaid =  9018.  c
 fatal error.  table data required for kcode, zaid = 90234.  c
 fatal error.  table data required for kcode, zaid = 91232.  c
 fatal error.  table data required for kcode, zaid = 95240.  c
 fatal error.  table data required for kcode, zaid = 95244.  c
```

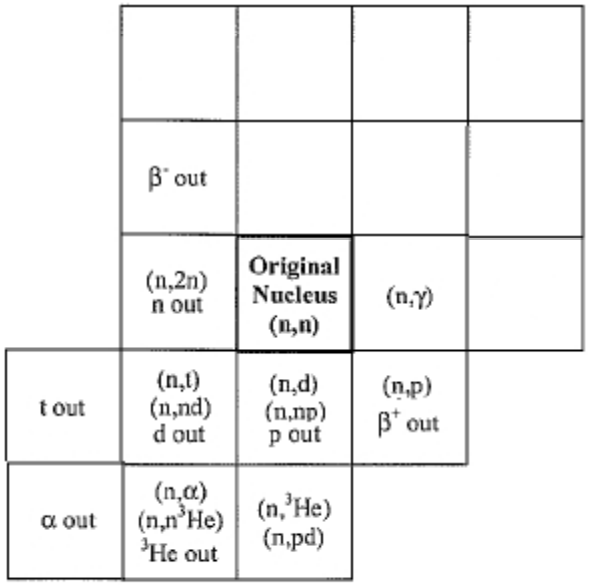
Two options for successful execution

- Run with Cross Section Models
  - B3 = 1
  - Cross section models were qualified for >200 MeV particles
- Use OMIT card
  - MCNPX no longer recalculates spatial reaction rates for isotopes on OMIT card
  - For the omitted isotopes, a 63-group flux from MCNPX is matched to a 63 group cross section set in CINDER90 to create an energy integrated reaction rate

Decay Chain Tracking

- MCNPX utilizes the Isotope Generator Algorithm to determine all the immediate daughter isotopes created from a burn material reaction, and tracks those isotopes during the transport process

- CINDER90 still tracks isotope concentrations for 3400 isotopes
  - Only those isotopes utilized in the steady state transport calculation contain isotope abundance data in the output file



n = neutron
p = proton
d = deuteron
t = triton
α = alpha particle
β⁻ = beta minus (negative electron)
β⁺ = beta plus (positron)
ε = electron capture

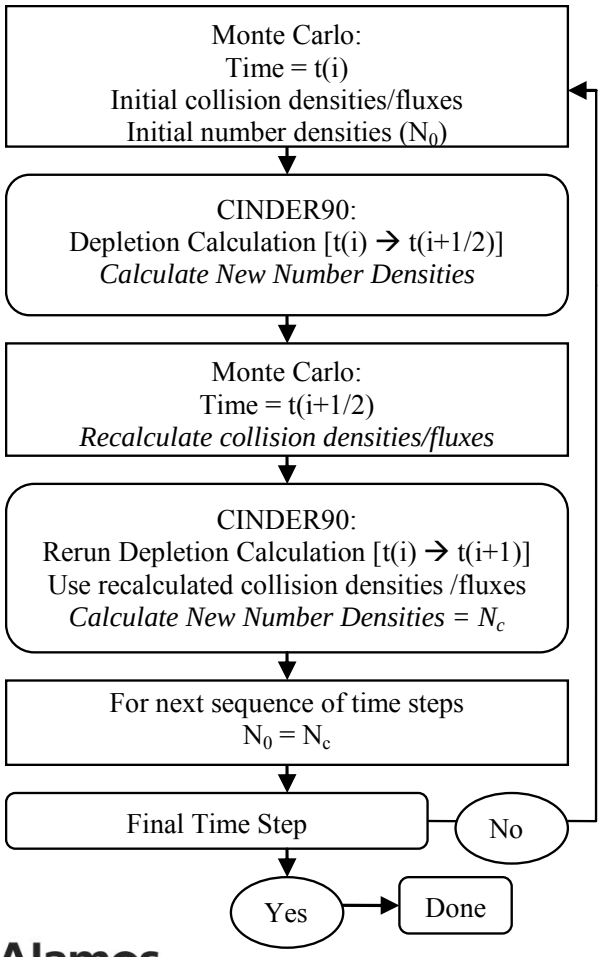
Cross Section Models

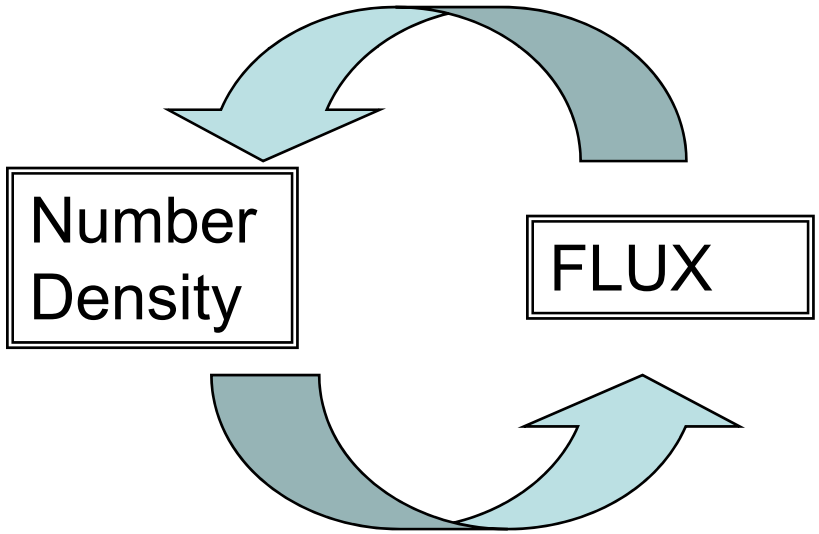
- Example 2C
  - Burn only the fuel region
  - Use fission product Tier 1
  - Ordering the output by zaid
  - Retrieving burnup output only at the end of the of run
