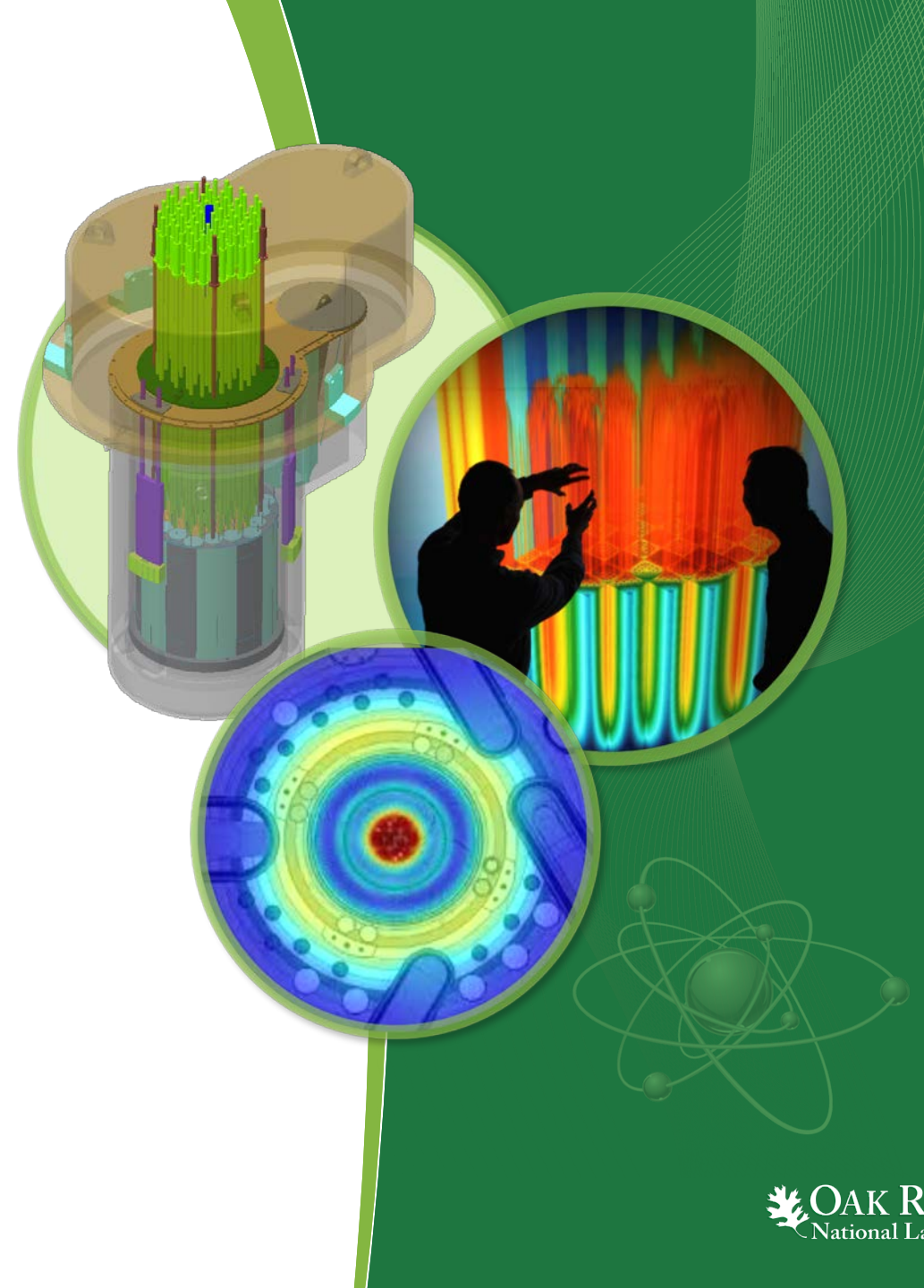


ORIGAMI Spent Fuel Characterization Tutorial

SCALE Users' Group Workshop
September 28, 2017

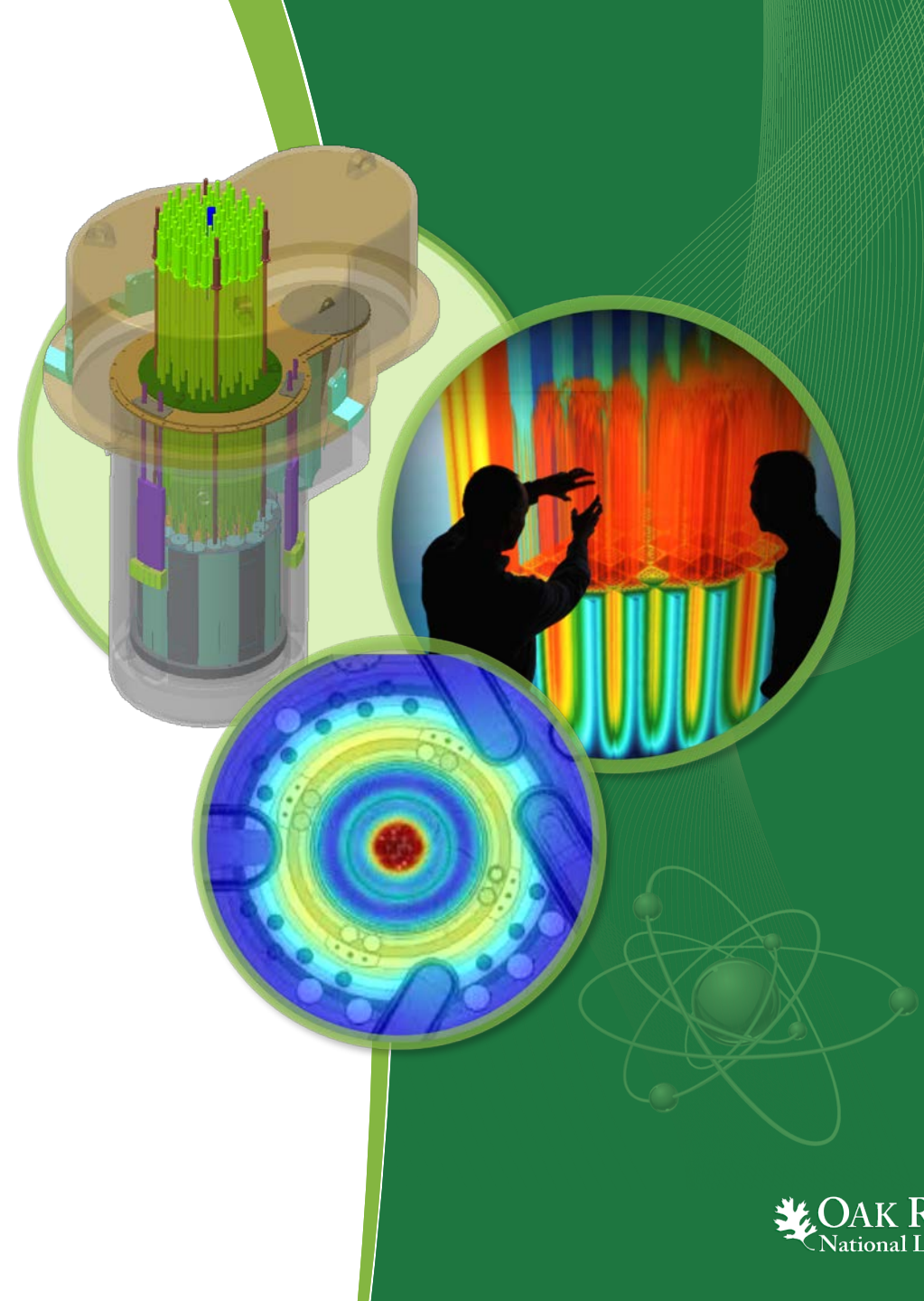
Instructors:
Will Wieselquist
Henrik Liljenfeldt



Outline

- Introduction to ORIGAMI
- ORIGAMI examples
 - Decay heat and activity for a typical W15x15 assembly
 - Calculate Pu content of a typical W17x17 assembly
 - Multicycle simulation with ORIGAMI

Introduction to ORIGAMI



ORIGAMI

- ORIGen AsseMbly Isotopics
- Motivation
 - perform many spent fuel calculations
 - U.S. Fuel Inventory analysis (200,000+ assemblies)
 - NRC Level 3 Probability Risk Assessment (3000+ assemblies)
 - SCALE 6.1 GUI (or any GUI impractical)
- In terms of SCALE modules:
ORIGAMI = ARP + ORIGEN w/ hint of TRITON
 - ARP to create a specific library
 - ORIGEN to solve problem
 - TRITON-style mixture and operating history specification

