

ORIGEN Reactor Libraries

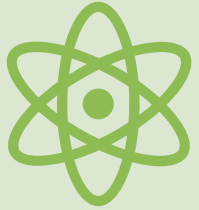
SCALE 6.3.1

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U.S. DEPARTMENT OF
ENERGY

Learning goals



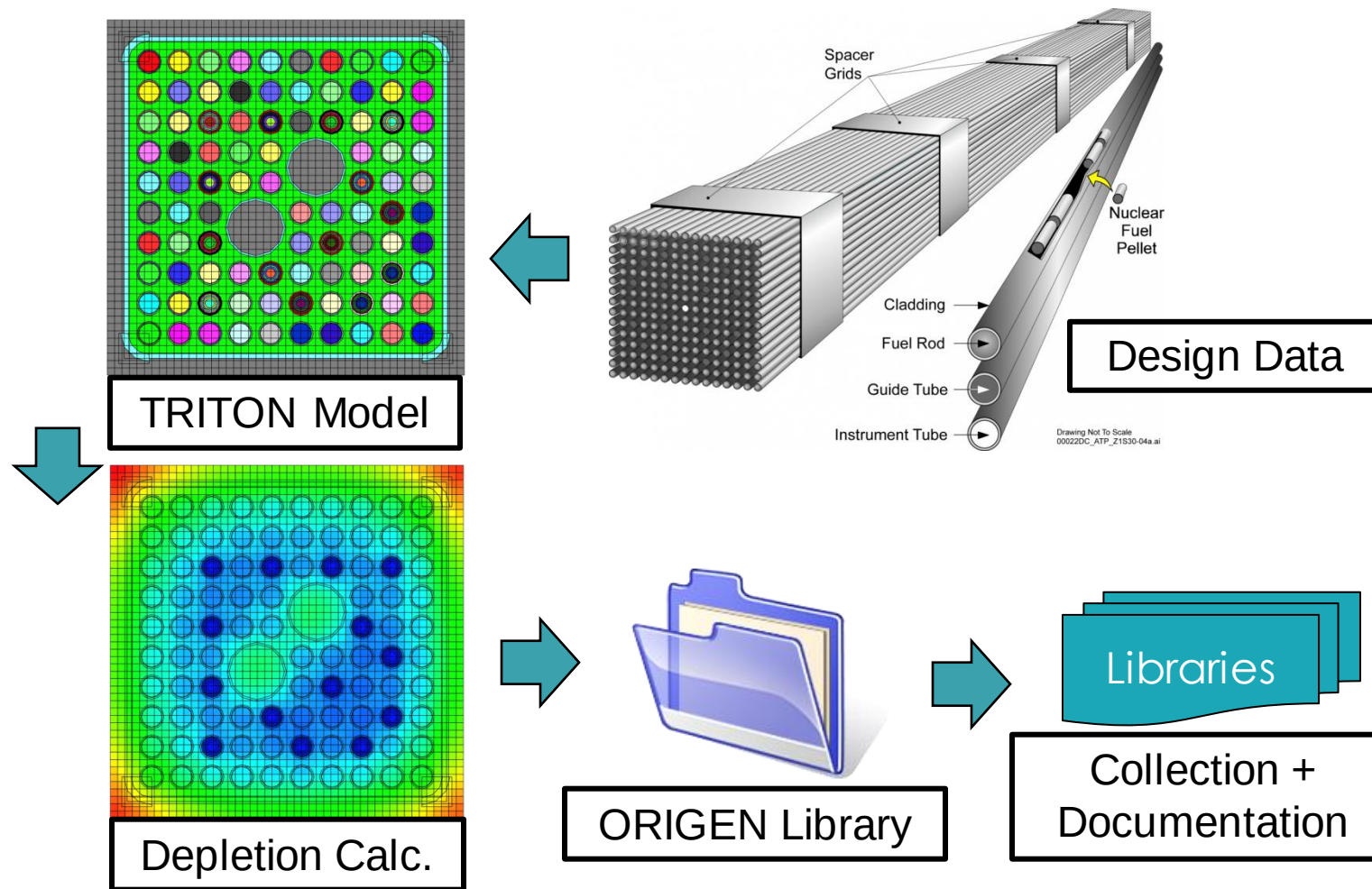
Understand ORIGEN reactor libraries

- **What they are** (what they physically represent)
- **How they are used** in depletion calculations
- **How they are created** using SCALE