  - **OMMITING from the calculation those isotopes that do not contain transport cross sections**

Example 2C

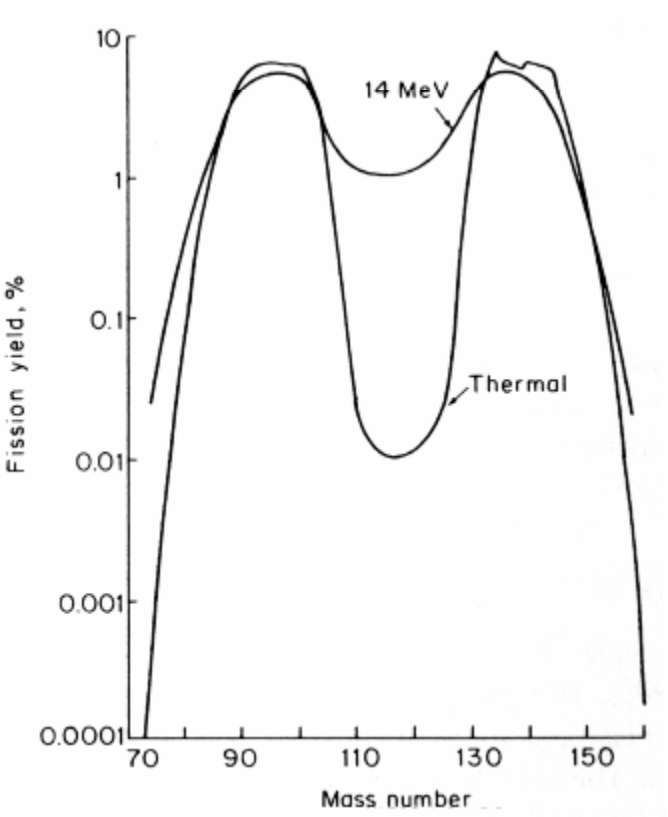
```
BURN TIME=50 500
     MAT=1
     POWER= 0.07
     PFRAC=1.0 1.0
     AFMIN= 1e-10 1e-4
     OMIT=1,8,6014,7016,8018,9018,90234,91232,95240,95244
     BOPT=1.0 4
```

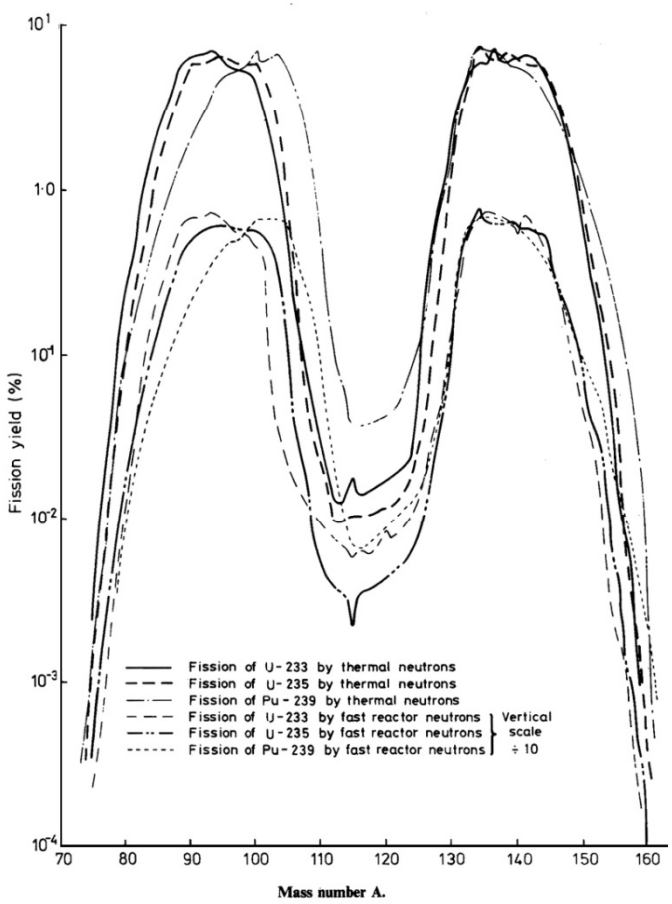
Cross Section Averaging





Fission Product Yields





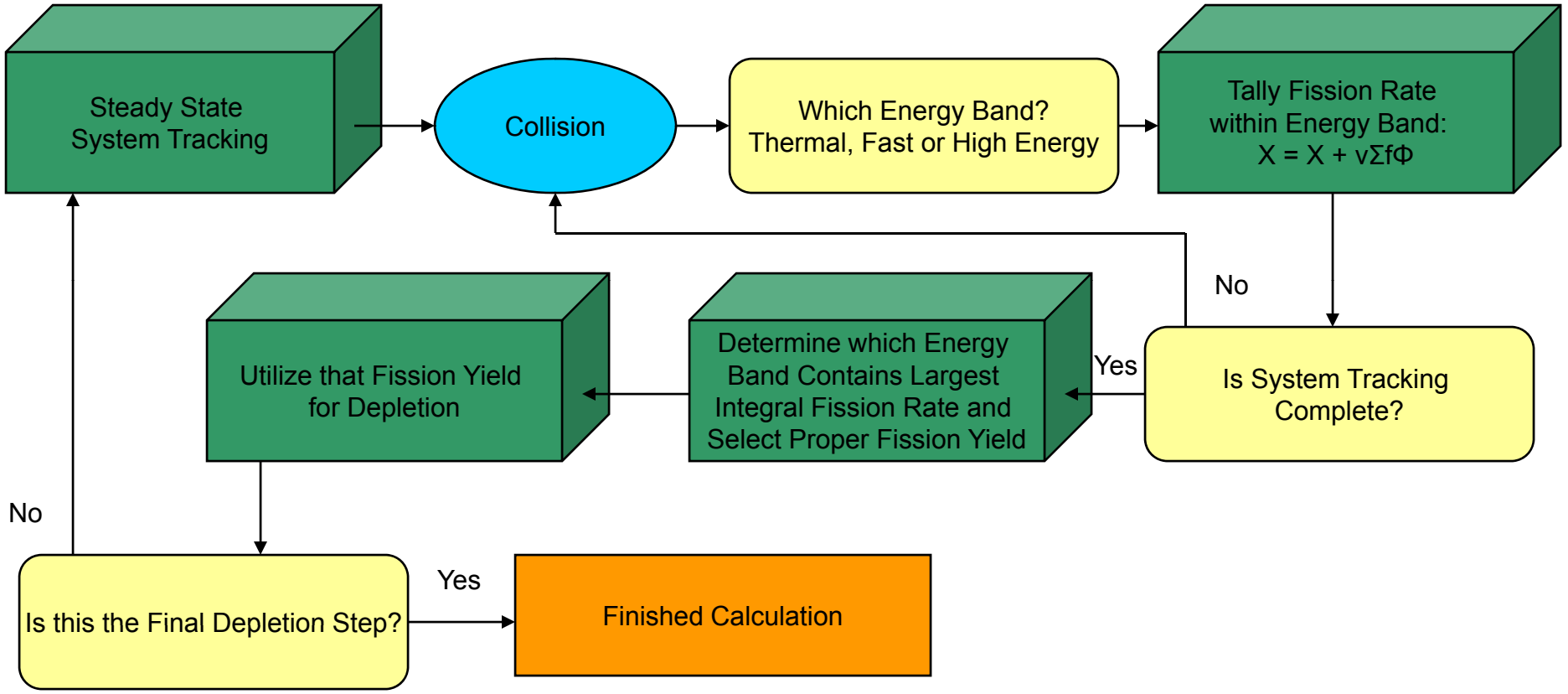
Yield Data Available

Element	Z	A	Thermal	Fast	HE	SF
Th	90	227	x			
Th	90	229	x			
Th	90	232		x	x	
Pa	91	231		x		
U	92	232	x			
U	92	233	x	x	x	
U	92	234		x	x	
U	92	235	x	x	x	
U	92	236		x	x	
U	92	237		x		
U	92	238		x	x	x
Np	93	237	x	x	x	
Np	93	238		x		
Pu	94	238		x		
Pu	94	239	x	x	x	
Pu	94	240	x	x	x	
Pu	94	241	x	x		
Pu	94	242	x	x	x	

Element	Z	A	Thermal	Fast	HE	SF
Am	95	241	x	x	x	
Am	95	242m	x			
Am	95	243		x		
Cm	96	242		x		
Cm	96	243	x	x		
Cm	96	244		x		x
Cm	96	245	x			
Cm	96	246		x		x
Cm	96	248		x		x
Cf	98	249	x			
Cf	98	250				x
Cf	98	251	x			
Cf	98	252				x
Es	99	253				x
Es	99	254	x			
Fm	100	254				x
Fm	100	255	x			
Fm	100	256				x

- Transmutation chain data for 3400 isotopes
- Fission Yield Data for 1325 isotopes
  - Thermal: 18 isotopes, Fast: 22 isotopes, HE: 11 isotopes, S.F.: 9 isotopes

Automatic Fission Yield Selection



- Automating the fission yield selection process eliminate computational cost associated with preliminary neutron spectrum calculation

FPs, Outputs, and Pfrac

