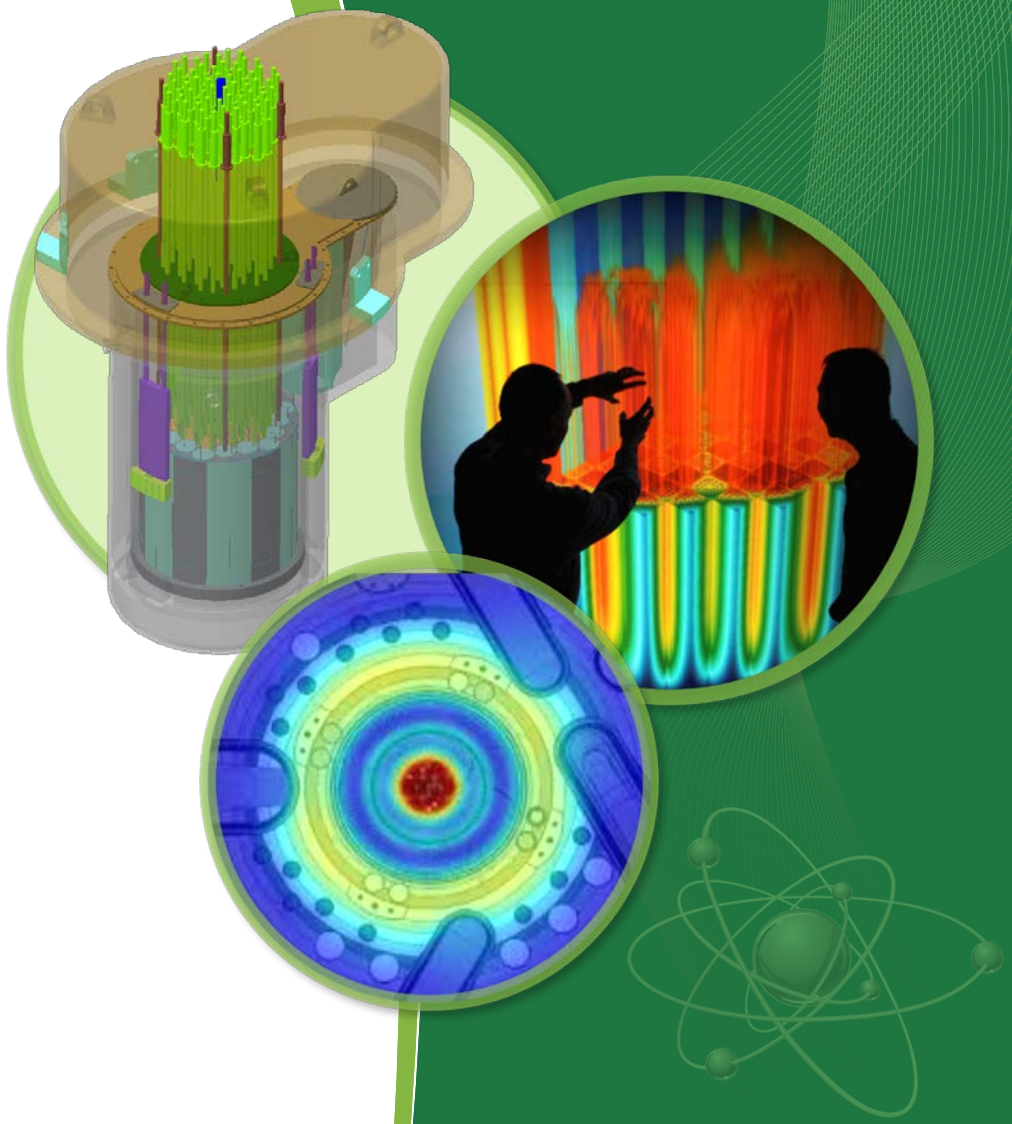
ORIGAMI Spent Fuel Characterization Tutorial