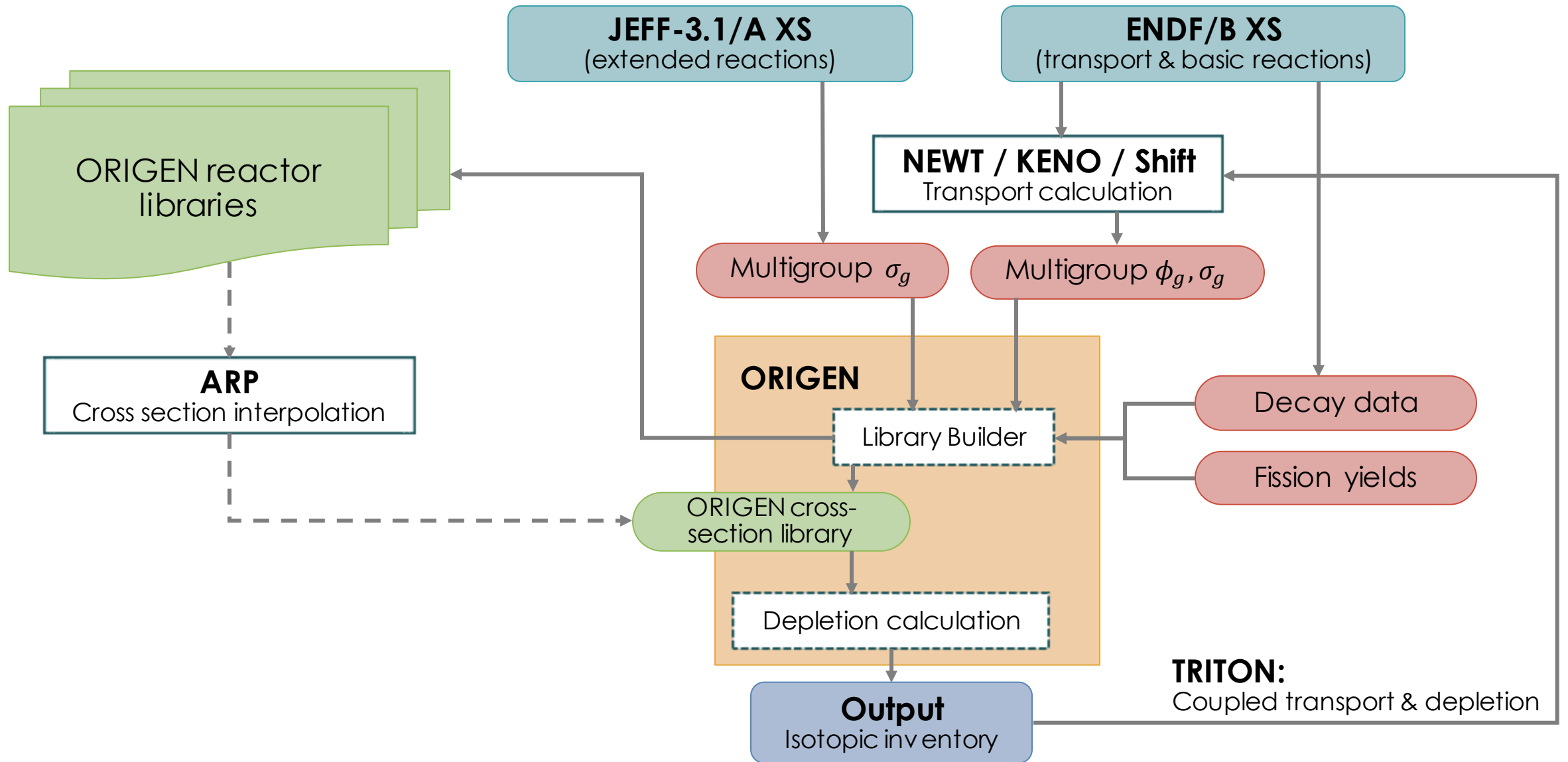


Familiarize users with the available pre-generated ORIGEN reactor libraries provided with SCALE

Generating ORIGEN reactor libraries



How ORIGEN uses nuclear data



What are ORIGIN cross section vs. ORIGIN reactor libraries?

ORIGIN cross section library

One F33 file containing burnup-dependent 1-group cross sections for one specific assembly design.

Note common terminology:

ORIGIN cross section library
= *ORIGIN library*
= *ORIGIN 1-group library*
= *F33 file*

ORIGIN reactor library

A **set** of ORIGIN cross section libraries for a specific reactor type and fuel assembly configuration, parametrized to, for example, the following:

- Enrichment
- Moderator density
- Pu content, ^{239}Pu values (MOX fuel)

Example

g10_e40w03.f33

One file corresponding to a specific BWR GE 10×10 fuel assembly model: 4.0 wt.% ^{235}U enrichment and 0.3 g/cm³ coolant density

Example

g10_e05w01.f33	...
g10_e05w03.f33	g10_e80w07.f33
g10_e05w07.f33	g10_e80w09.f33
g10_e05w09.f33	g10_e85w01.f33
g10_e15w01.f33	g10_e85w05.f33
g10_e15w03.f33	g10_e85w07.f33
...	g10_e85w09.f33

A set of files for a BWR GE 10×10 fuel assembly for different combinations of enrichment and moderator density

What are these libraries used for?

ORIGEN cross section library

One F33 file containing burnup-dependent 1-group cross sections for one specific assembly design.

Note common terminology:

ORIGEN cross section library
= *ORIGEN library*
= *ORIGEN 1-group library*
= *F33 file*

ORIGEN reactor library

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- Enrichment
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ORIGEN

Used by ORIGEN to run a single depletion calculation of a specific problem to obtain the time-dependent inventory for this exact problem.

ORIGAMI

Used by ORIGAMI to rapidly run a depletion calculation and generate inventory for varying parameters.

User input: reactor library name together with desired enrichment/moderator density and depletion history

ORIGAMI calculation: interpolation of cross sections from pre-generated libraries followed by depletion to generate inventory

Available ORIGEN reactor libraries

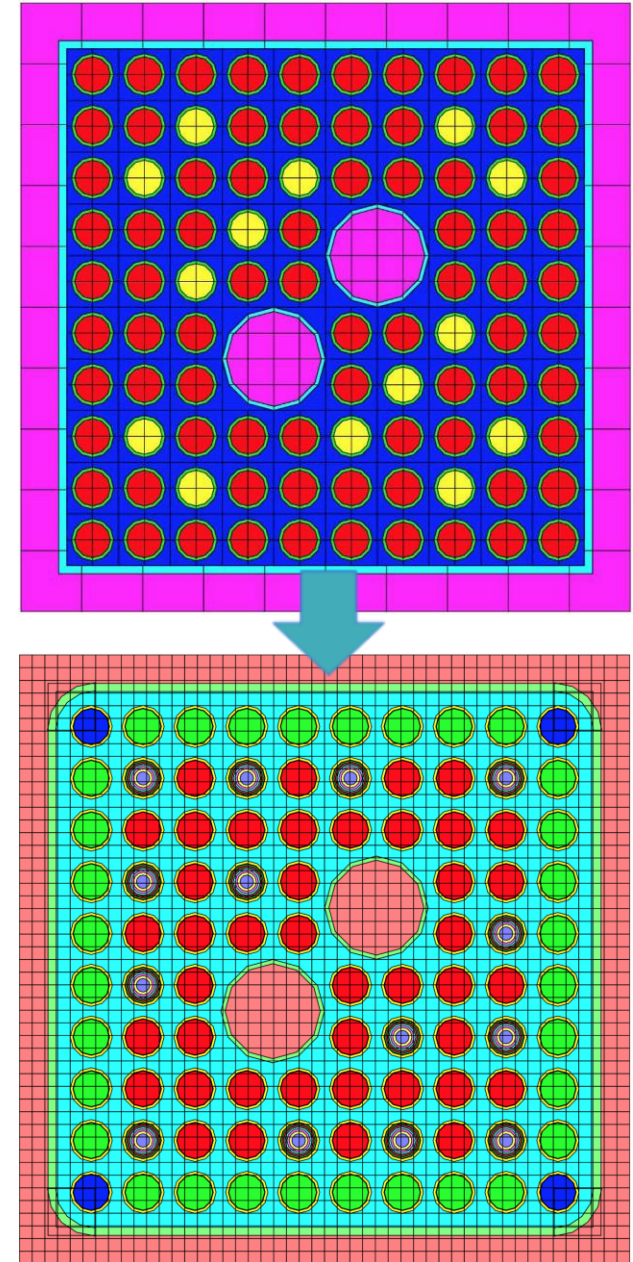


Libraries

- Available with SCALE 6.3 for:
 - Pressurized water reactors (PWRs)
 - Boiling water reactors (BWRs)
 - Mixed-oxide (MOX) for typical BWRs and PWRs
 - Russian VVER reactors
 - Russian RBMK reactors
 - Canadian CANDU reactors
 - UK advanced gas reactors (AGRs)
 - MAGNOX reactors
 - IRT reactors
- Other reactor libraries can be generated by ORNL or by the user, provided sufficient design information is available

