ORIGEN Reactor Libraries Generation

SCALE Users' Group Workshop
August 5, 2021

Briana Hiscox
Benjamin Betzler

Table of Contents

- Why should you use ORIGEN reactor libraries?
- TRITON vs ORIGEN (using reactor libraries)
- What are ORIGEN reactor libraries?
- *Common assemblies
- ORIGEN reactor libraries existing and coming soon
- Why generate your own ORIGEN library?
- How to make and use your own ORIGEN Library?
- Suggested parameters to generate ORIGEN libraries
- How to generate many ORIGEN libraries (SLIG python utility)?

Why should you use ORIGEN reactor libraries?

- Do you need to deplete a common* assembly?
- Do you want to save time?

- ORIGEN reactor libraries enable fast depletion simulations with ORIGEN (ORIGAMI).
- Depletion simulations that could take 12-90 hours to run with TRITON can be run with ORIGEN (ORIGAMI) in <5 minutes when using ORIGEN reactor libraries.
- For example, a CE14x14 TRITON run took 7 hours and 13 GB of memory and similar ORIGAMI run took 21 seconds and 62MB of memory

What are SCALE ORIGEN reactor libraries (1/3)

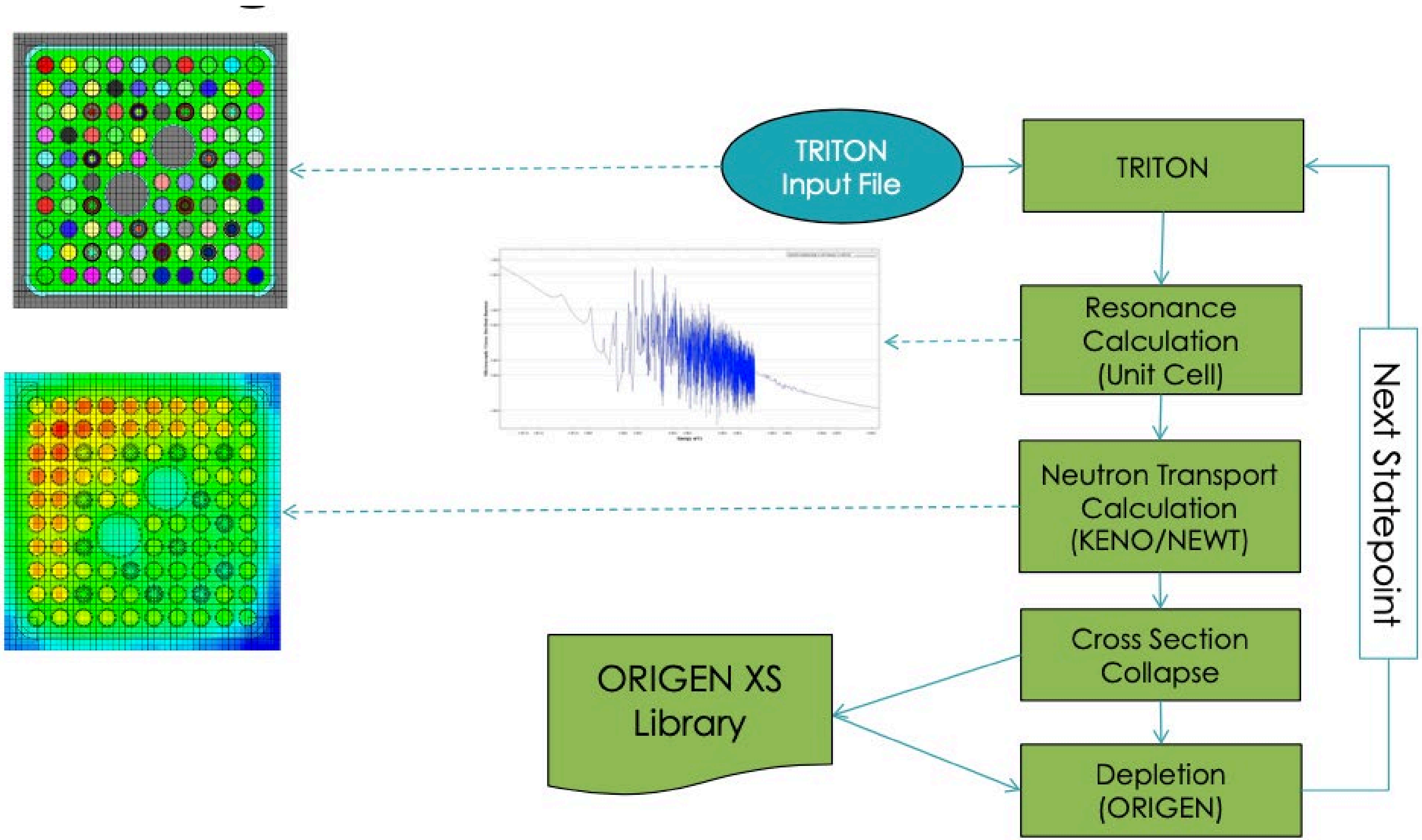
- ORIGEN libraries contain 1-group cross section data used to solve the depletion (Bateman) equation
- ORIGEN libraries are generated and used internally as part of the TRITON sequence
- Generating an ORIGEN library is as easy as generating the geometry to be simulated, and running the depletion calculation!
  - Using the flexible geometry definition available in TRITON, a user can generate an ORIGEN library for nearly any configuration
- Libraries are written to SCALE unit 33 – look for ***ft33f001*** in the temporary directory
  - In practice, ORNL staff use the ".f33" extension for these files