- The following examples address the effect of implementing different fission product tiers on criticality as well as the available options for ordering output and adjusting output frequency

- Example 3
  - Copy ex2C and rename to ex3
  - Use fission product tier 2
  - Order output by mass
  - Burn at 80% power for the final step
  - Alter output frequency so that burnup output is printed after each kcode run

Example 3

BURN TIME=50 500

MAT=1

POWER= 0.07

PFRAC=1.0 0.8

AFMIN= 1e-10 1e-4

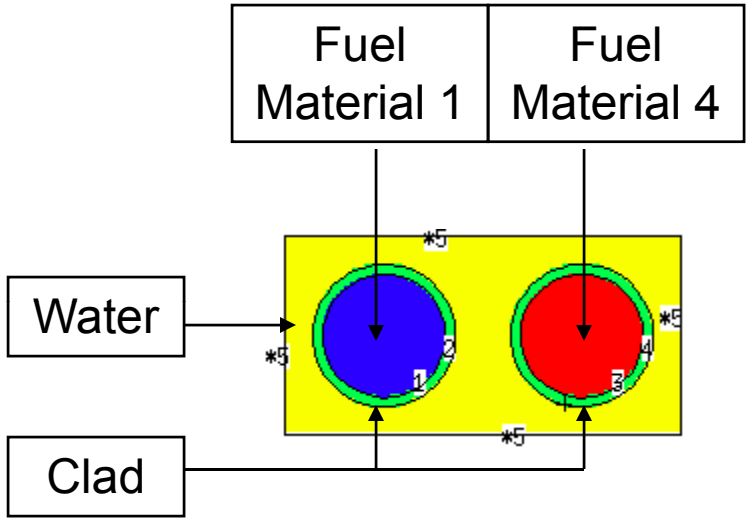
OMIT=1,9,6014,7016,8018,9018, 90234,91232,95240,95244

BOPT=1.0 -11

- How does the end of cycle k_{eff} of this case compare with Example 2C? Why?

Multiple Material Burning

- The following example addresses the multiple material burning capabilities
- Example 4
  - Open ex4 rename ex4a
  - Burn materials 1 and 4
  - Type in needed BURN card input




```
Infinitely Reflected PWR Fuel Pin
C  Cell Cards
1   1   6.87812e-2     -1   imp:n=1 vol=192.29 $ Fuel
3   2   4.5854e-2     1 -2 imp:n=1 vol=66.53  $ Clad
4   4   6.87812e-2     -3   imp:n=1 vol=192.29 $ Fuel
5   2   4.5854e-2     3 -4 imp:n=1 vol=66.53  $ Clad
6   3   7.1594e-2 2 4 -5 vol=748.34 imp:n=1 $ water box
7   0   5 imp:n=0 $ Outside Universe
```

Second entry on cell the card corresponds to material number

Example 4a

```
BURN TIME=50 500
     MAT=1,4
     POWER= 0.07
     PFRAC=1.0 1.0
     AFMIN=1e-10 1e-4
     OMIT=1,8,6014,7016,8018,9018, 90234,91232,95240,95244
          4,8,6014,7016,8018,9018, 90234,91232,95240,95244
     BOPT=1.0 4
```

SAVE THE OUTPUT OF THIS CASE FOR LATER USE!!!!