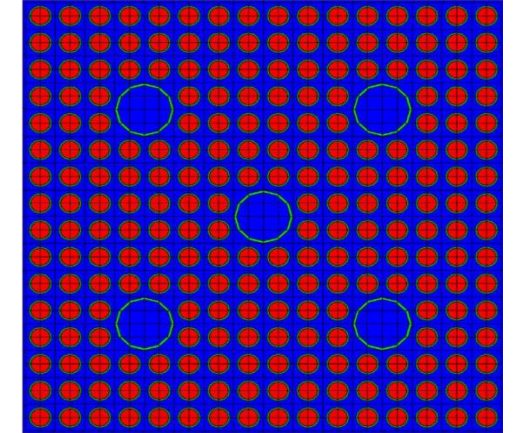
ORIGEN reactor libraries – SCALE 6.3

- Automation tools allow reactor libraries to be generated with each release of SCALE
- Generation of reactor libraries is based on ORNL modeling best practices
 - 252-group ENDF/B-VII.1 cross section library for the neutron transport solution
 - CENTRM cross section processing for the NEWT transport solver
 - Specialized Dancoff factors for BWR corner and edge pins
 - Adequate spatial solution grid
 - Sources of information provided
 - MOX assembly models with typical radial zoning
- **New in SCALE-6.3**
 - Extended enrichments (up to 8.5 wt % ^{235}U) and burnups (up to 82,500 MWd/MTU) for all PWR and BWR libraries

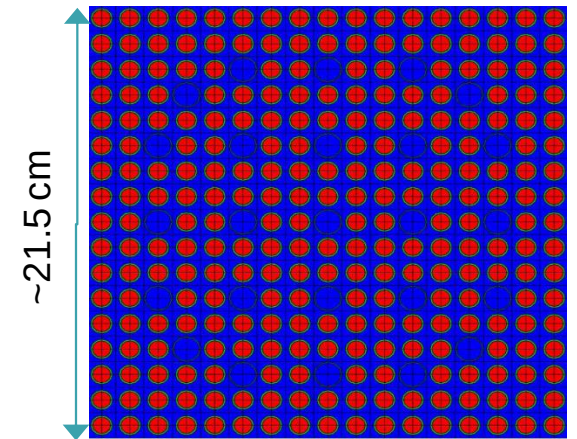


ORIGEN reactor libraries for PWRs

- PWRs operate under high pressure so that water does not boil
- Moderator (water) density is relatively constant in the reactor, $\sim 0.7 \text{ g/cm}^3$
- Coolant contains boron to control the reactor, 0–2500 ppm, depending on the time in the cycle
- Most reactors in the United States use 17×17 fuel assemblies



CE 16x16



W 17x17

ORIGEN PWR libraries in SCALE 6.3

Libraries

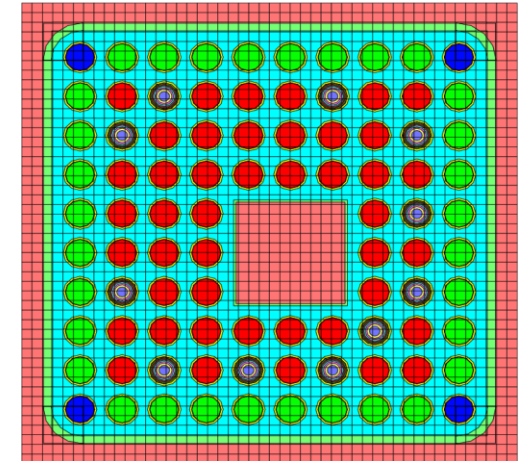
Assembly Design	Library Name	Enrichment (wt% ^{235}U)	Density (g/cc)
Westinghouse CE 14×14	ce14x14	0.5 – 8.5	0.7332
Westinghouse CE 16×16	ce16x16	0.5 – 8.5	0.7100
Westinghouse 14×14	w14x14	0.5 – 8.5	0.7264
Siemens 14×14	s14x14	0.5 – 8.5	0.7283
Siemens 18×18	s18x18	0.5 – 8.5	0.7283
Westinghouse 15×15	w15x15	0.5 – 8.5	0.7135
Westinghouse 17×17	w17x17	0.5 – 8.5	0.6700
Westinghouse 17×17 OFA	w17x17_ofa	0.5 – 8.5	0.6700

These libraries are based on 2D TRITON models (ENDF/B-VII.1 cross sections) with burnups to 82.5 GWd/MTU.

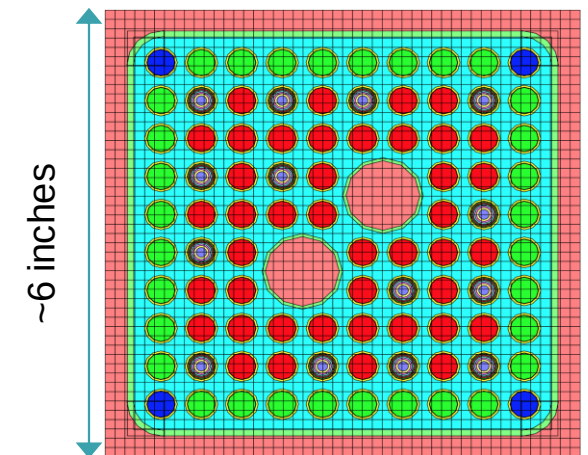
ORIGEN reactor libraries for BWRs

- BWRs operate at lower pressures (compared to PWRs)
- Water inside the channel boils, whereas water outside the channel remains at a relatively constant density
- Moderator density changes have a significant effect on the cross sections and, thus, fuel nuclide inventory
- BWRs typically contain many burnable poison rods (Gd_2O_3)
- Fuel enrichment and burnable absorber content can vary radially and axially
- GE14 (10×10) is the most common type of fuel in the United States; however, there are significantly more variations than are found in typical PWRs