ORIGAMI Capabilities

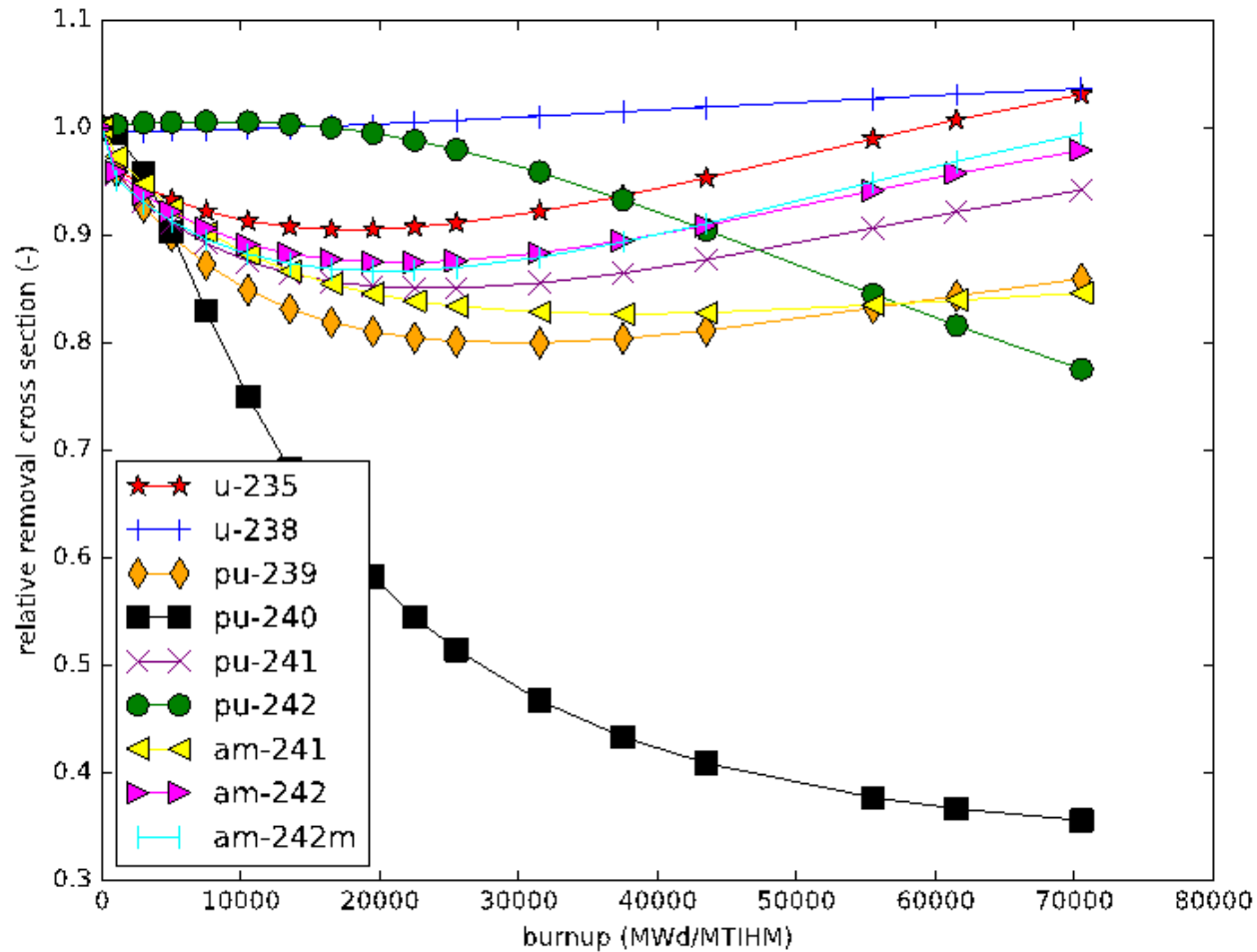
With a narrower scope, many convenient features

- Input capabilities
 - axial moderator density/power distributions
 - radial composition/ORIGEN library assignment (enables approximate pin-by-pin 3D depletion)
 - SCALE StdComp integration (e.g. zirc4)
- Output capabilities
 - produces complete f71 automatically
 - SCALE StdComp mix file
 - MCNP materials file
 - axial decay heat file

ORIGEN-ARP Methodology

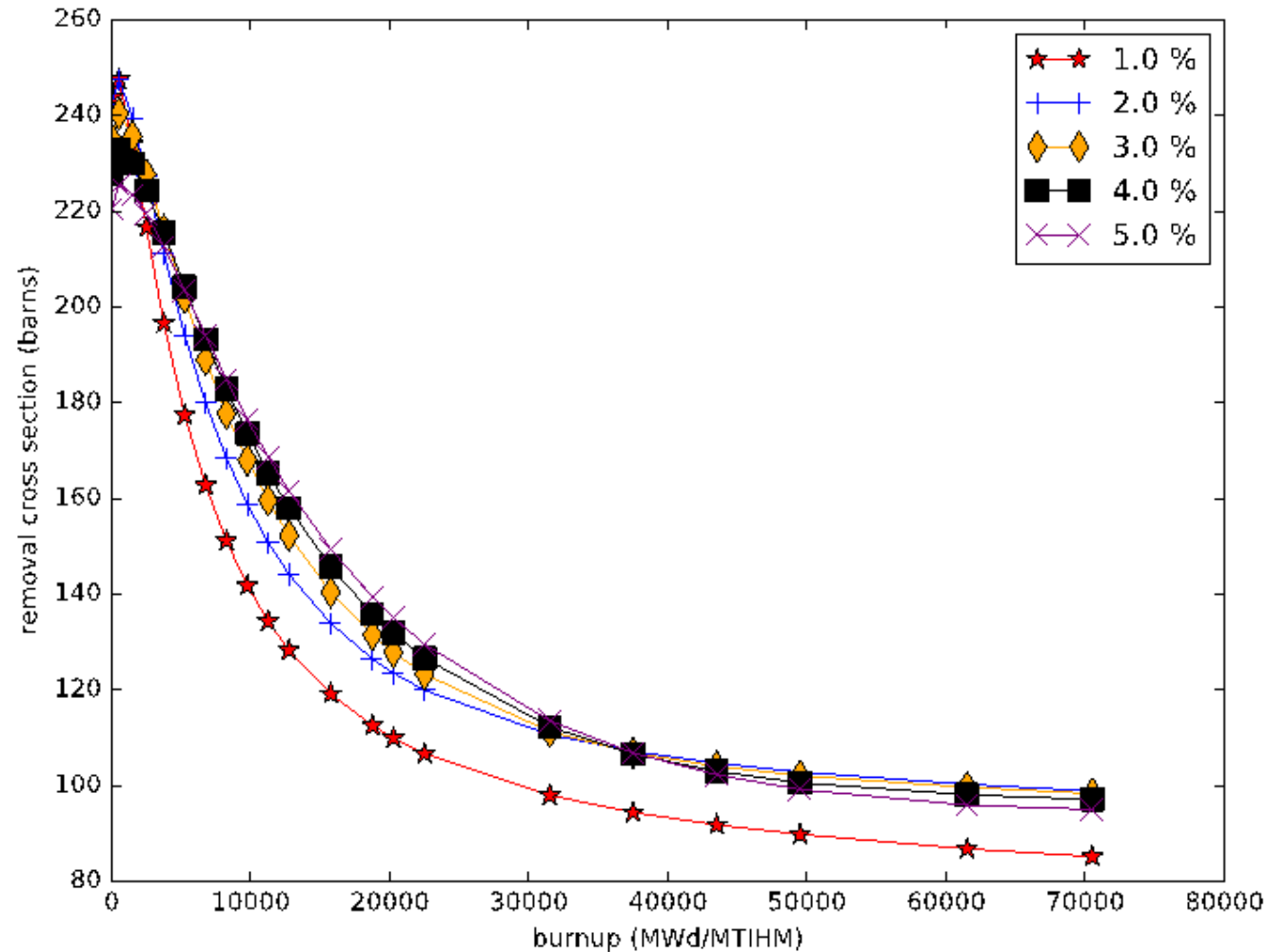
- Automated Rapid Processing (ARP)
- Developed as a way to use a set of TRITON calculations covering some space of assembly design/operation to predict isotopics at arbitrary burnups/decay times
- Could create isotopics "database" and interpolate
- Better to create cross section "database" and re-solve depletion for the new system (depletion is cheap)