SCALE Users' Group Workshop

September 28, 2017

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Henrik Liljenfeldt

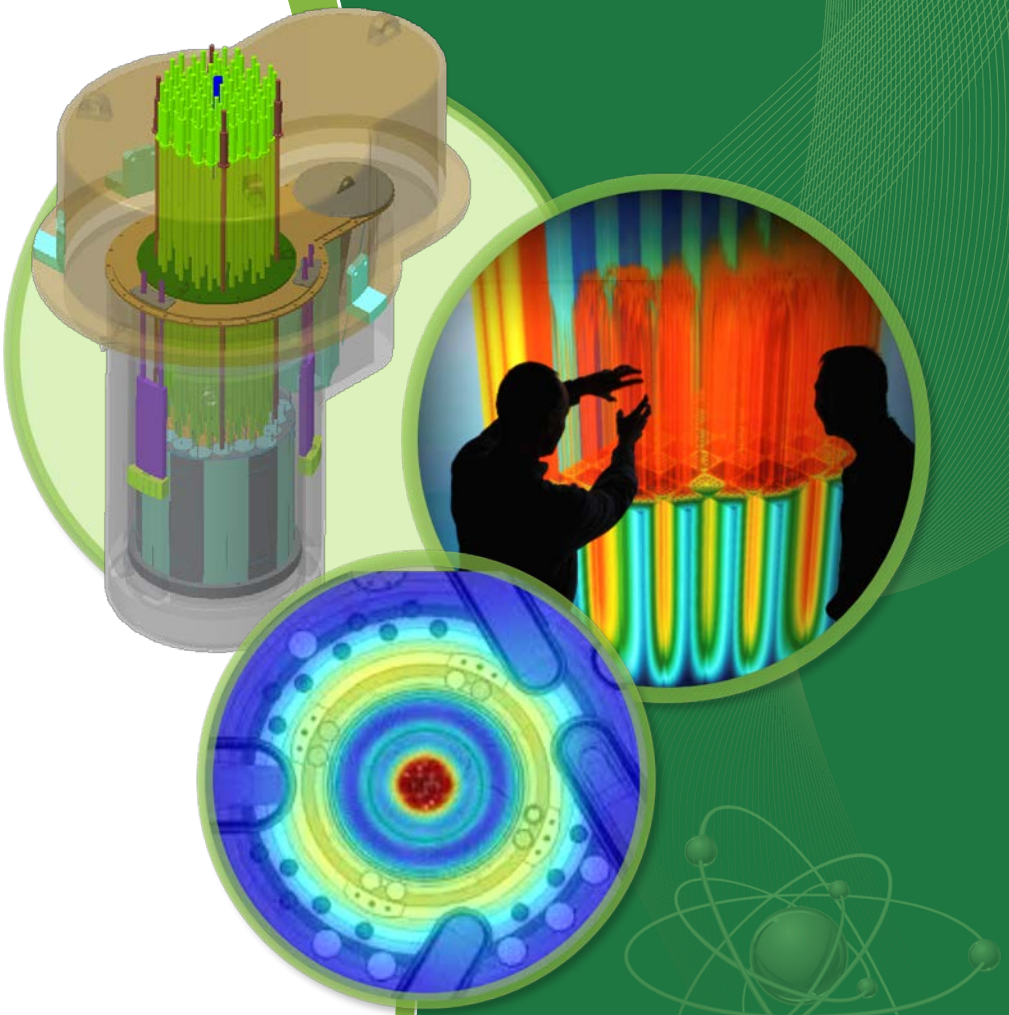
ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

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

- **ORIG**en **A**sse**M**bly **I**sotopics
- 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