Libraries



ATRUM 10



~6 inches

GE 10x10

ORIGEN BWR libraries in SCALE 6.3

Libraries

Assembly Design	Library Name	Enrichment (wt% U-235)	Density (g/cc)
GE 7×7	ge7x7-0	0.5 – 8.5	0.1 – 0.9
GE 8×8	ge8x8-1, ge8x8-2	0.5 – 8.5	0.1 – 0.9
ABB 8×8	abb8x8-1	0.5 – 8.5	0.1 – 0.9
GE 9×9	ge9x9-2	0.5 – 8.5	0.1 – 0.9
GE 10×10	ge10x10-8	0.5 – 8.5	0.1 – 0.9
ATRIUM-9	atrium9x9-9	0.5 – 8.5	0.1 – 0.9
ATRIUM-10	atrium10x10-9	0.5 – 8.5	0.1 – 0.9
SVEA-64	svea64-1	0.5 – 8.5	0.1 – 0.9
SVEA-100	svea100-0	0.5 – 8.5	0.1 – 0.9
SVEA-96	svea96-1	0.5 – 8.5	0.1 – 0.9

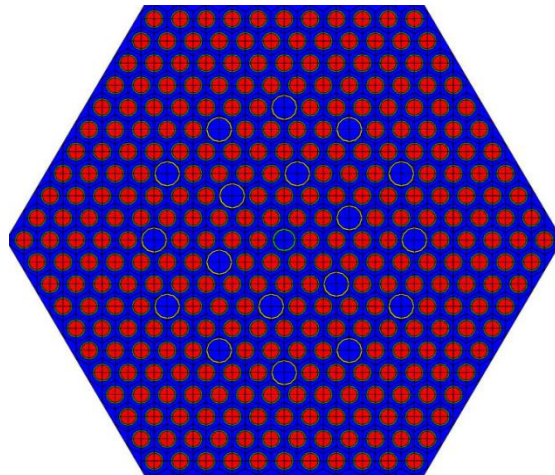
These libraries are based on 2-D TRITON models (ENDF/B-VII.1 cross sections) with burnups to 82.5 GWd/MTU.

ORIGEN VVER libraries in SCALE 6.3

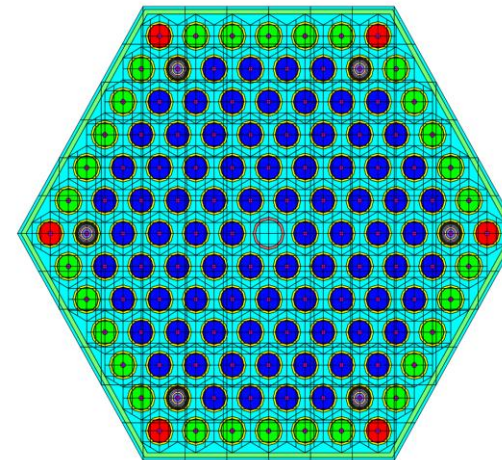
Libraries

Assembly Design	Library Name	Enrichment (wt% U-235)	Density (g/cc)
VVER-440 flat	vver440	1.6 – 3.6	0.73
VVER-440 profiled	vver440_3.82	3.82 average	0.73
VVER-440 profiled	vver440_4.25	4.25 average	0.73
VVER-440 profiled	vver440_4.38	4.38 average	0.73
VVER-1000	vver1000	0.5 – 8.5	0.7145

These libraries are based on 2D TRITON models (ENDF/B-VII.1 cross sections) with burnups to 82.5 GWd/MTU.

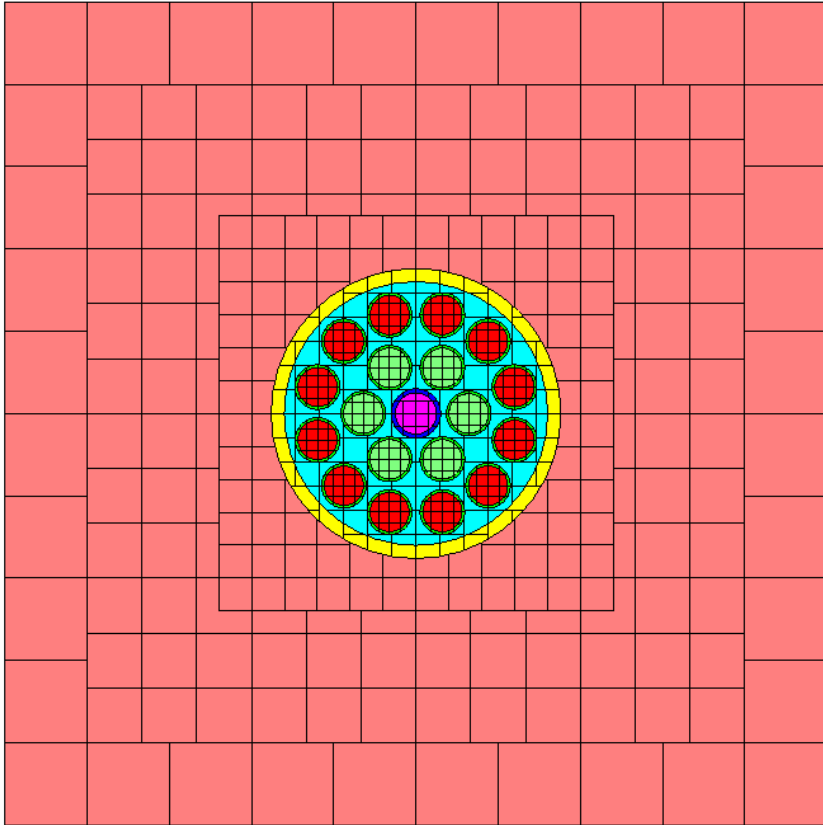


VVER-1000



VVER-440

ORIGEN RBMK libraries in SCALE 6.3



- Libraries generated based on design data representative of the Chernobyl Unit 4 reactor
- **Enrichment:** 1.8, 2.0, 2.2, 2.6, and 3.0 wt% ^{235}U
- **Coolant density:** 0.15, 0.28, 0.41, 0.54, 0.67, and 0.80 g/cm³
- **Burnup:** 0 to 24.375 GWd/MTU