Relative removal xs for various nuclides vs. burnup W17x17



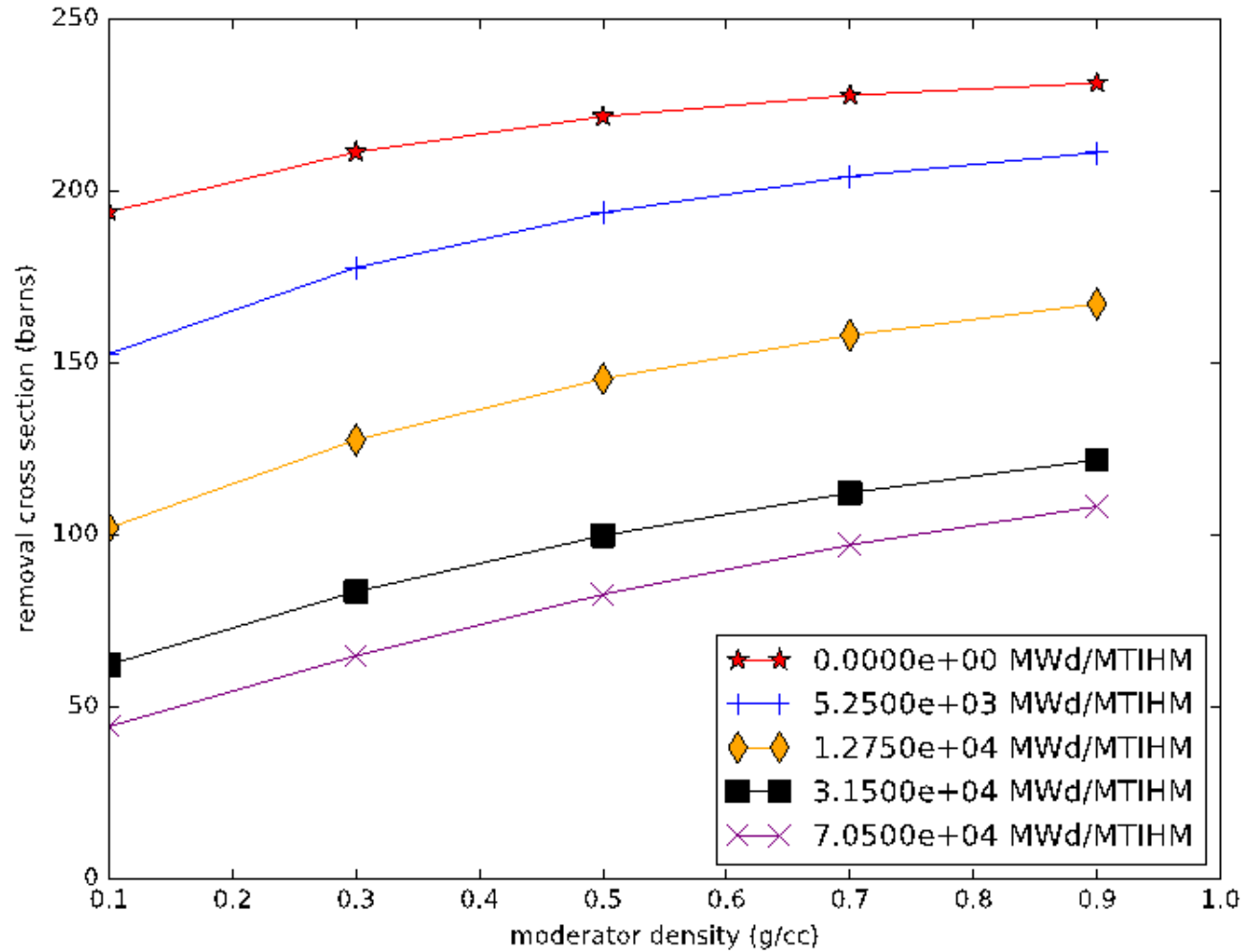
Pu-240 removal xs vs. burnup and enrichment

GE 10x10

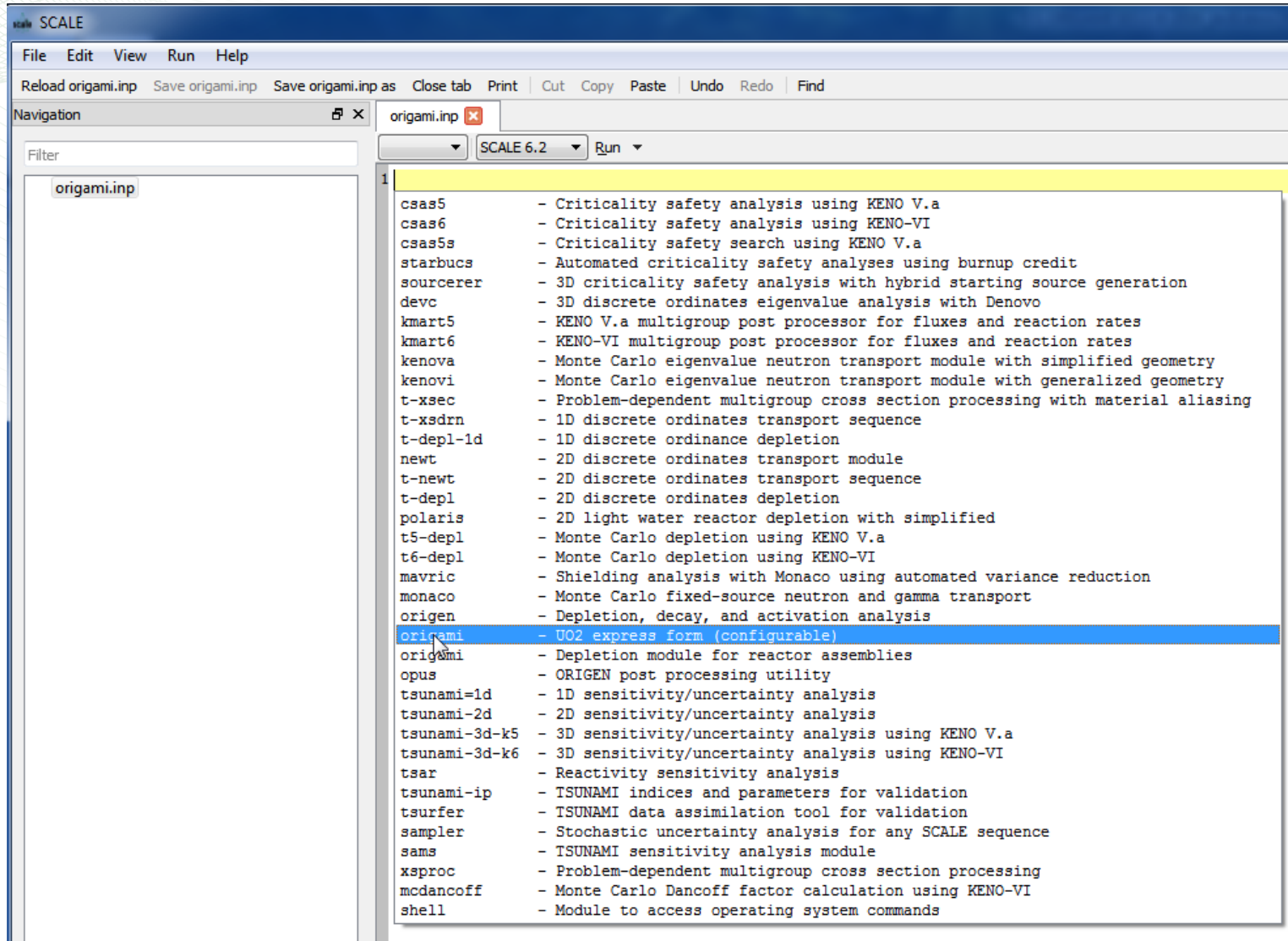


Pu-240 removal xs vs. burnup and moderator density

GE 10x10



ORIGAMI "Express Form"

