A Review of Basic Concepts and Tools for Fast Reactor Neutronic and Fuel Cycle Simulations

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TOC

Motivation

Fast reactors have several advantages over LWRs

- Harder spectrum allows breeding without suffering from FP poisons
- All actinides have lower α in harder spectrum, allowing waste transmutation
- Liquid metal coolants chemically compatible with metallic fuel
- Liquid metal coolant allows natural circulation decay-heat removal

And some disadvantages

- Exotic coolants often reactive with the natural environment
- Diminishing Σ_c at high energy leads to positive void coefficient
- Lower β_{eff}

Fast Reactor Analysis

Analysts are concerned with reaction rates.

$$M\phi = \frac{1}{k} B\phi \tag{1}$$

$$\frac{\partial}{\partial t} N = AN \tag{2}$$

Philosophy is to divide and conquer. We perform three levels of calculations to solve the transport,

- Library calculation
- Lattice calculation
- Global calculation

and use a quasistatic approach to perform depletion.

Homogenization

Long mean free path of fast neutrons allows accuracy for spatial homogenization.

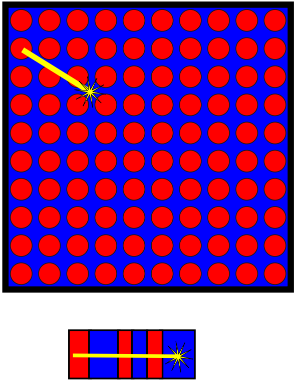

Figure: A LWR Assembly

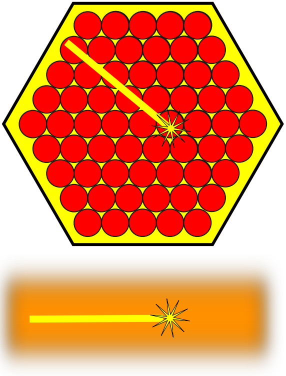

Figure: A SFR Assembly

Detailed energy calculations

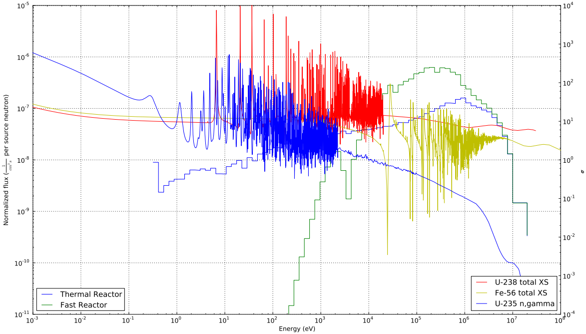

Figure: Characteristic neutron spectra

Microscopic Depletion

Macroscopic depletion:

- Cross sections are parameterized vs. temperature, burnup, fuel history, etc.
- Spectral history is poorly treated
- Typically sufficient in thermal reactor calculations

Microscopic depletion:

- Number densities are explicitly tracked
- Spectral history effects are remembered
- Requires 2x or more computational time and memory
- Necessary for fast reactor calculations

Lumped Fission Products

- An approximation to microscopic depletion
- One pseudo-nuclide for each yield set (different parents, burnups)
- High burnup problems present complications, inaccuracies
- Today's computers can do large cases with many FPs explicitly modeled
- Recommendation: Model the most important 15 FPs explicitly, lump the rest and/or make burnup dependent LFPs

Fast Reactor Tools

- ERANOS and MC^2–REBUS are CEA and Argonne's common-practice fast reactor neutronic tools
- MCNP has been coupled to burnup codes countless times
- Argonne is developing UNIC, an ultra hi-fi unstructured mesh finite element system that can run on >100,000 cores

REBUS

REBUS has many capabilities

- Many geometry options
- Diffusion or Variational Nodal Transport solvers
- Searches on critical enrichment, poison density, cycle length, burnup limit, equilibrium cycle
- Can model entire fuel cycle for one reactor, including multiple reprocessing plants
- Burnup dependent cross sections with polynomial fitting
- Arbitrary or repetetive fuel shuffling