Multi Material Burnup

Individual Material Burnup

Material #: 1

step	duration (days)	time (days)	power fraction	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	4.956E-01	0.000E+00
1	5.000E+01	5.000E+01	4.967E-01	9.945E-01
2	5.000E+02	5.500E+02	5.038E-01	1.096E+01

Material #: 4

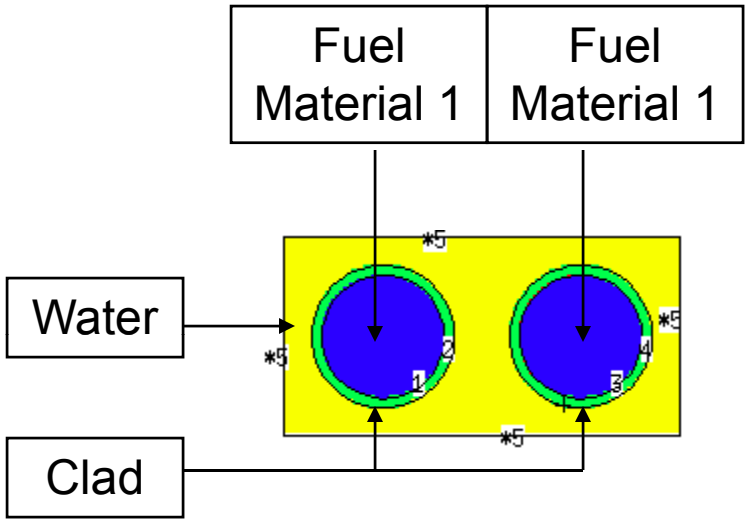
step	duration (days)	time (days)	power fraction	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	5.044E-01	0.000E+00
1	5.000E+01	5.000E+01	5.033E-01	1.012E+00
2	5.000E+02	5.500E+02	4.962E-01	1.111E+01

$$Burnup_i = Burnup_{i,previous\ step} + \frac{Power\ Level * \%\ Full\ Power * Time * Power\ Fraction}{MTHM_i}$$

$$Power\ Fraction = \frac{(volume)_j (atom\ density)_j \sum_i (\%\ isotope)_{i,j} \sigma_{f,i,j} Q_{i,j}}{\sum_j (volume)_j (atom\ density)_j \sum_i (\%\ isotope)_{i,j} \sigma_{f,i,j} Q_{i,j}}$$

Multiple Material Burning

- Example 4b
  - Rename ex4a to ex4b
  - Set both fuel cells as material 1
  - Burn material 1 only
    - Material 1 is located in cells 1 and 3




```
Infinitely Reflected PWR Fuel Pin
C  Cell Cards
1   1  6.87812e-2    -1  imp:n=1 vol=192.29 $ Fuel
3   2  4.5854e-2    1 -2 imp:n=1 vol=66.53  $ Clad
4   1  6.87812e-2    -3  imp:n=1 vol=192.29 $ Fuel
5   2  4.5854e-2    3 -4 imp:n=1 vol=66.53  $ Clad
6   3  7.1594e-2 2 4 -5 vol=748.34 imp:n=1 $ water box
7   0  5 imp:n=0 $ Outside Universe
```

Second entry on cell the card corresponds to material number

Example 4B

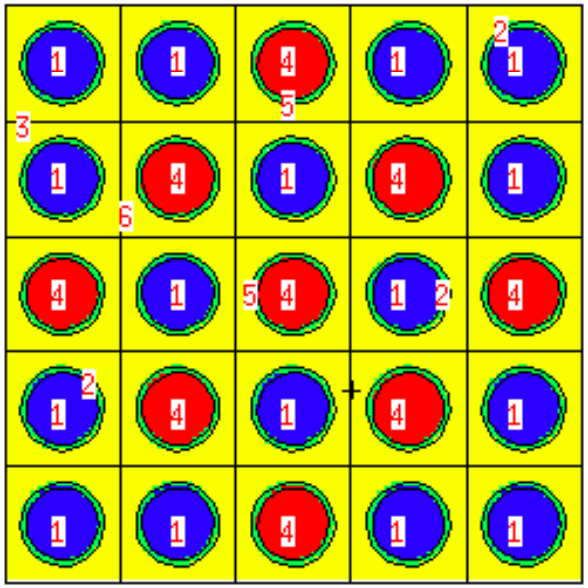
```
BURN TIME=50 500
     MAT=1
     POWER= 0.07
     PFRAC=1.0 1.0
     AFMIN=1e-10 1e-4
     OMIT=1,8,6014,7016,8018,9018, 90234,91232,95240,95244
     BOPT=1.0 4
```

- Are the results different from between the two runs? Why or why not?

Lattices

```
Infinitely Reflected PWR Fuel Pin
C  Cell Cards
1  1  6.87812e-2  -1   imp:n=1 vol=192.29 u=1 $ Fuel
2  2  4.5854e-2   1 -2 imp:n=1 vol=66.53  u=1 $ Clad
3  3  7.1594e-2   2    imp:n=1 vol=374.17 u=1 $ water box
4  4  6.87812e-2 -1    imp:n=1 vol=192.29 u=2 $ Fuel
5  2  4.5854e-2   1 -2 imp:n=1 vol=66.53  u=2 $ Clad
6  3  7.1594e-2   2    imp:n=1 vol=374.17 u=2 $ water box
7  0  -5 imp:n=1 lat=1  u=3 fill=0:4 0:4 0:0
                            1 1 2 1 1
                            1 2 1 2 1
                            2 1 2 1 2
                            1 2 1 2 1
                            1 1 2 1 1
8  0  -6 fill=3 imp:n=1 $ Lattice Bounds
9  0   6 imp:n=0        $ Outside Universe

C  Surface Cards
C Fuel Pin
1 RCC 0 0 0 0 0 365.0 0.4095
C Cladding
2 RCC 0 0 -0.0655 0 0 365.131 0.4750
C Water Box
5 BOX -0.65665 -0.65665 -0.1 1.3133 0 0 0 1.3133 0 0 0 367.0
*6 BOX -0.657 -0.657 -0.11 6.57 0 0 0 6.57 0 0 0 367.1
...