ORIGEN reactor libraries for MOX fuel

Libraries

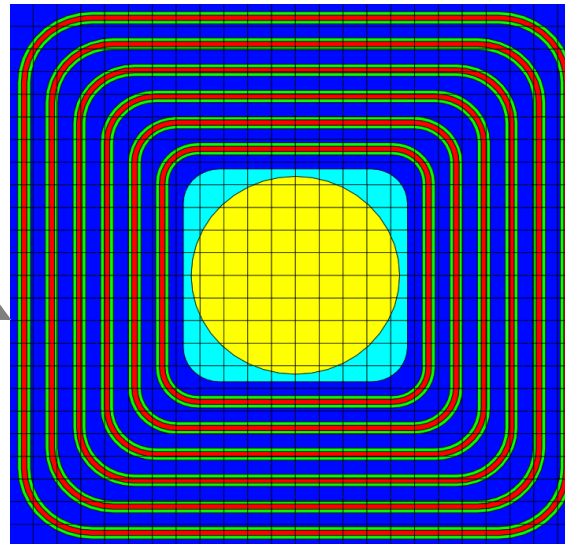
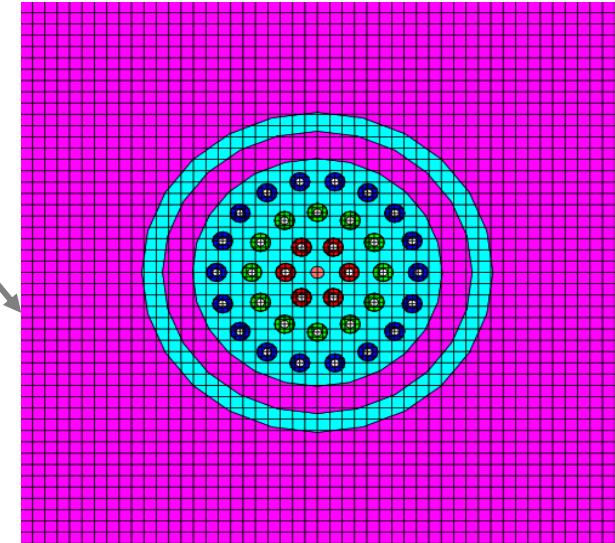
- MOX fuel PWR and BWR assemblies
 - PWR 14×14 , 15×15 , 16×16 , 17×17 , 18×18
 - BWR 8×8 , 9×9 , 10×10
 - Variable moderator density for all BWR MOX designs

Reactor Type	Lattice Type	No. of MOX Rods	No. of UO ₂ /Gd Rods	Fuel Pitch (cm)	Pellet diameter (mm)	Clad diameter (cm)	Assembly pitch (cm)
PWR	18 x 18	300	-	1.27	8.05	9.5	23
	17 x 17	264	-	1.26	8.19	9.5	21.5
	16 x 16	236	-	1.43	9.11	10.75	23
	15 x 15	205	-	1.43	9.13	10.75	21.6
	14 x 14	179	-	1.41	9.29	10.72	19.8
BWR	10 x 10 - 9	81	10	1.3	8.7	10.05	15.2
	9 x 9 - 9	60	12	1.43	9.5	10.8	15.2
	9 x 9 - 1	68	12	1.43	9.5	10.8	15.2
	8 x 8 - 2	62	14	1.63	10.3	12.3	15.2

Other ORIGEN reactor libraries in SCALE 6.3

Libraries

- CANDU – natural UO_2 , heavy water
- MAGNOX – natural U metal
- AGR
- IRT – research reactor fuel



Viewing ORIGIN reactor library file contents using OBIWAN:

OBIWAN info and
OBIWAN view



OBIWAN modes

```
obiwan <mode> <options> FILE
```

Tip: Redirect STDERR
to a log file: `2>log`

- **info** – print basic info about multiple files
- **view** – view a file
- **tag** – manipulate tags on a file
- **convert** – convert between versions of files
- **diff** – diff/compare two files
- **interp** – interpolate files
- **patch** – patch data in files

The following slides provide some of the most common or useful options for the different modes. Please see the manual or the help screen for all details.

OBIWAN operating modes & capabilities

convert

- Convert f33 libraries and F71 files between different SCALE formats (6.1 $\Leftrightarrow$ 6.2+)

diff

- Compare two ORIGEN binary files

info

- View file metadata (e.g., # of positions, format)

interp

- Interpolate a file along tags or burnup values

patch

- Rewrite / "patch" data on an existing file

tag

- Introduce metadata onto a binary file (used for identification and interpolation)

view

OBIWAN info: File metadata information

```
obiwan info [-type=TYPE] FILE
```

- Displays metadata about an ORIGEN binary file
 - Library (f33), StateSet / Concentrations (f71), Yield Resource (yld)
- **Example:** Display info for all w15_ assemblies in **\${DATA}/arplibs:**

```
obiwan info [path to data]/arplibs/w15*
```

fileName	dataType	numSets	fileFormat	fileType	file/sysEndian	appVersion
w15_e05.f33	Origen::Library	17	bof	binary	little/little	6.2.0
w15_e15.f33	Origen::Library	17	bof	binary	little/little	6.2.0
w15_e20.f33	Origen::Library	17	bof	binary	little/little	6.2.0
w15_e30.f33	Origen::Library	17	bof	binary	little/little	6.2.0
w15_e40.f33	Origen::Library	17	bof	binary	little/little	6.2.0
w15_e50.f33	Origen::Library	17	bof	binary	little/little	6.2.0
w15_e60.f33	Origen::Library	17	bof	binary	little/little	6.2.0

OBIWAN view: Library file output formats (`-format=`)

Transition matrix

coeff	output tabular transition coefficients
coefft	same as coeff but with transition ids
matrix	output full transition matrix

Neutron production

nprodr	neutron production ratio
genneu	neutron generation

One-group library cross sections

loxs	1-group effective disappearance cross section
fisxs	1-group fission cross section

Library metadata

tags	output file tags
nucl	nuclide list
burnups	output burnup list
reaction	allowed reactions