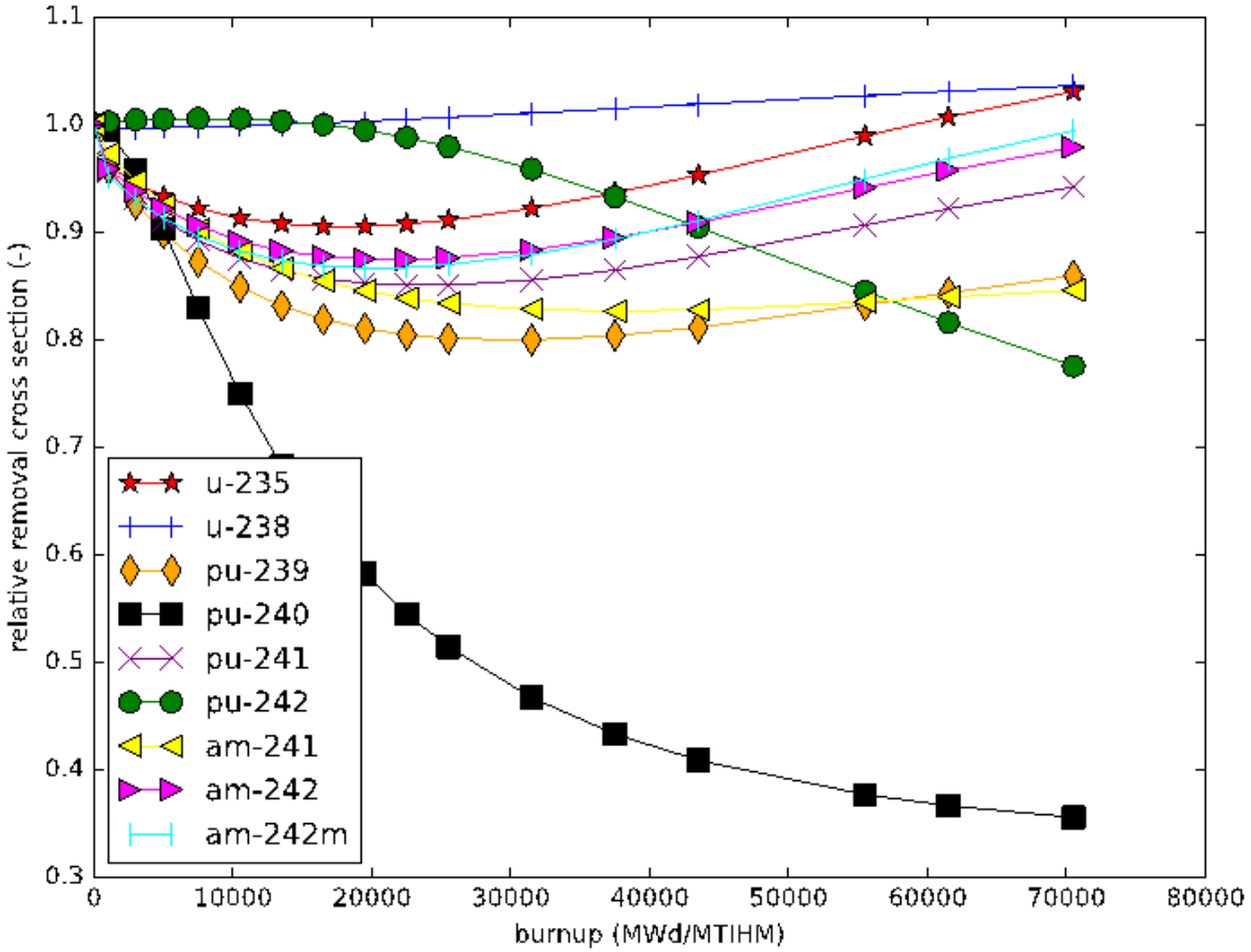
With a narrower scope, many convenient features