```



Repeated Structures Modeling

- Energy integrated reaction rates and normalization constants are tallied within each separate burn material using the track length estimator

$$\phi = \frac{1}{N}\sum_{n}\left(\frac{(l_n * w_n)}{V}\right)$$

- Due to limitations in the repeated structures mapping algorithm in MCNPX, the code cannot always determine the total volume of a plethora of repeated cells
  - Excessive time is also wasted trying to query and calculate the total volume

$$\phi = \frac{1}{NV}\sum_{n}(l_n * w_n)$$

MATVOL Keyword

MATVOL=V1,V2,V3,V4

- If a cell is used once a vol keyword is not needed on the BURN card
- Vi = Total volume of all cells containing material Mi.
- A Vi entry must be stated for each corresponding Mi entry or the user receives a fatal error
- If a VOL keyword is not stated, the code will try to determine total volume of burn cells employing each specific burn material
  - However the code will determine this incorrectly if the user is implementing repeated structures

Multiple Material Burning

- Example 4d
  - Open ex4c rename to ex4d
  - Burn material 1 and 4 in each lattice element
    - Material 1 is listed 16 times
    - Material 2 is listed 9 times
  - Use a MATVOL keyword to specify the total volume of all pins

Example 4d

```
BURN TIME=50 500
     MAT=1,4
     POWER= 0.07
     PFRAC=1.0 1.0
     AFMIN= 1e-10 1e-4
     OMIT=1,8,6014,7016,8018,9018,90234,91232,95240,95244
          4,8,6014,7016,8018,9018,90234,91232,95240,95244
     BOPT=1.0 4
     MATVOL=3076.6 1730.6
```

Manual Time-Dependent Concentration Changes

- To model real life systems, isotopes may have to be added or extracted in order to meet the conditions of the operating strategies
  - Boron dilution in PWR
  - Fission product extraction in molten salt or gaseous fuel reactor

- MCNPX depletion is capable of manually changing the concentration of a nuclide at any time step
  - Atom density
  - Weight density
  - Atom fraction
  - Weight fraction

MATMOD

MATMOD= $$NT,_1TS,_1NM,_1MT_1,_1K_1,_1Z_1^1,_1C_1^1,_1Z_1^2,_1C_1^2,\ldots,_1Z_1^{K_1},_1C_1^{K_1},$$
$$\ldots,_1MT_n,_1K_n,_1Z_n^1,_1C_n^1,_1Z_n^2,_1C_n^2,\ldots,_1Z_n^{K_n},_1C_n^{K_n},$$
$$_jTS,_jNM,_jMT_1,_jK_1,_jZ_1^1,_jC_1^1,_jZ_1^2,_jC_1^2,\ldots,_jZ_1^{K_1},_jC_1^{K_1},$$
$$\ldots,_jMT_n,_jK_n,_jZ_n^1,_jC_n^1,_jZ_n^2,_jC_n^2,\ldots,_jZ_n^{K_n},_jC_n^{K_n},$$

- NT = Number of time steps (1 through l)
- $_jTS$ = Time step (1..j) for which to manually change nuclide concentrations of material MT_i. Enter "1" for 2nd, etc. (If positive apply at discrete steps. If negative apply continuously and make linear interpolations for corrector step)
- $_jNM$ = Number of materials at time step "j" that incur nuclide concentration changes
- $_jMT_n$ = nth material number for which to manually change nuclides at time step "j". Positive value indicates atom/wt. fraction and negative value indicates atom/gram densities.
- $_jK_n$ = number of nuclides to manually change for the ith material

MATMOD

MATMOD= $NT,_1TS,_1NM,_1MT_1,_1K_1,_1Z_1^1,_1C_1^1,_1Z_1^2,_1C_1^2,\ldots,_1Z_1^{K_1},_1C_1^{K_1},$

$\ldots,_1MT_n,_1K_n,_1Z_n^1,_1C_n^1,_1Z_n^2,_1C_n^2,\ldots,_1Z_n^{K_n},_1C_n^{K_n},$

$_jTS,_jNM,_jMT_1,_jK_1,_jZ_1^1,_jC_1^1,_jZ_1^2,_jC_1^2,\ldots,_jZ_1^{K_1},_jC_1^{K_1},$

$\ldots,_jMT_n,_jK_n,_jZ_n^1,_jC_n^1,_jZ_n^2,_jC_n^2,\ldots,_jZ_n^{K_n},_jC_n^{K_n},$

- $_jZ_n^{K_n}$ = 1st, 2nd,.. K_nth nuclide of the MT_ith material at time step "j" for which a concentration will be specified. List as a ZAID value.