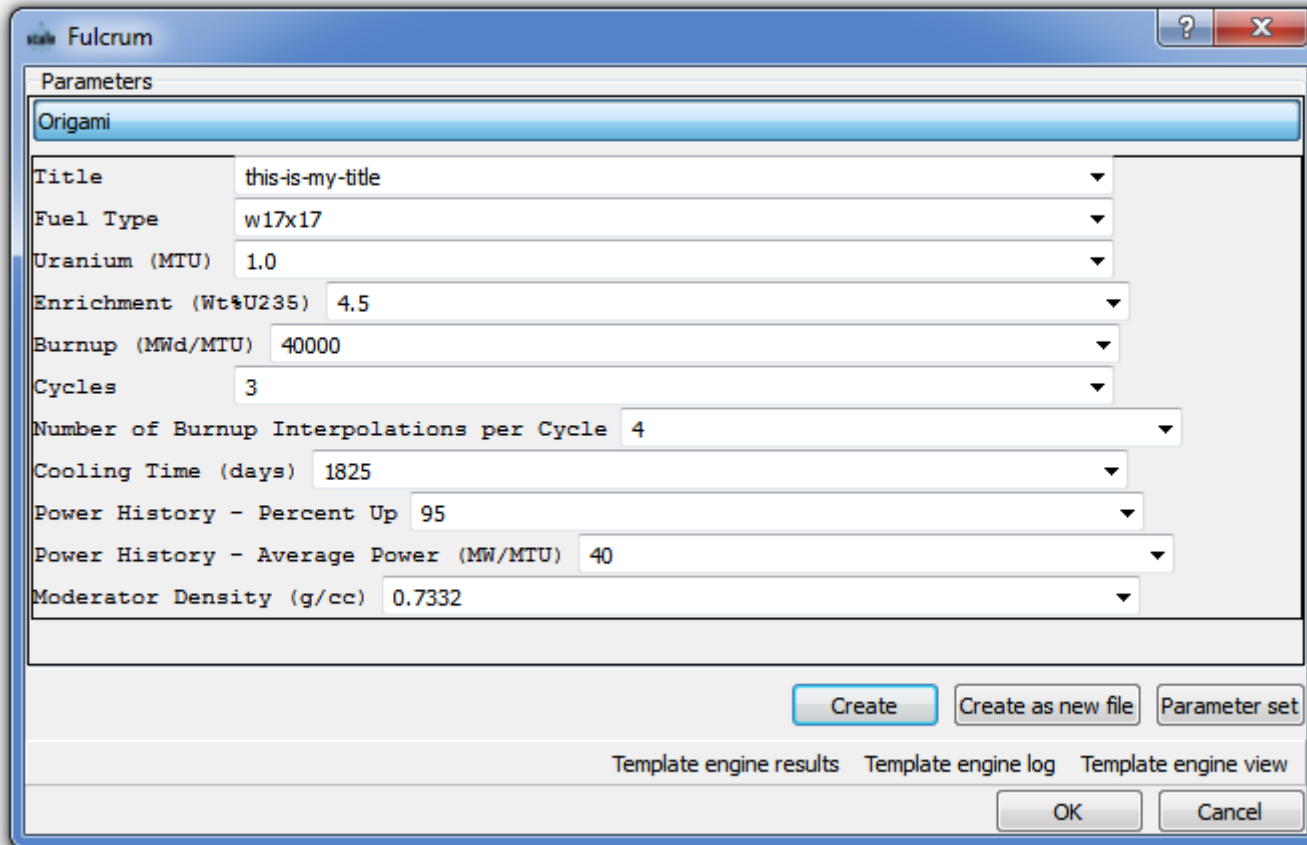


The screenshot shows the SCALE software interface. The main window displays a list of modules with their descriptions. The 'origami' module is highlighted in blue, indicating it is selected. The interface includes a menu bar (File, Edit, View, Run, Help), a toolbar with options like 'Reload origami.inp', 'Save origami.inp', 'Close tab', 'Print', 'Cut', 'Copy', 'Paste', 'Undo', 'Redo', and 'Find', and a 'Navigation' pane on the left showing the 'origami.inp' file. The main content area shows a list of modules with their descriptions:

```
1
csas5      - Criticality safety analysis using KENO V.a
csas6      - Criticality safety analysis using KENO-VI
csas5s     - Criticality safety search using KENO V.a
starbucs   - Automated criticality safety analyses using burnup credit
sourcerer  - 3D criticality safety analysis with hybrid starting source generation
devc       - 3D discrete ordinates eigenvalue analysis with Denovo
kmart5     - KENO V.a multigroup post processor for fluxes and reaction rates
kmart6     - KENO-VI multigroup post processor for fluxes and reaction rates
kenova     - Monte Carlo eigenvalue neutron transport module with simplified geometry
kenovi     - Monte Carlo eigenvalue neutron transport module with generalized geometry
t-xsec     - Problem-dependent multigroup cross section processing with material aliasing
t-xsdrrn   - 1D discrete ordinates transport sequence
t-depl-1d  - 1D discrete ordinates depletion
newt       - 2D discrete ordinates transport module
t-newt     - 2D discrete ordinates transport sequence
t-depl     - 2D discrete ordinates depletion
polaris    - 2D light water reactor depletion with simplified
t5-depl    - Monte Carlo depletion using KENO V.a
t6-depl    - Monte Carlo depletion using KENO-VI
mavric     - Shielding analysis with Monaco using automated variance reduction
monaco     - Monte Carlo fixed-source neutron and gamma transport
origen     - Depletion, decay, and activation analysis
origami    - UO2 express form (configurable)
origami    - Depletion module for reactor assemblies
opus       - ORIGEN post processing utility
tsunami-1d - 1D sensitivity/uncertainty analysis
tsunami-2d - 2D sensitivity/uncertainty analysis
tsunami-3d-k5 - 3D sensitivity/uncertainty analysis using KENO V.a
tsunami-3d-k6 - 3D sensitivity/uncertainty analysis using KENO-VI
tsar       - Reactivity sensitivity analysis
tsunami-ip - TSUNAMI indices and parameters for validation
tsurfer    - TSUNAMI data assimilation tool for validation
sampler    - Stochastic uncertainty analysis for any SCALE sequence
sams       - TSUNAMI sensitivity analysis module
xsproc     - Problem-dependent multigroup cross section processing
modancoff  - Monte Carlo Dancoff factor calculation using KENO-VI
shell      - Module to access operating system commands
```

- create empty file (origami.inp)
- CNTL+SPACE inside empty file
- choose "origami – UO2 express form (configurable)"

ORIGAMI "Express Form" (cont.)



The screenshot shows a software window titled "Fulcrum" with a sub-tab "Origami". The window contains a list of parameters for a nuclear reactor simulation, each with a text input field and a dropdown arrow. The parameters and their values are:

Parameter	Value
Title	this-is-my-title
Fuel Type	w17x17
Uranium (MTU)	1.0
Enrichment (Wt%U235)	4.5
Burnup (MWd/MTU)	40000
Cycles	3
Number of Burnup Interpolations per Cycle	4
Cooling Time (days)	1825
Power History - Percent Up	95
Power History - Average Power (MW/MTU)	40
Moderator Density (g/cc)	0.7332

At the bottom of the window, there are three buttons: "Create" (highlighted in blue), "Create as new file", and "Parameter set". Below these buttons are three tabs: "Template engine results", "Template engine log", and "Template engine view". At the very bottom, there are "OK" and "Cancel" buttons. A mouse cursor is visible near the bottom center of the window.