- 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

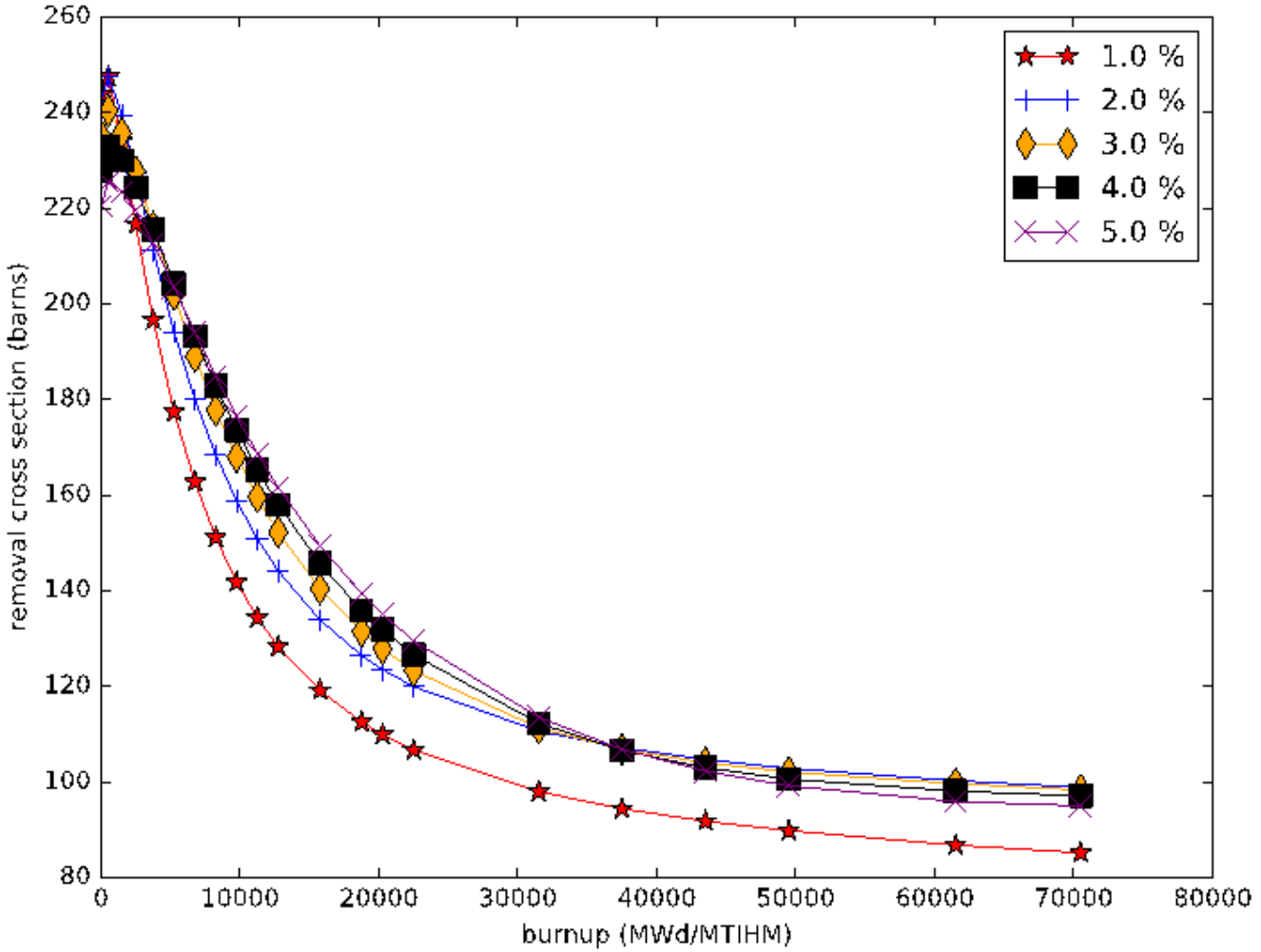
ORIGEN-ARP Methodology

- 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)

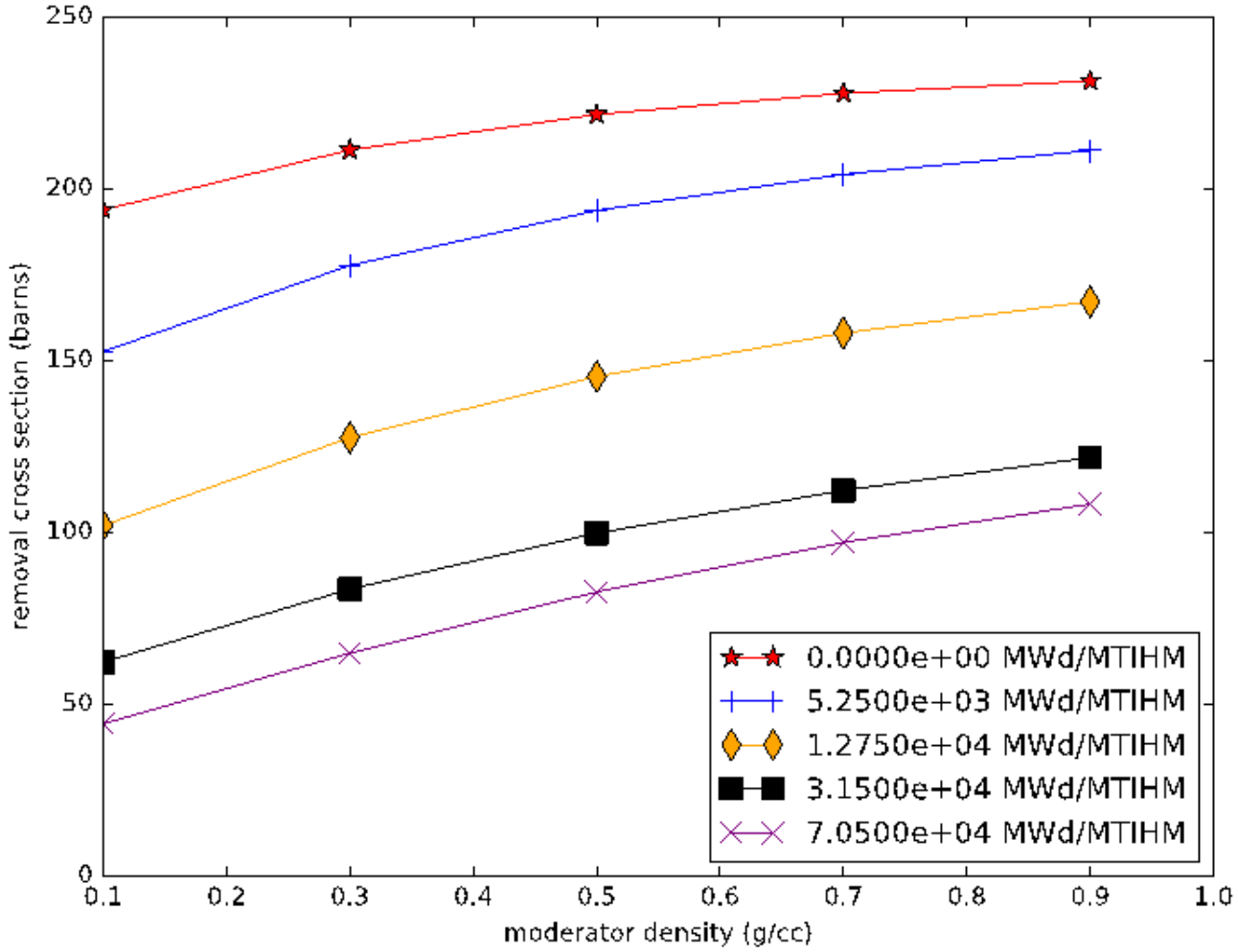
Relative removal xs for various nuclides vs. burnup
W17x17