$$\frac{dN_i}{dt} = \sum_{j=1}^{m} l_{ij}\lambda_j N_j + \bar{\Phi}\sum_{k=1}^{m} f_{ik}\sigma_k N_k - (\lambda_i + \bar{\Phi}\sigma_i + r_i)N_i$$

What are SCALE ORIGEN reactor libraries (2/3)

- During a TRITON calculation, ORIGEN libraries (ft33 files) are generated for each depletion mixture in the problem (all depletion sequences)
  - ft33f001.mixN, where "N" is the mixture ID used in the TRITON input file
- A "combined" ft33 file representing the weighted sum of all depletion mixtures is generated only when running the t-depl (NEWT-based) sequence
  - ft33f001.cmbined (not a typo, ".cmbined" not ".combined")

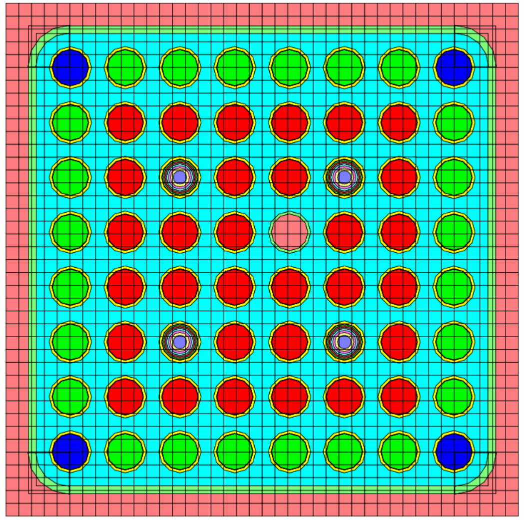
What are SCALE ORIGEN reactor libraries (3/3)



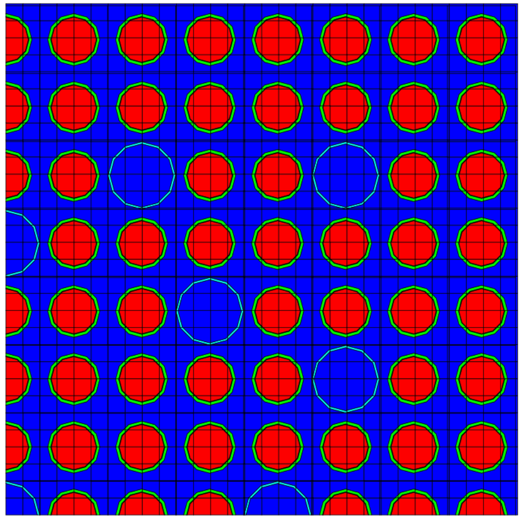
*Common assemblies

61 assembly types:

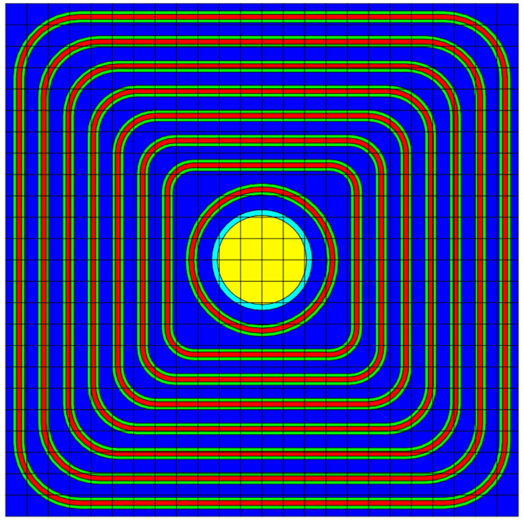
- 11 BWR assemblies
- 9 PWR assemblies
- 20 MOX assemblies (PWR, BWR)
- 3 CANDU
- 10 IRT
- 8 other – VVER, SVEA, RBMK, MAGOX, etc. **



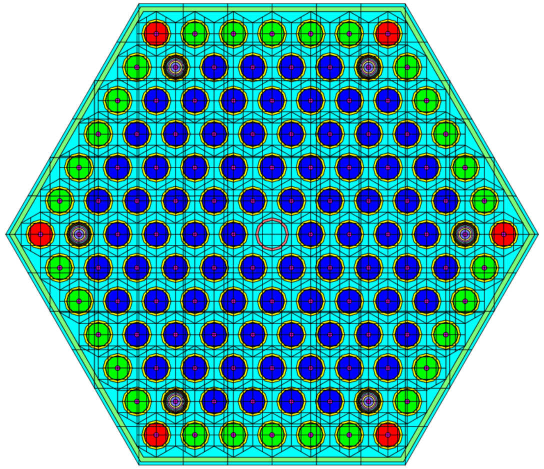
BWR - ABB8x8-1



PWR - W15x15



IRT3M8tubePoly



VVER440

** complete list available in bonus slides in this presentation

SCALE ORIGEN reactor libraries existing and coming soon

Updated version of Table 5.3.2 (SCALE 6.2.3 manual)

		SCALE 6.2			SCALE 6.3		
Assembly type	Coolant/moderator densities [g/cc]	Enrichments [%]	Maximum burnup [GWd/MTU]	Number of libraries	Enrichments [%]	Maximum burnup [GWd/MTU]	Number of libraries
PWR LEU	~0.73	0.5, 1.5, 2, 3, 4, 5, 6	70.5	7	0.5, 1.5, 2, 3, 4, 5, 6, 7, 8, 8.5	82.5	10
BWR LEU	0.1, 0.3, 0.5, 0.7, 0.9	0.5, 1.5, 2, 3, 4, 5, 6	70.5	35	0.5, 1.5, 2, 3, 4, 5, 6, 7, 8, 8.5	82.5	50
PWR MOX	~0.73	*	70.5	15	*	82.5	15
BWR MOX	0.1, 0.3, 0.5, 0.7, 0.9	*	70.5	75	*	82.5	75
AGR	1.65	0.5, 1.5, 2, 3, 4, 5	48.7	6	0.5, 1.5, 2, 3, 4, 5	48.7	6
CANDU	0.8445	0.711	13.7	3	0.711	13.7	3
IRT	0.989	19.75, 36, 80, 90	159	12	19.75, 36, 80, 90	159	12
Magnox	1.628	0.7, 0.8, 0.9, 1	13.7	4	0.7, 0.8, 0.9, 1	13.7	4
RBMK	0.15, 0.28, 0.41, 0.54, 0.67, 0.8	1.8, 2.2, 2.6, 3	24.3	24	1.8, 2.2, 2.6, 3	24.3	24
VVER440	0.73	1.6, 2.4, 3.6, profiled	70.5	6	1.6, 2.4, 3.6, profiled	82.5	6
VVER-1000	0.7145	0.5, 1.5, 2, 3, 4, 5, 6	70.5	7	0.5, 1.5, 2, 3, 4, 5, 6, 7, 8, 8.5	82.5	10

Why generate your own ORIGEN reactor library?