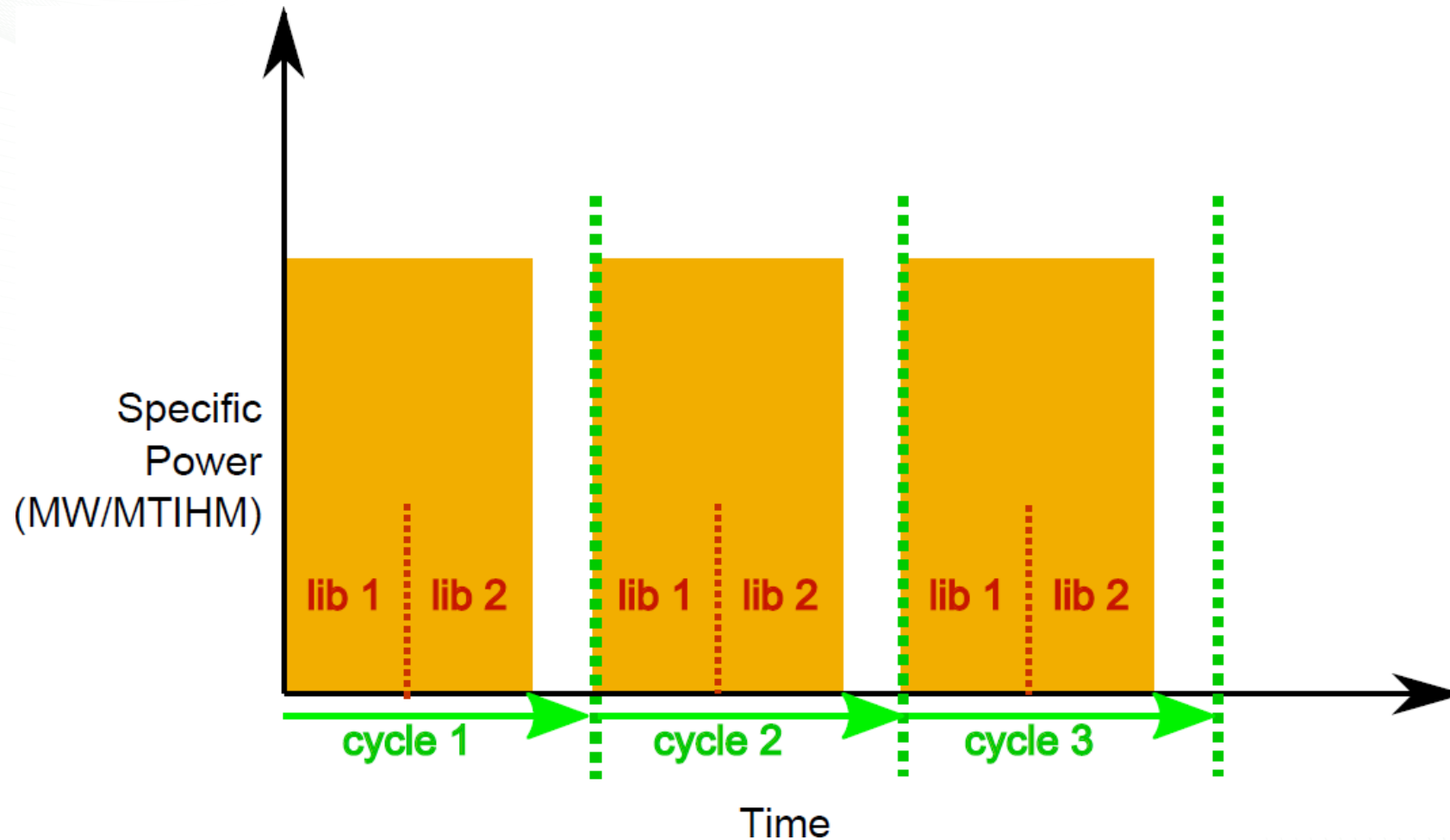
- window will appear
- click "Create"
- click "OK"

ORIGAMI "Express Form" (cont.)

```
origami.inp* x
document SCALE 6.2 Run
1 =origami
2
3 title="this-is-my-title"
4 options{ mtu=1.0 ft71=all}
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10 modz=[ 0.7332 ]
11 pz=[ 1.0 ]
12 hist[
13   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
14   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
15   cycle{ power=40 burn=333.33 nlib=4 down=0 }
16   cycle{ down=1825 }
17 ]
18
19 end
20
21
```

- This is a valid ORIGAMI input!
- click Run

Controlling Cross Section Interpolation (libraries per cycle)



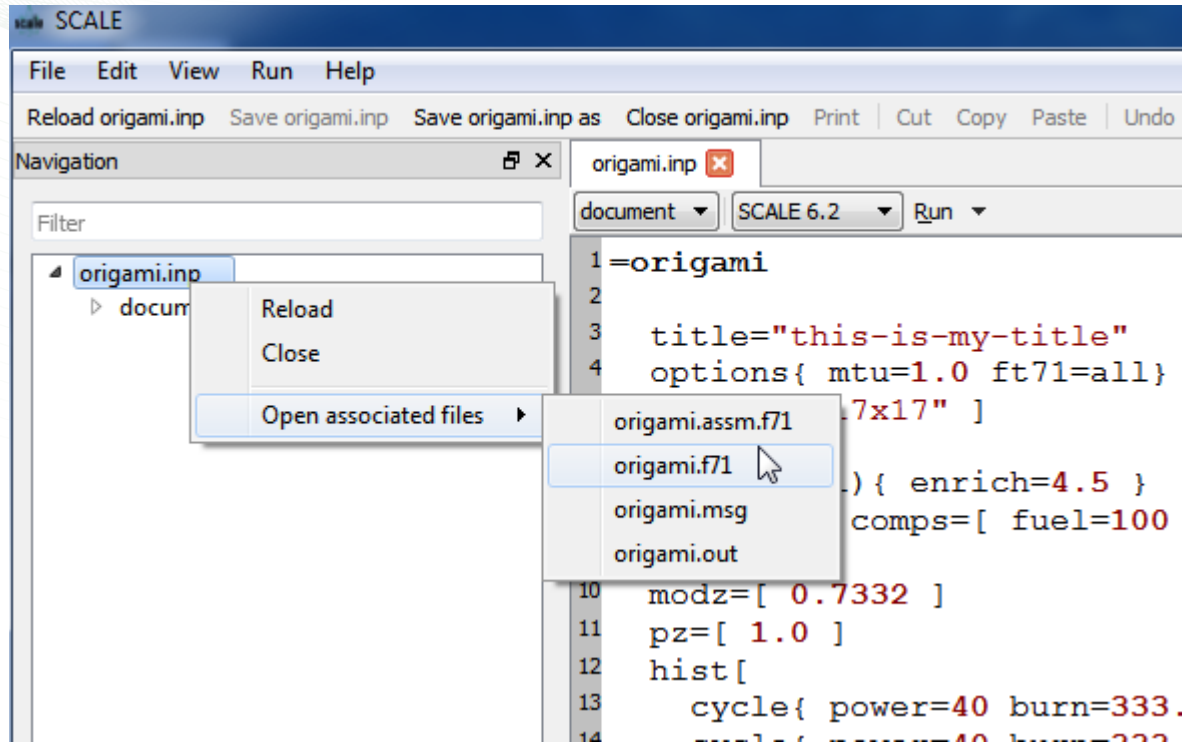
ORIGAMI "Express Form" (cont.)

```
Wed Feb 17 17:13:11 2016 x Wed Feb 17 17:19:44 2016 x
9 *
10 *           Reactor and Nuclear Systems Division *
11 *           Oak Ridge National Laboratory *
12 *
13 *           http://scale.ornl.gov *
14 *           scalehelp@ornl.gov *
15 *
16 *****
17 *****
18
19           Job Information
20           -----
21 Job started on PC0091974 on Wed 17/02/2016 17:19:44
22 Working directory: C:\Users\ww5\AppData\Local\Temp\scale.ww5.13016
23 Input file name   : C:\Users\ww5\Desktop\origami.inp
24 Output file name  : C:\Users\ww5\Desktop\origami.out
25 SCALE executable  : C:\SCALE-6.2\bin\scale
26
27 *****
28
29
30 Now depleting axial zone: 001, pin: 01-01
31
32
33 Scale job C:/Users/ww5/Desktop/origami.inp is finished.
34 Output is stored in C:\Users\ww5\Desktop\origami.out
35
36 Process finished with 0 return code; ran in 13 secs, finished at Wed Feb 17 17:19:57 2016
```

ORIGAMI takes a little while...