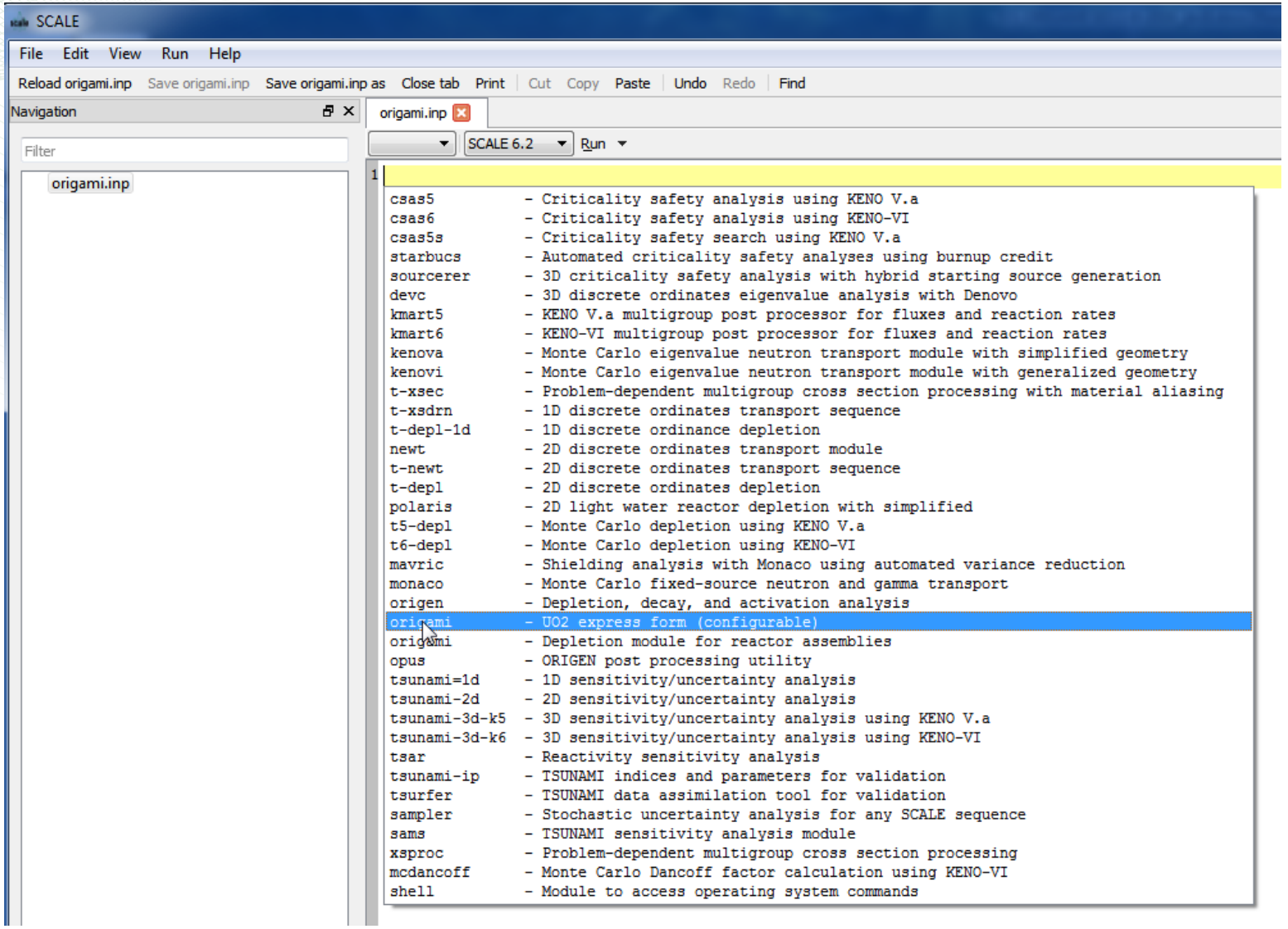
Pu-240 removal xs vs. burnup and enrichment
GE 10x10