Output formats for post-processing

json	output in JSON format
graphviz	output dot file transitions to STDOUT

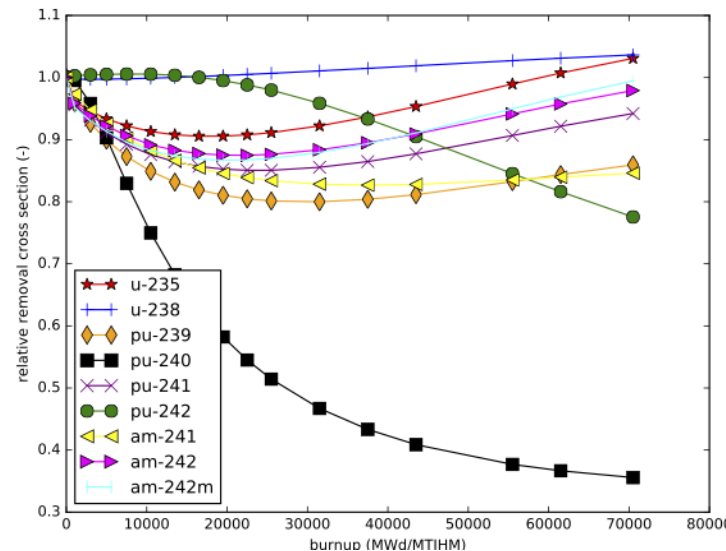
Example: Viewing ^{240}Pu loss XS as a function of burnup

```
obiwan view -format=loxs -symbols=1 ~/scale/data/arplibs/w17_e50.f33
```

```
...
AC:pu238  1.9918E+01  1.9426E+01  1.9117E+01  1.8876E+01  1.8700E+01  1.8550E+01  1.8445E+01  1.8403E+01
AC:pu239  1.5127E+02  1.4876E+02  1.4515E+02  1.4010E+02  1.3598E+02  1.3195E+02  1.2831E+02  1.2563E+02
AC:pu240  2.2669E+02  2.2674E+02  2.2551E+02  2.1707E+02  2.0451E+02  1.8794E+02  1.6994E+02  1.5479E+02
AC:pu241  1.2945E+02  1.2672E+02  1.2398E+02  1.2075E+02  1.1815E+02  1.1565E+02  1.1346E+02  1.1192E+02
...
```

```
obiwan view -format=burnup ~/scale/data/arplibs/w17_e50.f33
```

```
pos  MWd/MTIHM
1      0
2     40
3    1040
4    3000
5    5000
6    7500
7   10500
8   13500
...
```



Same method can be applied across different assembly dimensions (initial enrichment, moderator density, etc.).

Tutorial:

Exploring content of an
ORIGEN reactor library file (f33)



Exercise: Viewing an ORIGEN reactor library file (f33) content

Using the provided library file “**obiwan.f33**” (produced with TRITON):

1. Print the list of burnups contained in the library
2. Find the loss cross section of U-235, Pu-239 as a function of burnup
3. Print all the transition coefficients (yield x cross section) to daughter Te-135 (with `-format=coefft`)

Solution: List of burnup points on the library file

```
obiwan view -format=burnups obiwan.f33
```

pos	MWd/MTIHM				
		11	22500.0000	22	55500.0000
1	0.0000	12	25500.0000	23	58500.0000
2	40.0000	13	28500.0000	24	61500.0000
3	1040.0000	14	31500.0000	25	64500.0000
4	3000.0000	15	34500.0000	26	67500.0000
5	5000.0000	16	37500.0000	27	70500.0000
6	7500.0000	17	40500.0000	28	73500.0000
7	10500.0000	18	43500.0000	29	76500.0000
8	13500.0000	19	46500.0000	30	79500.0000
9	16500.0000	20	49500.0000	31	82500.0000
10	19500.0000	21	52500.0000		

Solution: Loss XS for U-235, Pu-239 as a function of burnup

```
obiwan view -format=loxs -sizzzaaa=92235 -symbols=1 -transpose=1 obiwan.f33
```

```
obiwan view -format=loxs -sizzzaaa=94239 -symbols=1 -transpose=1 obiwan.f33
```

burnupAC:u235				burnupAC:pu239			
	3.7500e+04	3.0899e+01			3.7500e+04	9.0775e+01	
0.0000e+00	3.2040e+01	4.0500e+04	3.1126e+01	0.0000e+00	1.0965e+02	4.0500e+04	9.0957e+01
4.0000e+01	3.1489e+01	4.3500e+04	3.1375e+01	4.0000e+01	1.0820e+02	4.3500e+04	9.1244e+01
1.0400e+03	3.1104e+01	4.6500e+04	3.1643e+01	1.0400e+03	1.0624e+02	4.6500e+04	9.1626e+01
3.0000e+03	3.0816e+01	4.9500e+04	3.1929e+01	3.0000e+03	1.0360e+02	4.9500e+04	9.2095e+01
5.0000e+03	3.0608e+01	5.2500e+04	3.2233e+01	5.0000e+03	1.0140e+02	5.2500e+04	9.2645e+01
7.5000e+03	3.0407e+01	5.5500e+04	3.2553e+01	7.5000e+03	9.9101e+01	5.5500e+04	9.3269e+01
1.0500e+04	3.0237e+01	5.8500e+04	3.2889e+01	1.0500e+04	9.6874e+01	5.8500e+04	9.3960e+01
1.3500e+04	3.0135e+01	6.1500e+04	3.3238e+01	1.3500e+04	9.5119e+01	6.1500e+04	9.4715e+01
1.6500e+04	3.0092e+01	6.4500e+04	3.3600e+01	1.6500e+04	9.3750e+01	6.4500e+04	9.5525e+01
1.9500e+04	3.0100e+01	6.7500e+04	3.3973e+01	1.9500e+04	9.2700e+01	6.7500e+04	9.6387e+01
2.2500e+04	3.0151e+01	7.0500e+04	3.4356e+01	2.2500e+04	9.1914e+01	7.0500e+04	9.7295e+01
2.5500e+04	3.0240e+01	7.3500e+04	3.4749e+01	2.5500e+04	9.1350e+01	7.3500e+04	9.8245e+01
2.8500e+04	3.0363e+01	7.6500e+04	3.5147e+01	2.8500e+04	9.0977e+01	7.6500e+04	9.9227e+01
3.1500e+04	3.0516e+01	7.9500e+04	3.5551e+01	3.1500e+04	9.0770e+01	7.9500e+04	1.0024e+02
3.4500e+04	3.0695e+01	8.2500e+04	3.5957e+01	3.4500e+04	9.0708e+01	8.2500e+04	1.0127e+02