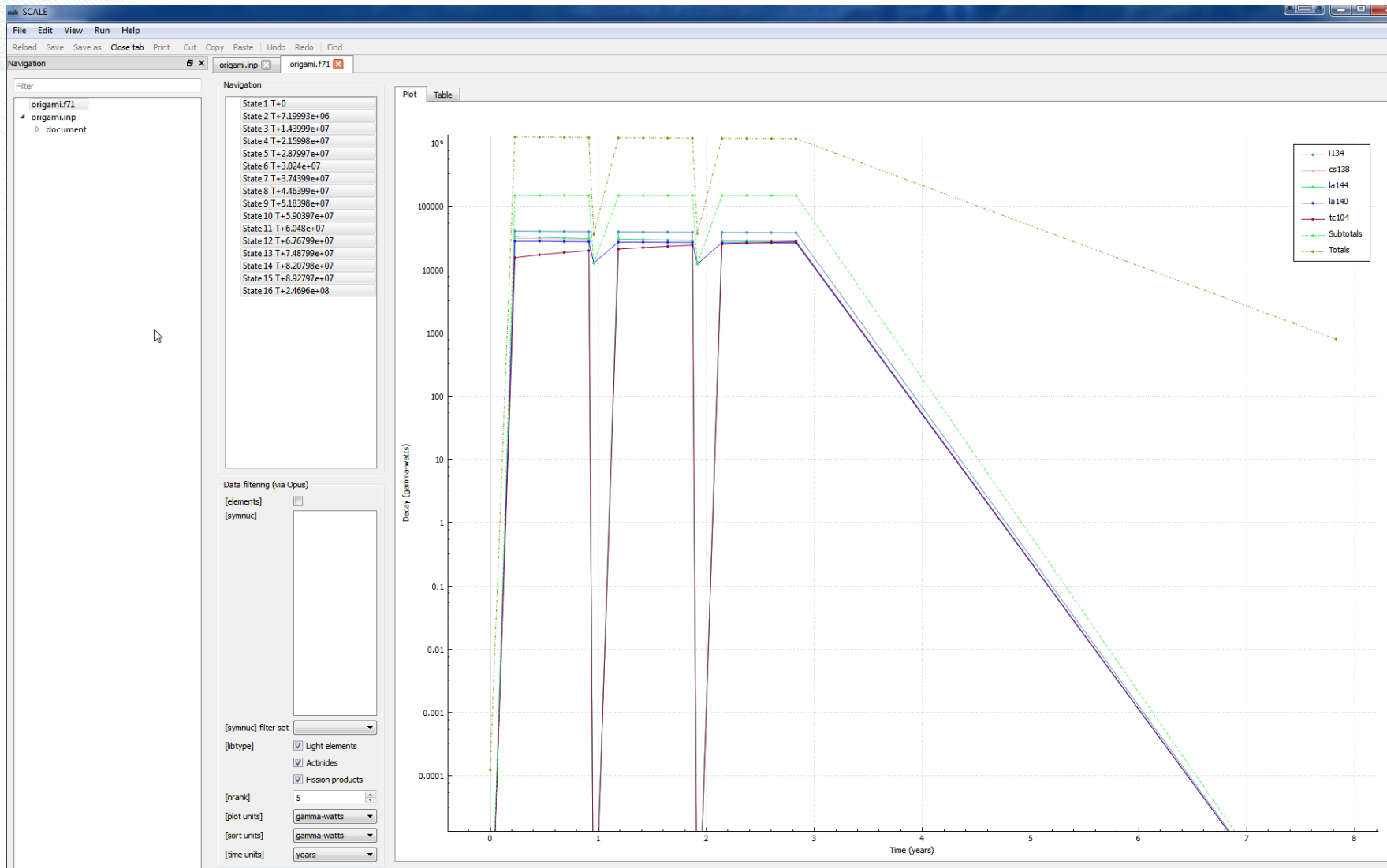
- performs by default 10 substeps
 - depletion equal length
 - decay rule of 3s
- nlib=4 would require 4 cases in ORIGEN
- the input to the left is $(4+4+4+1)*10=130$ depletion solves

ORIGAMI "Express Form" (cont.)



- ORIGAMI produces .f71 and .assm.f71 by default
- open .f71
 - right-click on origami.inp in navigation pane
 - open associated files
 - origami.f71

ORIGAMI "Express Form" (cont.)



- .f71 has all regions, all times
- .assm.f71 has only final time for each axial zone and total

ORIGAMI Input

```
origami.inp* x
document SCALE 6.2 Run
1 =origami
2
3 title="this-is-my-title"
4 options{ mtu=1.0 ft71=all}
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10 modz=[ 0.7332 ]
11 pz=[ 1.0 ]
12 hist[
13   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
14   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
15   cycle{ power=40 burn=333.33 nlib=4 down=0 }
16   cycle{ down=1825 }
17 ]
18
19 end
20
21
```

- **title** – set a descriptive title
- **options** – various global options
- **fuelcomp** – declare mixtures (single mixture problems use 1)
- **modz** – axial moderator density
- **pz** – axial power shape
- **hist** – operating history

ORIGAMI Input: power history

```
origami.inp* x
document SCALE 6.2 Run
1 =origami
2
3 title="this-is-my-title"
4 options{ mtu=1.0 ft71=all}
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10 modz=[ 0.7332 ]
11 pz=[ 1.0 ]
12 hist[
13   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
14   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
15   cycle{ power=40 burn=333.33 nlib=4 down=0 }
16   cycle{ down=1825 }
17 ]
18
19 end
20
21
```

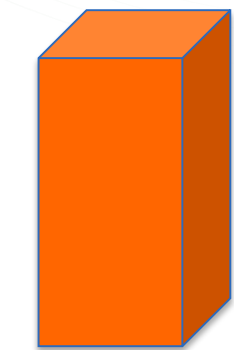
TRITON-style operating history

- **cycle**

- **power** assembly-average specific power in MW/MTIHM
- **burn** time in days at power
- **nlib** number of times to re-interpolate cross sections to current burnup
- **down** time in days of decay

ORIGAMI spatial variation

- power shape \rightarrow axial & radial $\rightarrow p(z) \times p(x, y)$
- moderator density \rightarrow axial only $\rightarrow m(z)$
- fuel composition \rightarrow radial only $\rightarrow c(x, y)$



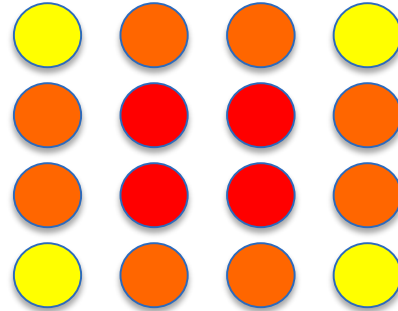
\bar{p}
 \bar{m}
 \bar{c}

0D
assembly



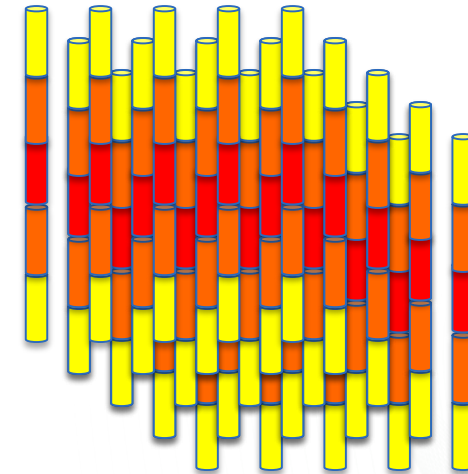
$p(z)$
 $m(z)$
 \bar{c}

1D
assembly



$p(x, y)$
 \bar{m}
 $c(x, y)$

2D
assembly



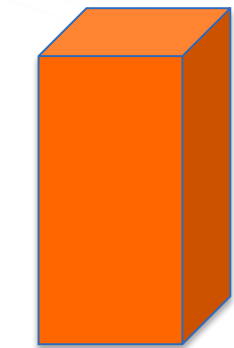
$p(x, y) \times p(z)$
 $m(z)$
 $c(x, y)$

3D
assembly

ORIGAMI spatial variation

- limitations

- *no time-dependence*
- *axially-dependent compositions really needed for BWRs*



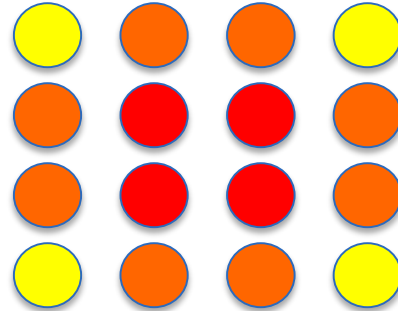
\bar{p}
 \bar{m}
 \bar{c}

0D
assembly



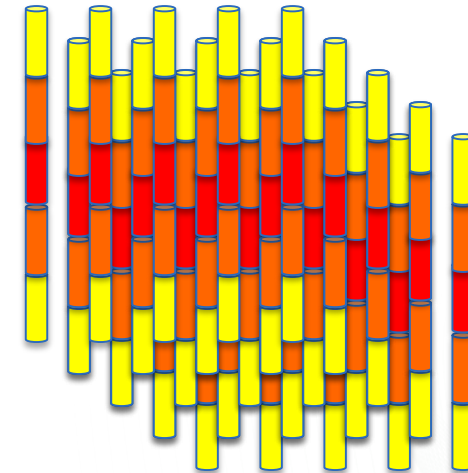
$p(z)$
 $m(z)$
 \bar{c}

1D
assembly



$p(x, y)$
 \bar{m}
 $c(x, y)$

2D
assembly



$p(x, y) \times p(z)$
 $m(z)$
 $c(x, y)$

3D
assembly

ORIGAMI Input: fuel composition

```
origami.inp* x
document SCALE 6.2 Run
1 =origami
2
3 title="this-is-my-title"
4 options{ mtu=1.0 ft71=all}
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10 modz=[ 0.7332 ]
11 pz=[ 1.0 ]
12 hist[
13   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
14   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
15   cycle{ power=40 burn=333.33 nlib=4 down=0 }
16   cycle{ down=1825 }
17 ]
18
19 end
20
21
```

TRITON-inspired mixtures

- **mix(N)**
 - N mixture index
 - **comps** array of composition names and wt. %
- **uox(name){...}**
 - creates a SCALE StdComp UO₂ Mixture
- StdComp has everything (zirc4, gd2o3, etc.)