Pu-240 removal xs vs. burnup and moderator density
GE 10x10

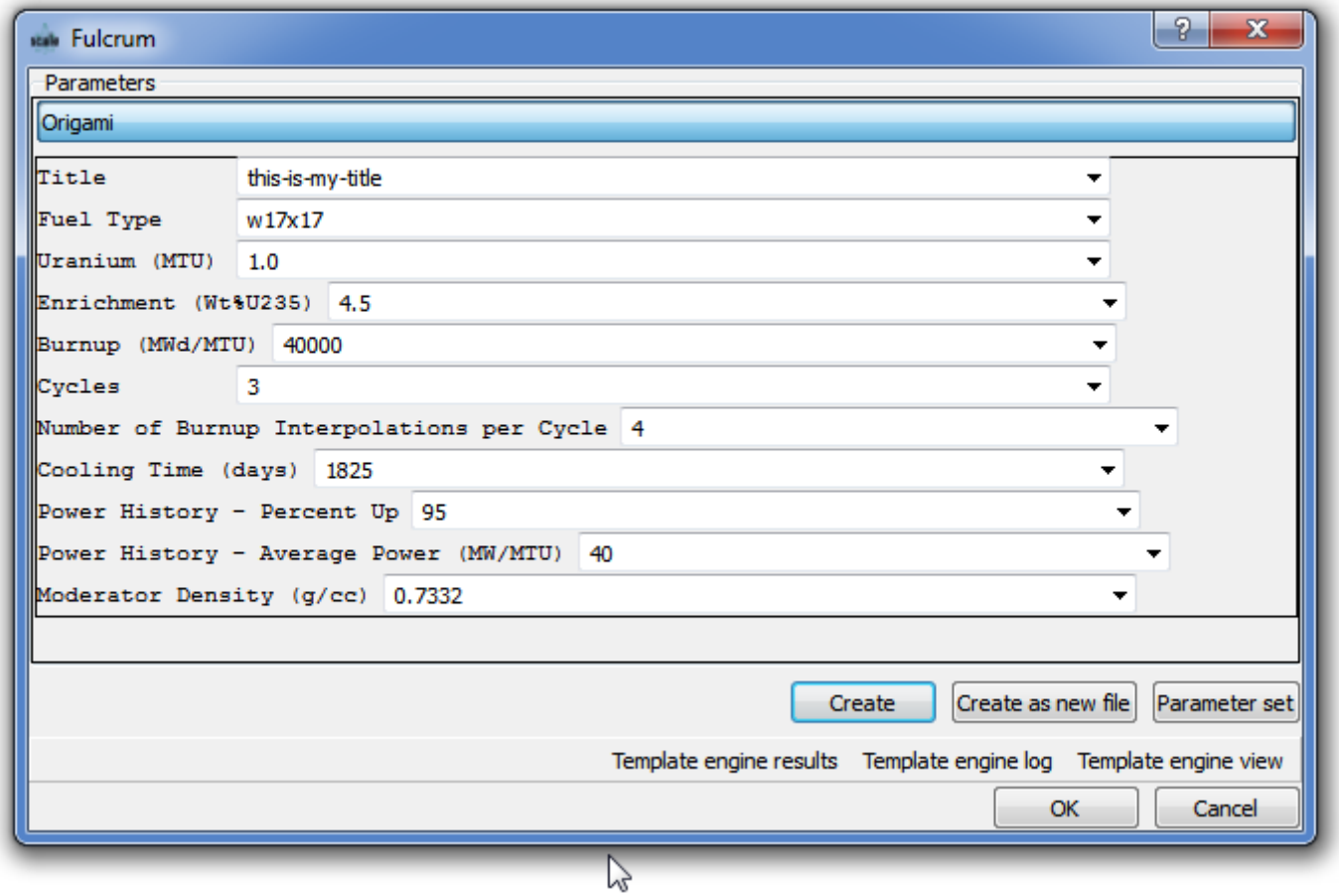


ORIGAMI "Express Form"



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

ORIGAMI "Express Form" (cont.)



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

ORIGAMI "Express Form" (cont.)

origami.inp*