- $_jC_n^{K_n}$ = concentration for the nth isotope in material MT_i at time step "j". Enter positive values for atom fractions or atom densities, and enter a negative value for wt. fractions or gram densities. See sign of MT_i to specify either fraction or density

Example 5

- Example 5
  - Copy ex4d rename to ex5
  - At the first time step change the atom density of U-235 to 7.0e-2 for both materials
  - At the second time step make U-238 97% atom fraction for material 1

MATMOD

```
BURN TIME=50 500
          MAT=1 4
          POWER= 0.07
          PFRAC=1.0 1.0
          AFMIN= 1e-10 1e-4
          OMIT=1,8,6014,7016,8018,9018,90234,91232,95240,95244
               4,8,6014,7016,8018,9018,90234,91232,95240,95244
          BOPT=1.0 4
          MATVOL=3076.6 1730.6
     MATMOD=2,
            1,
              2,-1,1,92235,7e-2
                -4,1,92235,7e-2
             2,
                1,1,1,92238,0.97
```

Time step Determination

$$\frac{dN_m(r,t)}{dt} = -N_m(r,t)\beta_m + \bar{Y}_m + \sum_{k \neq m} N_k(r,t)\gamma_{k \to m}$$

- Even with cross section averaging methods, without proper selection of time steps, inaccurate conclusion can be made about time dependant results
- As the flux shape changes by "ε," more burn steps are needed in order to determine accurate reaction rates
  - Dictated by the buildup and depletion of highly absorbing isotopes
    - How does one determine which isotopes have a threshold worth of implementing more burn steps?
- Time-steps are usually chosen by trial-and-error and/or engineering operating experience
  - Benchmarking!
  - However, can this process by automated?

Time Step

- Example 6
  - Take previous example and break up the 500 day time step into 5 100 day time steps
  - Why would the results be expected to be different?

Metastable Representation

Metastable isotopes ZA will now be represented using the following equation:

$$A' = (A+300) + (m*100)$$

$$m=1,2,3,4$$

Example:

Ag-110m = 47510

$$47510 = 47110 + 1^{st} \text{ metastable}$$

File 9 MT 102

Treating Metastable Isomer Branching in MCNPX 2.7.B

$$Collision\ Rate\ of\ Isomer\ State\ i = \int_G Y(E)_i \sigma(E)_R \Phi(E) dE$$

What we do to adjust:

1. Tally (n,g)total in MCNPX = $\left(\sigma_{n,\gamma}\Phi\right)_{MCNPX}$
2. Allow CINDER90 to calculate and energy integrate the M(n,g)L* = $\left(\sigma_{n,\gamma^*}\Phi\right)_{CINDER90}$
3. Use the equation listed below to adjust M(n,g)L

$$Corrected\ M(n,\gamma)N = \left(1 - \frac{\left(\sigma_{n,\gamma^*}\Phi\right)_{CINDER90}}{\left(\sigma_{n,\gamma}\Phi\right)_{MCNPX}}\right) \times \left(\sigma_{n,\gamma}\Phi\right)_{MCNPX}$$

Recoverable Energy per Fission

$$Q_{recoverable} = Q_{prompt} + Q_{delayed} + (\bar{\nu}(E) - k_{eff}) * Q_{capture\ \gamma} - Q_{neutrino}$$

- Prompt Q value is usually determined from ENDF tape
  - File 1 MT 458
- Delayed Q value may be estimated assuming local energy deposition
  - Deposited gamma energy may need adjustment
    - 207 of 390 isotopes contain capture gamma data in ENDF VII.0

Emitted and recoverable energy for fission of U-235

Form	Emitted Energy (MeV)	Recoverable Energy (Mev)
Fission Fragments	168	168
Fission Product Decay		
γ -rays	8	8
β-rays	7	7
neutrinos	12	--
Prompt gamma rays	7	7
Fission neutrons (kinetic energy)	5	5
Capture γ-rays	**--**	**3-12**
Total	**207**	**198-207**

Future Work for Burnup

- New Data
- CINDER90 version 8