Solution: Transition coefficients for Te-135

```
obiwan view -format=coefft -symbols=1 obiwan.f33 | grep te135
```

```
FP:te135 <--[decay,beta-|-2]-- FP:sb135 3.2201e-01 3.2201e-01 3.2201e-01 ... 3.2201e-01 3.2201e-01 3.2201e-01
FP:te135 <--[decay,beta-,neutron|-26]-- FP:sb136 3.5814e-01 3.5814e-01 3.5814e-01 ... 3.5814e-01 3.5814e-01 3.5814e-01
FP:te135 <--[fission|18]-- AC:th227 3.1997e-01 3.1626e-01 3.1352e-01 ... 3.2551e-01 3.2788e-01 3.3027e-01
FP:te135 <--[fission|18]-- AC:th229 2.9720e-01 2.9668e-01 2.9619e-01 ... 2.8938e-01 2.8957e-01 2.8977e-01
FP:te135 <--[fission|18]-- AC:th232 9.5584e-04 9.5732e-04 9.5907e-04 ... 9.6253e-04 9.6160e-04 9.6069e-04
FP:te135 <--[fission|18]-- AC:pa231 6.0233e-03 6.0323e-03 6.0412e-03 ... 6.0172e-03 6.0108e-03 6.0044e-03
FP:te135 <--[fission|18]-- AC:u232 8.0034e-02 7.9714e-02 7.9541e-02 ... 8.4851e-02 8.5161e-02 8.5468e-02
FP:te135 <--[fission|18]-- AC:u233 6.2912e-01 6.2154e-01 6.1601e-01 ... 6.5611e-01 6.6118e-01 6.6629e-01
FP:te135 <--[fission|18]-- AC:u234 1.0625e-02 1.0640e-02 1.0655e-02 ... 1.0598e-02 1.0587e-02 1.0575e-02
FP:te135 <--[fission|18]-- AC:u235 7.9705e-01 7.8172e-01 7.7099e-01 ... 8.7605e-01 8.8701e-01 8.9806e-01
FP:te135 <--[fission|18]-- AC:u236 1.2414e-02 1.2428e-02 1.2356e-02 ... 1.0736e-02 1.0717e-02 1.0699e-02
FP:te135 <--[fission|18]-- AC:u237 7.1777e-02 7.1809e-02 7.1841e-02 ... 7.3530e-02 7.3547e-02 7.3570e-02
FP:te135 <--[fission|18]-- AC:u238 4.7928e-03 4.8002e-03 4.8085e-03 ... 4.8074e-03 4.8023e-03 4.7972e-03
...
FP:te135 <--[n,p|103]-- FP:i135 0.0000e+00 0.0000e+00 0.0000e+00 ... 0.0000e+00 0.0000e+00 0.0000e+00
FP:te135 <--[n,2p|111]-- FP:xe136 5.2420e-28 5.5115e-28 9.5624e-28 ... 3.9169e-25 4.1051e-25 4.2891e-25
FP:i135 <--[decay,beta-|-2]-- FP:te135 3.6482e-02 3.6482e-02 3.6482e-02 ... 3.6482e-02 3.6482e-02 3.6482e-02
```

Comparison of ORIGIN library files:

OBIWAN diff



OBIWAN diff: Comparing ORIGEN library files

```
obiwan diff -format=y [opts] file1 file2
```

Option	Description	Default
-reltol	Relative tolerance threshold (%)	-reltol=0.01
-pos	File position to compare upon (0 = all positions)	-pos=1
-format=y	Smart format (side-by-side comparison)	} Difference indicated via return (status) code
-format=genneu	Neutron generation (by nuclide)	
-format=eq	Exact match (no output)	
-format=approx_eq	Fast comparison (no output)	

OBIWAN diff: Comparing ORIGEN binary files

```
obiwan diff -format=String(y) [opts] file1 file2
```

- Works for any binary ORIGEN file format
 - YieldResource, DecayResource
 - StateSet (f71)
 - Library (f33)
- Tolerance can be adjusted to look only for differences above a threshold

Tutorial:

Comparing library files for an
ORIGEN BWR library



Exercise: Transition coefficient differences for GE10x10-8

For the GE10x10-8 BWR library:

1. Between 1.5 and 3.0% enrichment (0.5 g/cc coolant density), how many transition coefficients change by:
 - a) > 5%?
 - b) >10%?
 - c) >50%?
2. Between 0.3 and 0.5 g/cc moderator density (at 3.0% enrichment), how many transition coefficients change by:
 - a) > 5%?
 - b) >10%?
 - c) >50%?

Tip: GE10x10-8 variants in `${DATA}/arplibs/` are named as `g10-eXX-wYY.f33`, where **XX** is the initial U-235 enrichment (wt.%) and **YY** is the moderator density (Y.Y g/cc).

Hints:

- Use “grep” to look for transitions with a difference over the threshold
- You can also use “wc -l” to get the number of lines in a file

Solution: Transition coefficient differences for GE10x10-8

```
obiwan diff -reltol=5.0
```

```
${DATA}/arplibs/g10_e15w05.f33
```

```
${DATA}/arplibs/g10_e30w05.f33 | grep DIFF | wc -l
```

1. GE10x10-8: 1.5 vs. 3.0% enrichment (coolant density = 0.5 g/cc)

- a) 15,175
- b) 2,308
- c) 2,096

2. GE10x10-8: 0.3 vs. 0.5 g/cc moderator density (enrichment = 3.0%)

- a) 14,984
- b) 1,458
- c) 328

The future format of
ORIGEN reactor libraries:

“Archive” format for multi-
dimensional libraries

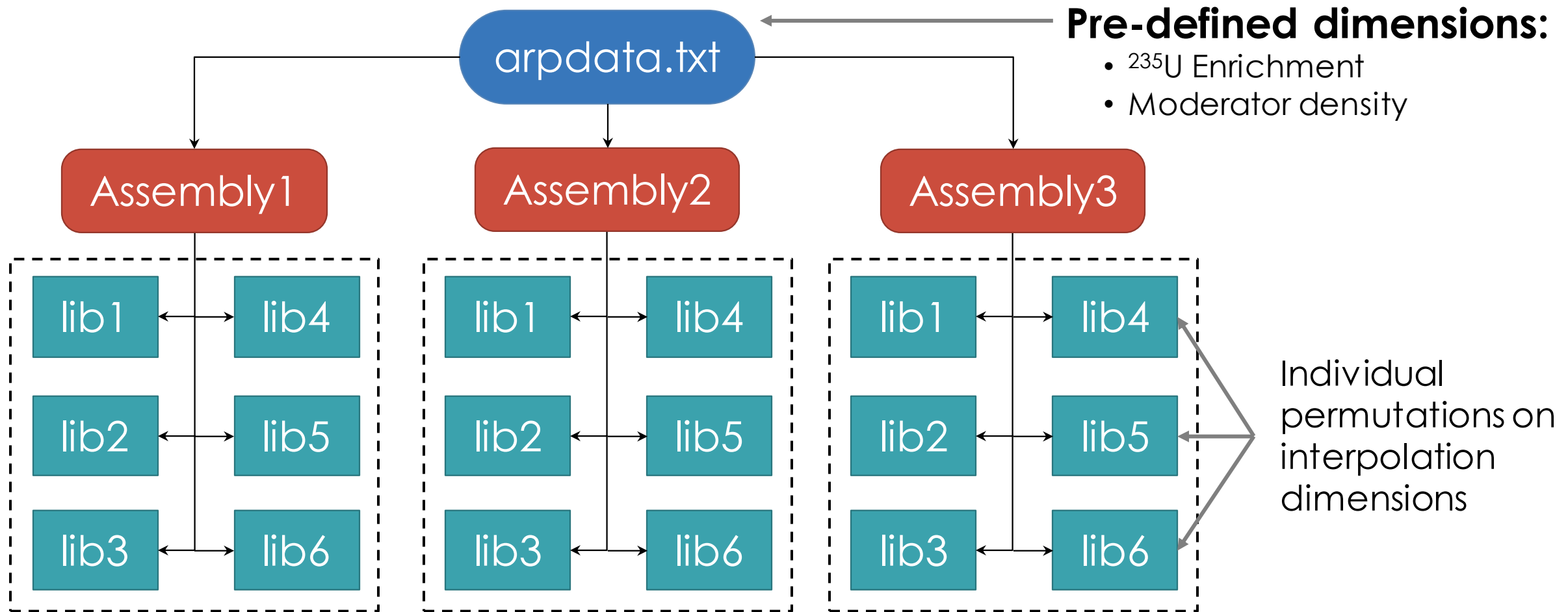


ORIGEN “Archive” format

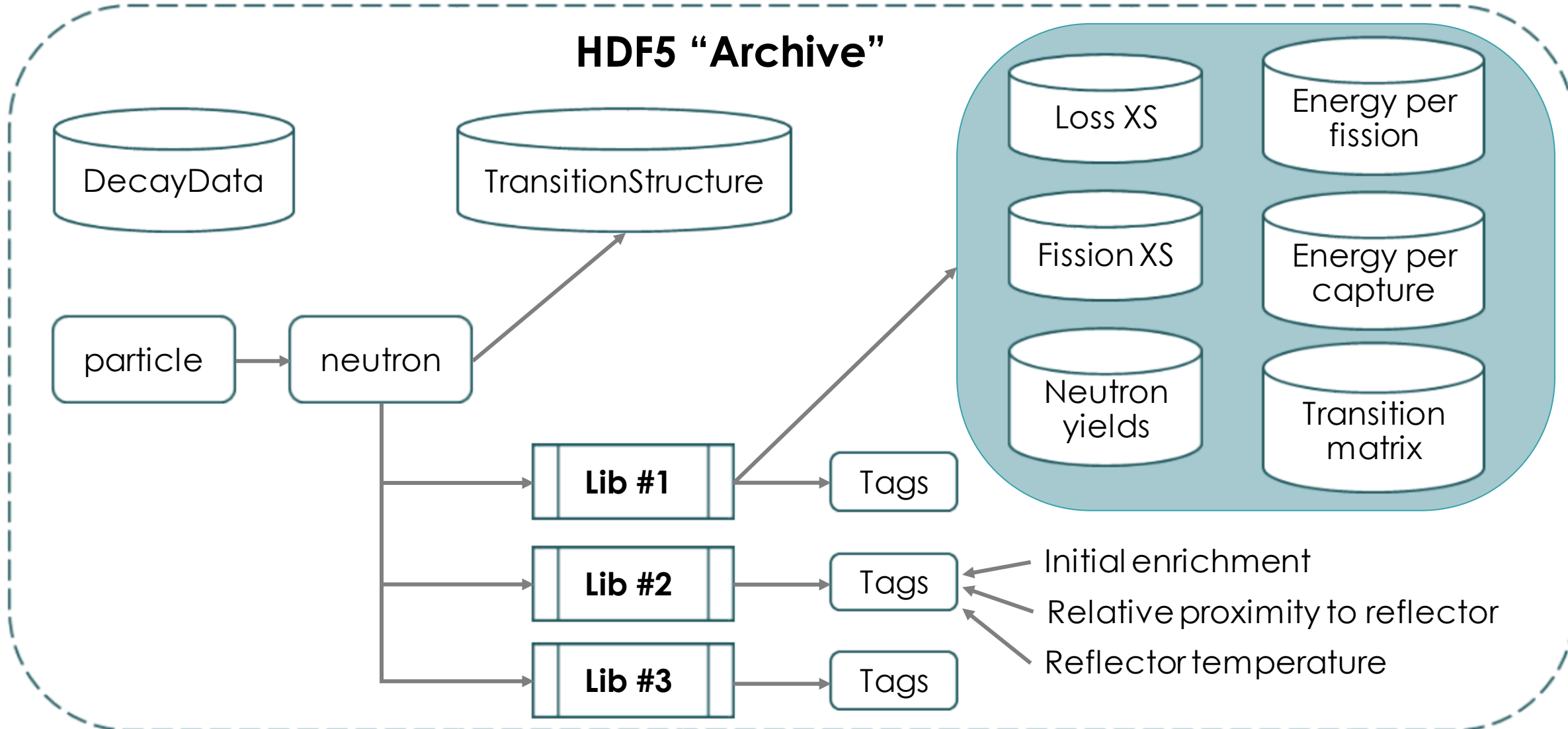
- ORIGIN and ORIGAMI in SCALE 7.0 will rely on HDF5-formatted “Archives” with descriptive interpolation data written on the file
- Flexible Archive data format allows for run-time specification & checking of interpolation parameters
- OBIWAN in SCALE 6.3.1 already supports conversion of libraries to the “archive” format
- Users can **convert** existing LWR libraries in `arpdata.txt` for use with ORIGAMI

```
obiwan convert -format=hdf5 -alias=[lib_alias][path_to_arpdata.txt]
```

ORIGEN reactor library interpolation relies on an ASCII database with hard-coded interpolation dimensions



New HDF5-based “Archive” format is designed to accommodate arbitrary interpolation dimensions



New ORIGIN “Archive” format will pair with HDF5 to facilitate consolidated storage & interpolation

- **Motivation:**

- How can we collect “similar” libraries together into a collection for interpolation?
- How can we “archive” a set of similar libraries to disk as a consolidated archive?