1. You want to use the pre-made libraries but need to make some changes such as:

- Higher burnup/enrichments
- Different IFBA or Gd patterns
- Different cladding
- Different geometries
- Different temperatures and densities
- To add enrichment zoning

2. You need to run several similar files from the same assembly or might have to re-run several times

How to make and use your own ORIGEN library 1/5

- 1. At the end of TRITON input file type:

```
=shell
  cp ${TMPDIR}/ft33f001.cmbined ${OUTDIR}/namelibrary.f33
end
```

- * ft33f001.cmbined is not a typo, “.cmbined” not “.combined”

- 2. Run Triton

How to make and use your own ORIGEN library 2/5

- 3. Open arpdata.txt
  - If SCALE is local on Mac, Applications/Contents/Resources/data/arpdata.txt
  - If you are on a cluster you must copy arpdata.txt from the SCALE install location to your directory to be able to edit

How to make and use your own ORIGEN library 3/5

- Note 1: To find the burnup values for arpdata.txt search "Library Burnup" in the Triton output file. The column on the right will show the library burnup values in MWd/MTIHM.
- Note 2: Library Burnup is at the midpoint of each depletion interval so if you edit the template* to say the last 2 burnups are 81 and 84 the max library burnup will be 82.5

Sub-Interval No.	Depletion Interval	Sub-interval in interval	Specific Power(MW/MTIHM)	Burn Length (d)	Decay Length (d)	Library Burnup (MWd/MTIHM)
0	****Initial Bootstrap Calculation****					0.00000E+00
1	1	1	25.000	2.000	0.000	2.50000e+01
2	1	2	25.000	38.000	0.000	5.25000e+02
3	1	3	25.000	40.000	0.000	1.50000e+03
4	1	4	25.000	40.000	0.000	2.50000e+03
5	1	5	25.000	60.000	0.000	3.75000e+03
6	1	6	25.000	60.000	0.000	5.25000e+03

* more on templates later

How to make and use your own ORIGEN library 4/5

- 4. Add the data for your new library to the arpdata.txt file.
- 5. Save arpdata.txt file
- 6. Make sure your new library is in the right folder
  - Note: the libraries do not go in the same folder as arpdata.txt they go in a subfolder called arplibs

arpdata.txt

```
!BH_w15
 2 1 31
 4.0000   5.0000
 0.7332
 'w17_e30_extra.f33' 'w17_e40_extra.f33' 'w17_e50_extra.f33'
      0.00      40.00    1040.00    3000.00    5000.00
   7500.00   10500.00   13500.00   16500.00   19500.00
  22500.00   25500.00   28500.00   31500.00   34500.00
  37500.00   40500.00   43500.00   46500.00   49500.00
  52500.00   55500.00   58500.00   61500.00   64500.00
  67500.00   70500.00   73500.00   76500.00   79500.00
  82500.00
!BH_w17
 3 1 31
 3.0000   4.0000   5.0000
 0.7332
 'w17_e30_extra.f33' 'w17_e40_extra.f33' 'w17_e50_extra.f33'
      0.00      40.00    1040.00    3000.00    5000.00
   7500.00   10500.00   13500.00   16500.00   19500.00
  22500.00   25500.00   28500.00   31500.00   34500.00
  37500.00   40500.00   43500.00   46500.00   49500.00
  52500.00   55500.00   58500.00   61500.00   64500.00
  67500.00   70500.00   73500.00   76500.00   79500.00
  82500.00
```

How to make and use your own ORIGEN library 5/5

- 7. Open ORIGAMI and put the name of your new library in libs=[“newlib”]
- 8. Run ORIGAMI

```
=origami
  title="example for Users group"
  options{ mtu=1.0e-03 ft71=all decayheat=yes}
  libs=["BH_w17"]

  fuelcomp{
    uox(fuel){ enrich=3.453 }
    mix(1){ comps=[ fuel=100 ] }
}
```

Example of the beginning of an origami file

Suggested parameters to generate libraries

- When SCALE 3.0 is released 1,665 ORIGEN reactor libraries files will be included. They were generated with these parameters :