ORIGAMI Input: libs

```
origami.inp* x
document SCALE 6.2 Run
1 =origami
2
3 title="this-is-my-title"
4 options{ mtu=1.0 ft71=all}
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10 modz=[ 0.7332 ]
11 pz=[ 1.0 ]
12 hist[
13   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
14   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
15   cycle{ power=40 burn=333.33 nlib=4 down=0 }
16   cycle{ down=1825 }
17 ]
18
19 end
20
21 NOTE: pinmap controls radial distribution of libraries
    DEFAULT: pinmap=[1]
```

ORIGEN reactor library names in ARPDATA.txt

- **libs= ["w17x17"]**
 - declares library 1 to be "w17x17", i.e. could be anything in ORIGEN reactor libraries
 - with radial layout, can have different libraries for each radial ("pin") location
- a single entry is typical

ORIGAMI Input: modz & pz

```
origami.inp* x
document SCALE 6.2 Run
1 =origami
2
3 title="this-is-my-title"
4 options{ mtu=1.0 ft71=all}
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10 modz=[ 0.7332 ]
11 pz=[ 1.0 ]
12 hist[
13   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
14   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
15   cycle{ power=40 burn=333.33 nlib=4 down=0 }
16   cycle{ down=1825 }
17 ]
18
19 end
20
21
```

axial power and moderator distribution

- **modz**

- density in g/cm^3 of moderator (used to interpolate the cross sections for T/H feedback)
- NOTE: not all reactor libraries have density variations

- **pz**

- axial power shape (unitless)
- renormalized by default

ORIGAMI Input: options

```
origami.inp* x
document SCALE 6.2 Run
1 =origami
2
3 title="this-is-my-title"
4 options{ mtu=1.0 ft71=all}
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10 modz=[ 0.7332 ]
11 pz=[ 1.0 ]
12 hist[
13   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
14   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
15   cycle{ power=40 burn=333.33 nlib=4 down=0 }
16   cycle{ down=1825 }
17 ]
18
19 end
20
21
```

miscellaneous input

- **mtu**
 - metric tons of initial heavy metal (not just U)
 - used to convert to power in MW
 - DEFAULT: 1 MTU
- **ft71**
 - flag to write f71 file last/cycle/all
- **other options**
 - **stdcomp** write SCALE StdComp blocks
 - **mcnp** write MCNP materials cards

Axial Distribution Example

```
1 =origami
2
3 title="W17x17 Assembly wtih Axial Distribution"
4 options{ mtu=1.0 ft71=all }
5 libs=[ "w17x17" ]
6 fuelcomp{
7   uox(fuel){ enrich=4.5 }
8   mix(1){ comps=[ fuel=100 ] }
9 }
10
11 meshz=[0    50    100    200    300    350]
12 modz  =[ 0.73  0.72  0.71   0.70  0.69   ]
13 pz    =[ 0.80  0.90  1.00   0.85  0.75   ]
14
15 hist[
16   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
17   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
18   cycle{ power=40 burn=333.33 nlib=4 down=0 }
19   cycle{ down=1825 }
20 ]
21
22 end
```

5 axial zones

- **meshz**
 - heights of zones (cm)
- **modz**
 - decreases from bottom to top of core
- **pz**
 - peak in middle

Axial Distribution Uses

```
1 =origami
2
3  title="W17x17 Assembly wtih Axial Distribution"
4  options{ mtu=1.0 ft71=all }
5  libs=[ "w17x17" ]
6  fuelcomp{
7    uox(fuel){ enrich=4.5 }
8    mix(1){ comps=[ fuel=100 ] }
9  }
10
11 meshz=[0    50    100    200    300    350]
12 modz  =[ 0.73  0.72  0.71  0.70  0.69  ]
13 pz    =[ 0.80  0.90  1.00  0.85  0.75  ]
14
15 hist[
16   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
17   cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
18   cycle{ power=40 burn=333.33 nlib=4 down=0 }
19   cycle{ down=1825 }
20 ]
21
22 end
```

- produce axial decay heat sources
- evaluate impact of moderator density variations
- fork detector modeling for non-destructive assay

ORIGAMI Disclaimers

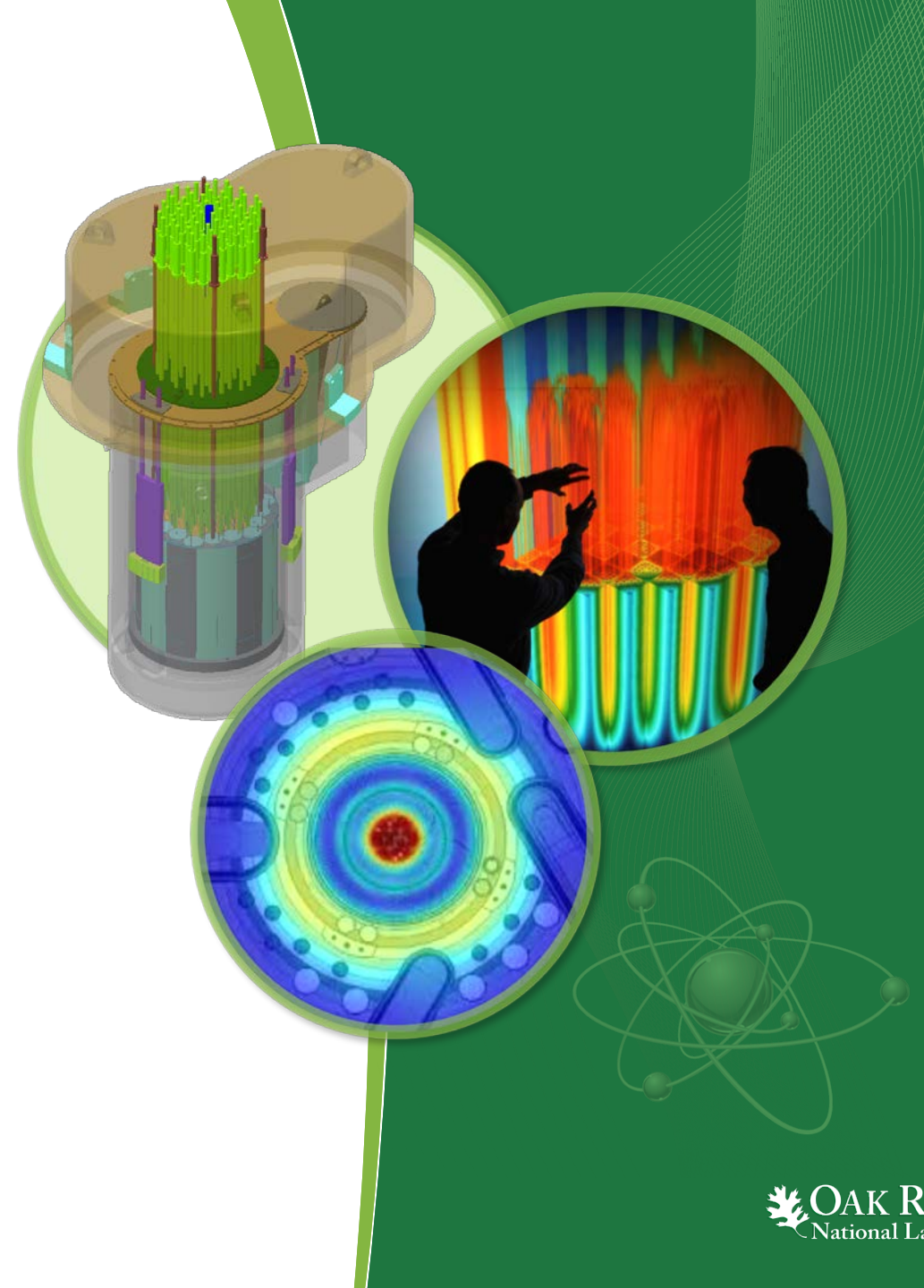
- ORIGEN reactor libraries distributed with SCALE are assembly-average cross sections from 2D TRITON calculations
 - axial distributions make sense
 - "pin-by-pin" radial distributions really need pin-average libraries (which you can also get from TRITON!)
- ORIGAMI composition input not checked for consistency with library
 - for high-fidelity, must be similar to the original TRITON composition
 - similar = not introduce any strong spectral or self-shielding differences