Compiling Argonne's codes on a modern PC

- Compiler choice is the key
- G95 and GCC can compile DIF3D 8.0 with info from web
- Probably REBUS-PC too, but process still unknown
- REBUS-PC and MC^2-2 can be compiled on Windows with Lahey/Fujitsu Express 7.2 FORTRAN and Borland C++ 5.5

```
lf95 -c -O1 mcc2.f
lf95 -c -O1 seglib.f
lf95 -c -O1 syslib.f
C:\Borland\BCC55\Bin\bcc32.exe -c sun.aug97.syslib.c*
lf95 -out mc2.exe *.obj
```

- Runs in Linux under WINE. LF95-linux not tested
- Intel compiler method may require a bit more work

Code Modifications to MC^2-2

- Find and replace QLOG $\rightarrow$ DLOG
- Find and replace REAL*16 $\rightarrow$ REAL*8
- Insert an extra space on line 44534 of mcc2.f to get standard FORTRAN
- Change CALL ERROR to CALL ERROR1 in all files
- Rename SUBROUTINE ERROR to SUBROUTINE ERROR1 in sun.aug97.syslib.c
- Remove include sys/time.h and sys/resource.h statements in *syslib.c
- Remove functions that don't have underscores in their names in the C sources
- Comment out contents of tleftc_ and add return(3.1415926); or something.

Compiling REBUS-PC

Binary runs on modern PCs, but you can get benefits by recompiling.

- A small fix can speed your larger cases up drastically.
- NUC031 module in norm1.f fixes a normalization problem from REBUS-3.
- But it spins the I/O system for EVER
- Arne Olson confirmed bug in code in July 09, suggested fix.

```
      CALL REED(ICOMPX,I0,DUM,I0,I0)
      PC(K,J)=WORK(NWDS)
  110 CONTINUE
  100 CONTINUE
```

```
            PC(K,J)=WORK(NWDS)
  110 CONTINUE
  100 CONTINUE
C     CLOSE DATA SET COMPXS
      CALL REED(ICOMPX,I0,DUM,I0,I0)
```

Compiling DIF3D 8.0

Compiles easily with instructions on web. Easy to add more rows.
`http://www.corephysics.com/dif3d_pc.html`

- DIF3D limited to 99999 regions. Easy to extend with global find and replace.
- find *.f -exec sed -i 's/FORMAT(16I5/FORMAT(16I10/g'
- 99999 limit changed to 9999999999. Should be plenty.

Other Bugs

MC^2-2 library contains undocumented AM242M nuclide. Use it instead of documented AM2425.

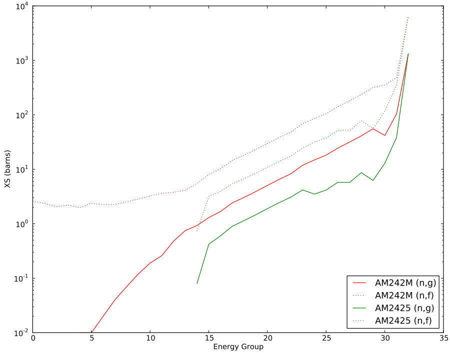

Figure: Comparison of AM-242m cross sections

Other Bugs

MC^2-2 library κ values are not accurate. Override with card 22 and ENDF-VII values for proper normalization (changes flux by $\sim$2%).

Nuclide	ENDF/B-VII	MC^2-2
U-235	193.48 MeV	198.53 MeV
U-238	198.03 MeV	193.44 MeV
Pu-239	198.84 MeV	198.03 MeV
Pu-240	199.47 MeV	194.44 MeV
Pu-241	201.98 MeV	199.83 MeV

Table: Comparison between MC**2 and ENDF/B-VII of values of κ_f for key nuclides

Summary

Fast reactor codes:

- Can get away with more spatial homogeneity
- Require detailed energy calculations
- Require hi-fi burnup systems

Additionally,

- REBUS and MC^2 can now be compiled on a PC
- A REBUS-PC bug fix speeds large calculations by 3 orders of magnitude
- Several MC^2-2 bugs have been identified

Find this presentation online at:
`http://www.whatisnuclear.com/docs/frBasics_ans2010.pdf`