- =t-depl parm=(centrm, addnux=4)
- v7-252
- centrmdata alump=0 pmc_dilute=1e30 pmc_omit=0 end centrmdata
- sn=8
- cell_tol=1e-8
- Sides=18
- Boundary mesh 6 mesh bins per pin

How to generate many libraries (SLIG Python utility)

- Location on selected ORNL clusters: /projects/scale/release/6.2.4/linux/etc/slig/src
- Location locally: Applications/SCALE-6.2.4/Contents/Resources/etc/slig/src

- Basics:
- 1. Edit your template files
- 2. run "./slig.py –gs"
- 3. run a submitSLIGjobs* file

```
' --------------------------------------------------------------
'  template to generate libraries for ORIGEN-S
'  parameters are: u235wt%        - wt% U235
'                  u234wt%        - wt% U234
'                  u236wt%        - wt% U236
'                  u238wt%        - wt% U238
'                  ddd            - coolant density (g/cc)
'                  dancoff1       - dancoff factor 1
'                  dancoff2       - dancoff factor 2
'                  namelibrary    - name of generated ORIGEN library
'                  specpow        - average specific power
'                  daystoburn     - depletion interval in days
'  options are:    name           - abb_
'                  enrichment     - 0.5, 1.5, 2.0, 3.0, 4.0, 5.0, 6.0
'                  cool. density  - 0.1, 0.3, 0.5, 0.7, 0.9
'                  dancoff1       - 0.4686, 0.3429, 0.2651, 0.2122,
'                                   0.1742
'                  dancoff2       - 0.3103, 0.2316, 0.1823, 0.1484,
'                                   0.1237
'                  spec. power    - 25.0
'                  burnups        - 0, 1, 2, 3, 4.5, 6, 7.5, 9,
'                                   10.5, 12, 13.5, 15, 16.5, 18,
'                                   19.5, 21, 24, 27, 30, 33, 36,
'                                   39, 42, 45, 48, 51, 54, 57, 60,
'                                   63, 66, 69, 72
' --------------------------------------------------------------
```

Figure 5.A.1. A typical BWR template header.

Acknowledgements

- Many thanks to Ben Betzler and Brian Ade for their input and for providing several of the figures in this presentation.

Bonus Slides

Helpful resources

1.SCALE 6.2.3 manual (2018) section 5.A

(https://www.ornl.gov/sites/default/files/SCALE_6.2.3.pdf)

B. T. Rearden and M.A. Jessee, Eds., ***SCALE Code System***, ORNL/TM-2005/39, Version 6.2.3, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2018). Available from Radiation Safety Information Computational Center as CCC-834.

2. ORIGEN_Reactor_Libraries.pdf (2016)

(/projects/scale/release/6.2.4/linux/docs/Additional Documents/ORIGEN_Reactor_Libraries.pdf)

B. Ade, B. Betzler, ***ORIGEN Reactor Libraries***, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2016).

3. sligManual.pdf (2015)

(/projects/scale/release/6.2.4/linux/etc/slig/docs)

B. R. Betzler, B. J. Ade, ***SCALE/ORIGEN Library (SLIG) Manual***, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2015).

Common assemblies details

- The complete list of the ORIGEN reactor libraries is shown below. This information is shown in section 5.3.1 in the SCALE 6.2.3 manual.
- BWR 7×7, 8×8-1, 8×8-2, 9×9-2, 9×9-9, 10×10-9, 10×10-8, SVEA-64, SVEA-96, and SVEA-100;
- PWR 14×14, 15×15, 16×16, 17×17, 18×18;
- CANDU reactor (19-, 28-, and 37-element bundle designs);
- Magnox graphite reactor;
- Advanced Gas-Cooled Reactor (AGR);
- VVER 440 and VVER 1000;
- RBMK;
- IRT;
- MOX BWR 7×7, 8×8-1, 8×8-2, 9×9-2, 9×9-9, 10×10-9, 10×10-8, SVEA-64, SVEA-96, and SVEA-100;
- MOX PWR 14×14, 15×15, 16×16, 17×17, 18×18.