- Large sized problems and message passing
- Error propagation
  - Toshikazu Takeda, Naoki Hirokawa and Tomohiro Noda "*Estimation of Error Propagation in Monte-Carlo Burnup Calculations*" Journal of Nuclear Science and Technology, Vol 36, No. 9, September 1999.
- Minor actinide fission yields
- Q value
  - File 1 MT 458 (Prompt Q)
  - Capture Gamma
    - 207 of 390 isotopes contain capture gamma data in ENDF VII.0
- Fission product lumps
- Critical Spectra
- Thermohydraulic feedback
- Isomer branching ratio File 9 MT 102
- Automatic burn step generation
- Domain decomposition Monte Carlo

Fixed Source Detector Calculations

- Sources
- Tallies and Tagging

Sources

- GENERAL
- CRITICALITY
- SURFACE
- USER-SUPPLIED
  - ENERGY
  - TIME
  - DIRECTION u,v,w
  - POSITION x,y,z
  - PARTICLE TYPE
  - WEIGHT
  - cell/surface if any

SDEF

KCODE/KSRC

SSW/SSR

SDEF Card

SDEF <var_1=$spec_1$> <var_2=$spec_2$>…

DEFAULT:

A 14 MeV isotropic point source from position 0,0,0 at time = 0 and weight = 1

SDEF ERG = 14 (*MeV*) pos = 0 0 0 tme = 0 (*shakes* = 10^{-8} *s*) wgt = 1

SDEF Variables Used for this Exercise

- SCALAR

  PAR, CEL, EXT and RAD

- VECTOR *(must specify x,y,z)*
  - POS reference point for sampling position
  - AXS reference vector for EXT and RAD

SDEF Specification Types

SPECIFICATION can have 3 forms:

- explicit value: SDEF Par = a
- distribution number: SDEF Pos = D1
- a function of another variable:

SDEF POS=D1 Par FPOS D2

SI (Source Information) Card

Distribution numbers: SDEF EXT = D1

SIn option entries

n = distribution number from D specification

H - histogram bin upper boundaries (default)
L - discrete values follow
A - points where probability density distribution is defined
S - distribution numbers follow

SP (Source Probability) Card

Distribution numbers: SDEF POS = D1

SPn option entries

n = distribution number from D specification

d - bin probabilities (default)
c - cumulative bin probabilities
v - probability proportional to volume
f - built-in function (FOR CYINDERS use -21 1)

DS (Dependent Source) Card

SDEF POS = D1 Par = fpos = d2

DSn option entries

```
SI1      L     0 0 0   11 0 0
SP1            1         1
DS2    L       a          t
```

Or…

```
DS2    S              3         4
```

H -- values for continuous distribution

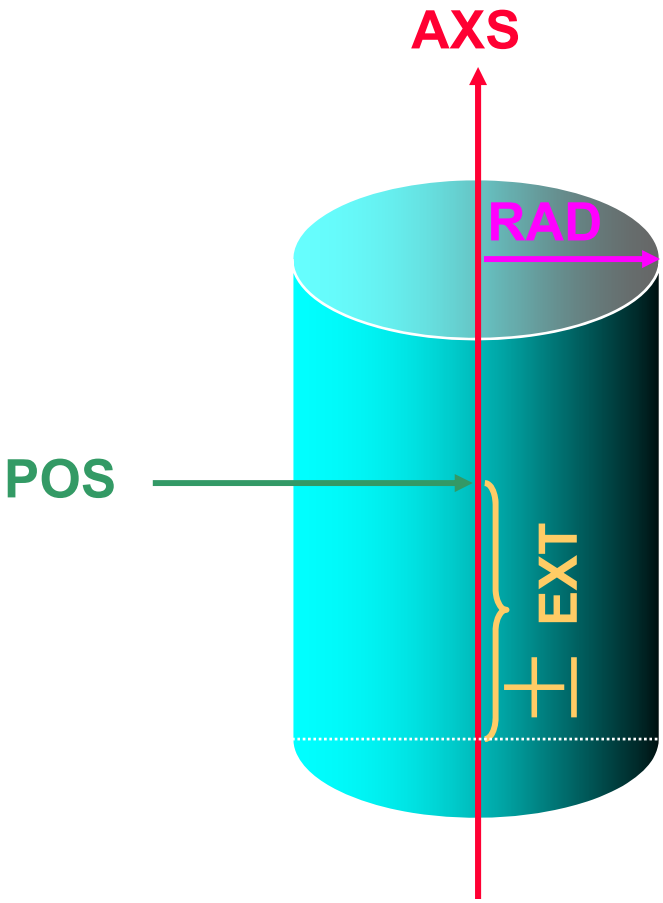
L -- discrete values

S -- more distribution numbers

T -- independent value dependent value

Q -- independent value distribution #

CYLINDRICAL VOLUME



AXS vector u v w

POS vector x y z

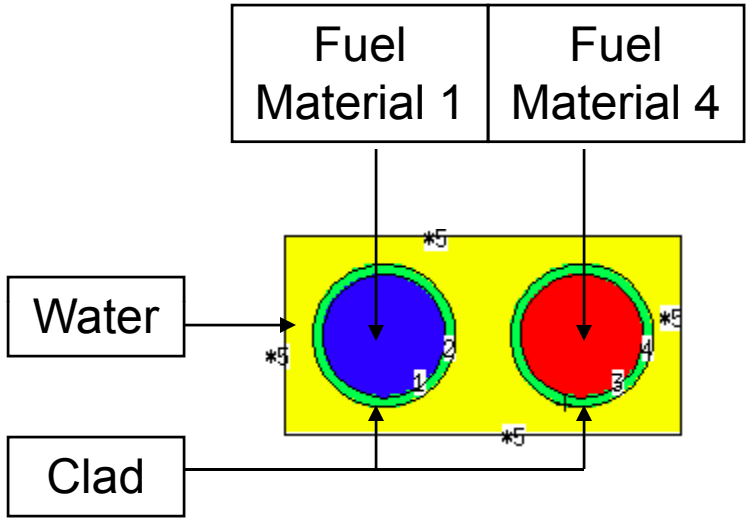
RAD distribution Dn

for cylinder

EXT distribution Dn

Spontaneous Fission Source from Two Cylinders

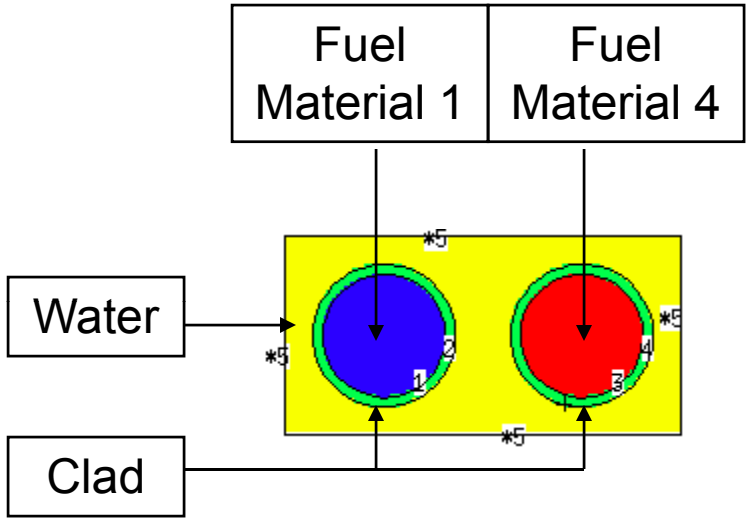
- Geometry of Ex4b
- Emit a spontaneous fission source par=sf from each fuel pin
- Cells 1 and 4 contain fuel pins cel = ?; d#
- Position is a function of cell location; pos=fcel=?
- Each fuel pin is 0 → 365 cm tall; ext = ?; d#
- Each fuel pin is 0 → 0.4095 cm diameter; rad = ?; d#; sp# -21 1
- Each fuel pin is oriented on the z-axis; axs = ?



What would the SDEF card for this passive spontaneous fission source look like?

Spontaneous Fission Source from Two Cylinders

```
SDEF par=sf cel=d1 pos=fcel=d2
        ext=d3 rad=d4 axs=0 0 1
SI1 L 1 4
SP1 1 1
ds2 L 0 0 0 1.3133 0 0
SI3 0.001 364.99
SP3 0 1
SI4 0 0.40949
SP4 -21 1
```



We will use this source later!!!