document | SCALE 6.2 | Run

```
=origami

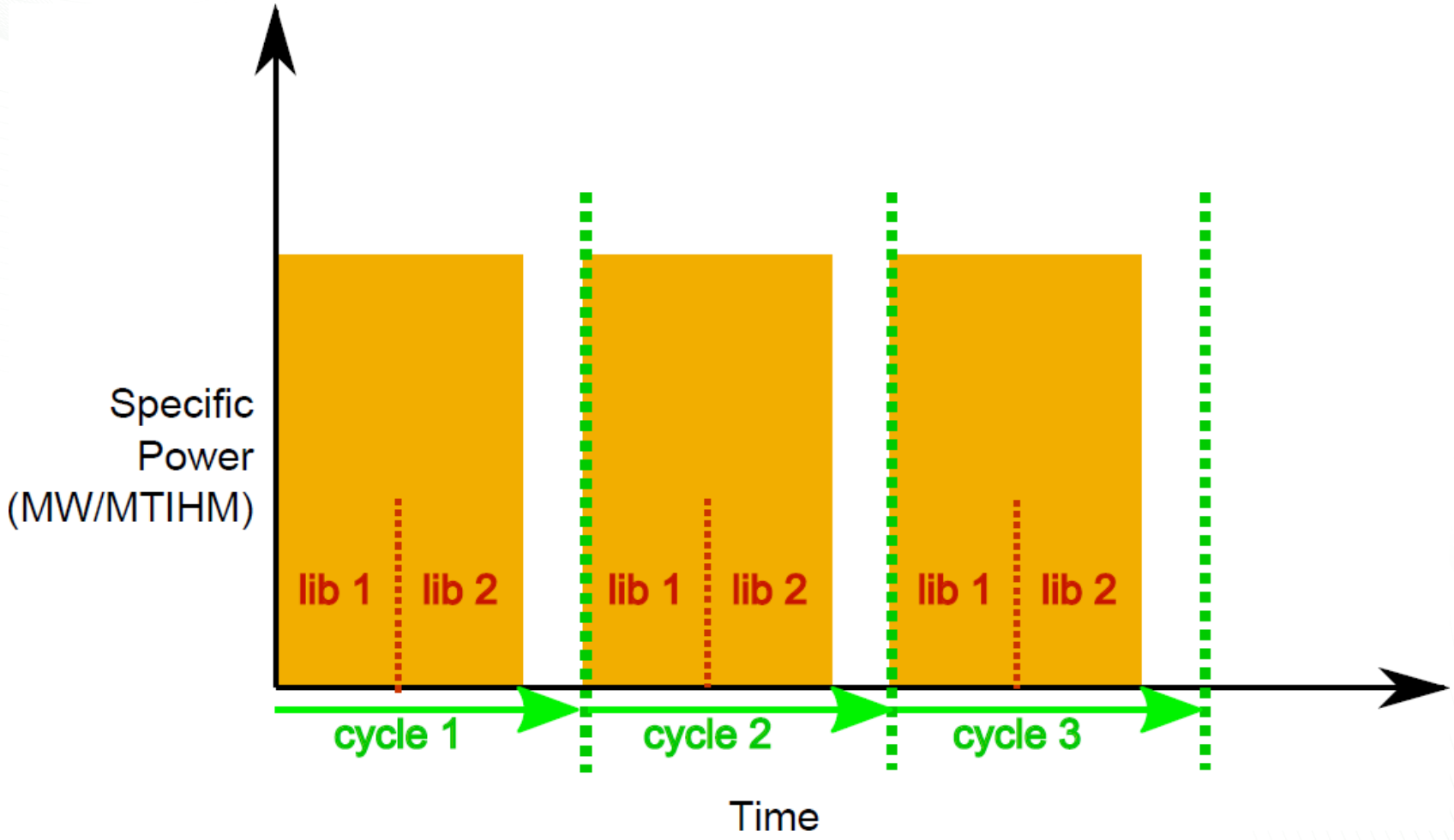
  title="this-is-my-title"
  options{ mtu=1.0 ft71=all}
  libs=[ "w17x17" ]
  fuelcomp{
    uox(fuel){ enrich=4.5 }
    mix(1){ comps=[ fuel=100 ] }
  }
  modz=[ 0.7332 ]
  pz=[ 1.0 ]
  hist[
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

end