ORIGAMI Summary

- Short, concise interface to ARP+ORIGEN for spent fuel calcs
- Good default parameter settings for LWR UO₂
- Allows axial variations to be investigated (radial, too)
- Produces f71 file automatically
 - readily viewed in Fulcrum
 - used to seed an ORIGEN calculation
 - post-processing with OPUS

ORIGAMI Examples

Problem description



Problem 1 Decay heat and activity for W15x15

- Use Origami express form to calculate radioactivity (Becquerels) and total decay heat (Watts) for a Westinghouse 15x15 fuel assembly:
 - 2.5 wt % U-235 enrichment
 - 3 cycles
 - 45,000 MWd/MTU burnup
 - 10 year cooling
 - 90% uptime
 - 32 MW/MTU average power
- Express results at 10 year cooling time

Problem 2: Pu content of typical W17x17 assembly

- Calculate the Pu content for a typical W17x17 assembly at 15, 30, and 45 GWd/MTU discharge burnups at 0 and 10 years cooling time (6 cases total)
 - kg Pu/MTU
 - fissile Pu content as weight % $(^{239}\text{Pu} + ^{241}\text{Pu})/\text{Pu}$
- Input data:
 - enrichment 4.5 wt% ^{235}U
 - power 30 MW/MTU
 - keep default for everything else

Problem 3 Origami multicycle problem

- Assume a W17x17 reactor library
- Fuel enrichment 5.0 wt% U-235
- Initial fuel composition in grams/basis (basis 1MTU)

$$\text{U-234} = 445$$

$$\text{U-235} = 50000$$

$$\text{U-236} = 230$$

$$\text{U-238} = 949325$$

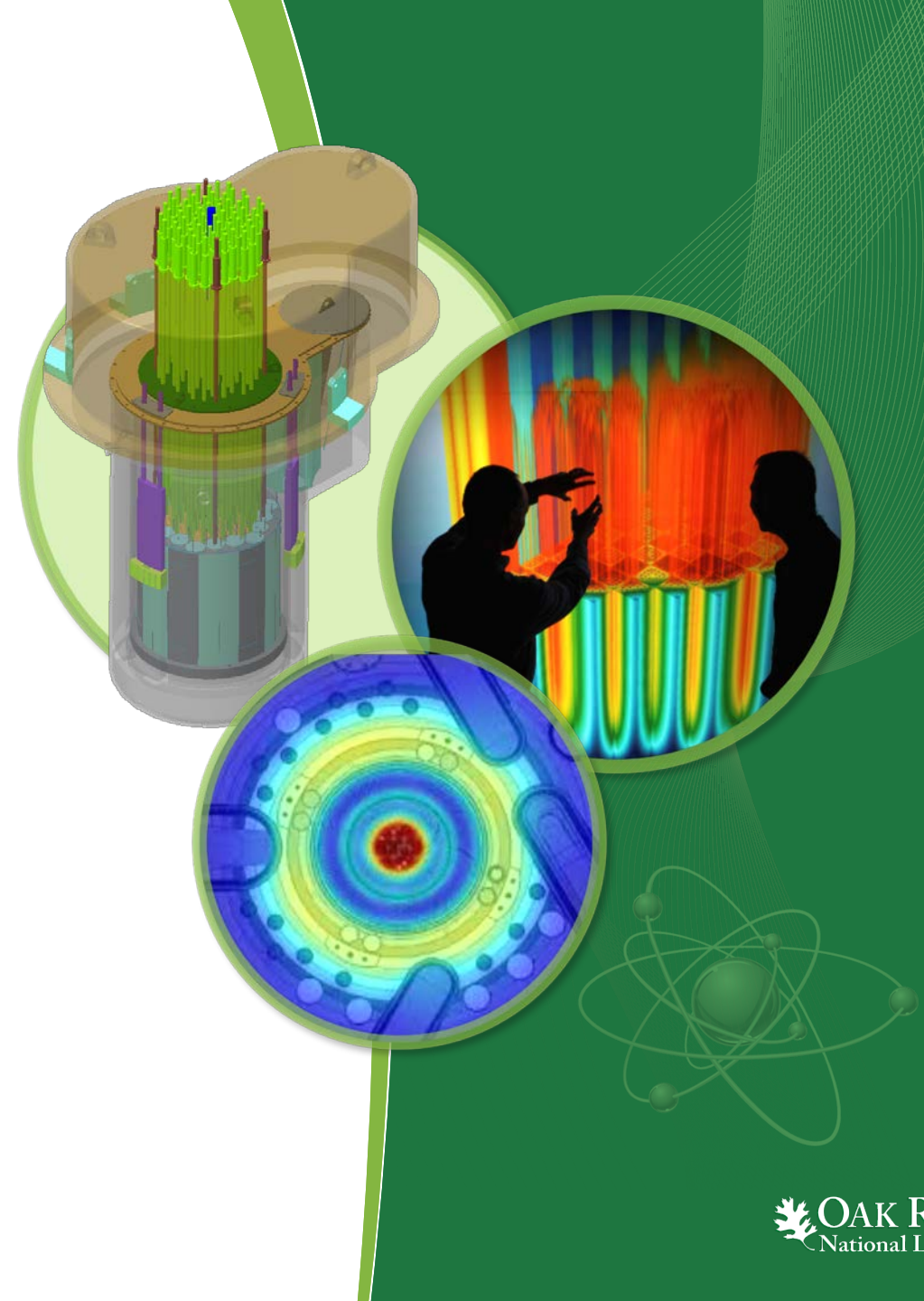
$$\text{O} = 1.34432\text{e}5$$

Problem 3 Origami multicycle problem (cont.)

- Irradiation history data
 - 3 cycles
 - Cycle length: 540 days
 - Downtime between cycles: 30 days
 - Cooling time (after 3d cycle): 10 years
 - Specific power (MW/MTU) for each cycle: 20, 19, 18
 - Number of libraries per cycle: 2, 2, 1
- Print isotopic compositions (in grams/basis) for selected actinides and fission products at 10 years cooling time
 - U-235, Pu-238, Pu-239, Pu-240, Pu-241, Am-241, Cm-244
 - Cs-134, Cs-137, Sm-149, Gd-155

ORIGAMI Examples

Solutions



Problem 1 Decay heat and activity for W15x15

- Decay heat = 1724.76 W/MTU at 10 years cooling
- Activity = $1.87e+16$ Bq ($5e+05$ Ci) at 10 years cooling

Problem 2: Pu content of typical W17x17 assembly

Discharge burnup (GWd/MTU)	Cooling time (years)	
	0	10
15	5.589 kg/MTU (85.33% fissile)	5.501 kg/MTU (85.10% fissile)
30	9.094 kg/MTU (76.52% fissile)	8.740 kg/MTU (75.56% fissile)
45	11.420 kg/MTU (68.92% fissile)	10.870 kg/MTU (67.22% fissile)

Problem 3 Origami multicycle problem

Nuclide	g/MTU
U-235	2.193E+04
Pu-238	1.148E+02
Pu-239	6.070E+03
Pu-240	1.711E+03
Pu-241	6.608E+02
Am-241	4.642E+02
Cm-244	5.275E+00
Cs-134	2.613E+00
Cs-137	8.843E+02
Sm-149	3.494E+00
Gd-155	4.457E+00