Tally Types

Tally Type		Fn: Units
F1:	Surface Current	#
F2:	Surface Fluence	#/cm2
F4:	Cell Fluence	#/cm2
F5:	Detector Fluence	#/cm2
F6:	Energy Deposition	MeV/gm
+F6:	Energy Depos. (all particles)	MeV/gm
F7:	Fission Energy Deposition	MeV/gm
F8:	Pulse Height	pulses

Tally Format

Simple Form: Fn:<*pl*> $S_1\ S_2\ .\ .\ .\ S_k$

General Form: Fn:<*pl*> $S_1\ (S_2\ .\ .\ .\ S_3)\ (S_4\ .\ .\ .\ S_5)\ S_6$ . . .

n = tally number

<*pl*> = particle type (IPT Symbol Only)

( ) -> total over the specified range

Examples

```
F2:n    3                   $ fluence on surface 3 (neutron)

F104:u  2                   $ fluence in cell 2 (neutrino)
        (5 6 7 8)           $ total fluence, cells 5, 6, 7, 8
```

Tally Test

Further Examples:

Tally neutrons crossing surface 2

F___:_ _____

Tally the volumetric flux for neutrons entering volume 4, have a separate tally determine neutrons entering volume 6

F___:_ _____

F___:_ _____

Tally Tagging

FT*n* TAG *a*

n = tally number

a = specifies how scatter is to be treated when tagging

a=1 all collided particles will lose their tag and bremsstrahlung and annihilation photons will be included in the bin of collided particles

a=2 indicates that all collided particles will lose their tag, but that bremsstrahlung and annihilation photons will be given special tags that allow them to be segregated

a=3 indicates that all collided particles will retain their production tag

Tally Tagging (Binning)

FU*n* CCCCCZZAAA.RRRRR

CCCCC = cell location (i.e. 400000 → cell 4)
ZZ = atomic number
AAA = atomic mass
RRR = reaction type (MT number)

Example:
1426056.00102 →tag all (n,g) reactions with iron 56 in cell 14 that contribute to detection in tally number n

Special Tags for Our Examples

-0000000001	or -1	Source particle tag for all cells
-CCCCC00001		Source (i.e., uncollided) particle tag for cell CCCCC
0000000000	or 0	Scattered particle tag
10000000000	or	1e10 everything else tag

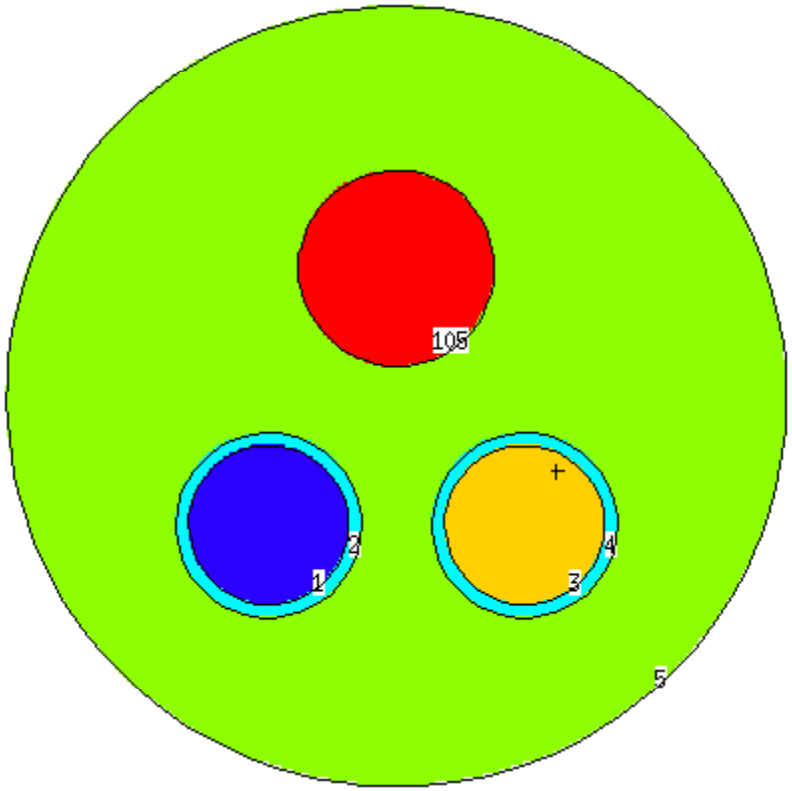
Example:

```
F4:n  3
FT4  TAG  3
FU4  400000.00018  -400001 400000 1e10
```

Tag neutrons were detected in cell 3 and came from cell 4 by fission, any other inelastic reaction, or source neutrons. Also tag everything else.

Example 7

- Example 7
  - Open ex7 rename to ex7a
  - Open ex4a.o
  - Take the material information for the final burn step for ex4b for materials 1 and 4 and make new material cards for ex7 materials 1 and 4
  - Add your previously generated passive neutron source definition; SDEF card
  - Create a volumetric neutron flux tally in the detector region; F_:n _; cell 105; duplicate this tally using another number F_:n _.
  - Use tally tagging to determine all neutrons sources and induced fissions that were detected in cell 105



Example 7

```
…
C SDEF Cards
SDEF par=sf cel=d1 pos=fcel=d2 ext=d3 rad=d4 axs=0 0 1
SI1 l 1 4
SP1 1 1
ds2 l 0 0 0 1.3133 0 0
SI3 0.001 364.99
SP3 0 1
SI4 0 0.40949
SP4 -21 1
C  Material Cards
…
…
print
f4:n 105
f14:n 105
FT14 TAG 3
FU14 400000.00018 100000.00018 -400001 -100001 1e10
FMULT 94236 WIDTH = 1.1 WATT = .2 4 SFYIELD 1
FMULT 96246 WIDTH = 1.1 WATT = .2 4 SFYIELD 1
nps 100000
mode n
phys:n  100 100 0 -1 20 1 0
```

Questions?