```

- This is a valid ORIGAMI input!
- click Run

Controlling Cross Section Interpolation (libraries per cycle)



ORIGAMI "Express Form" (cont.)

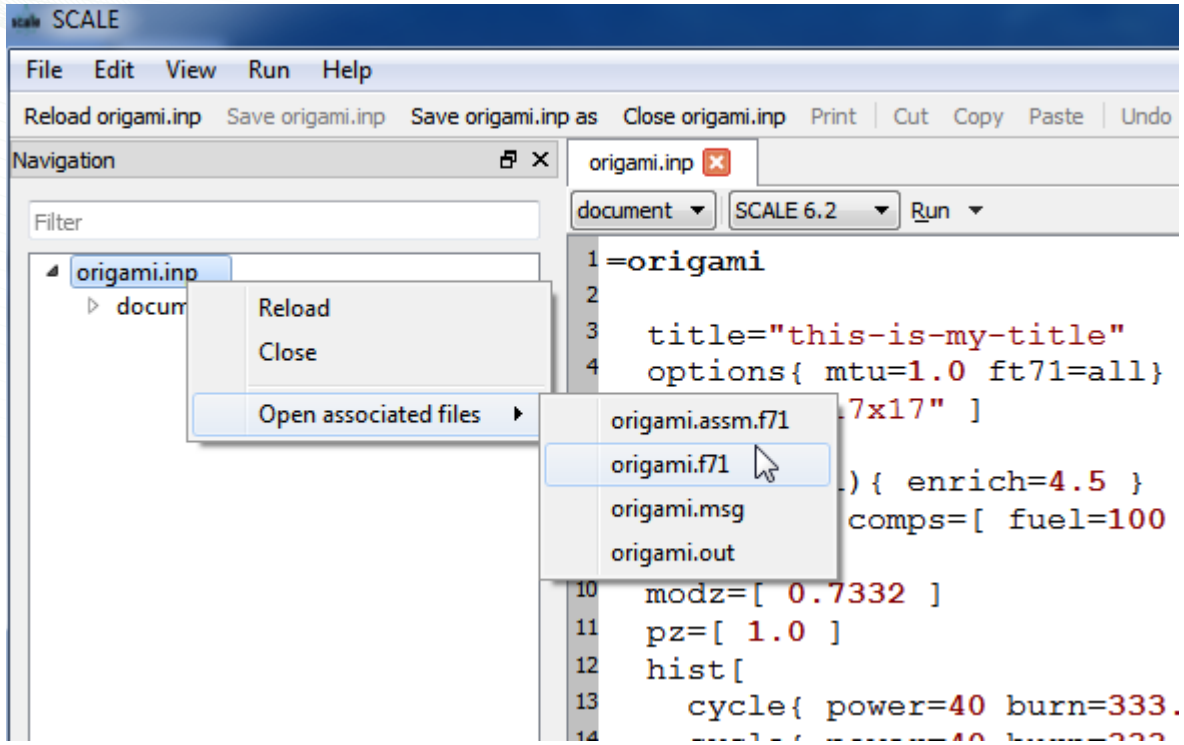
Wed Feb 17 17:13:11 2016 | Wed Feb 17 17:19:44 2016

```
 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…

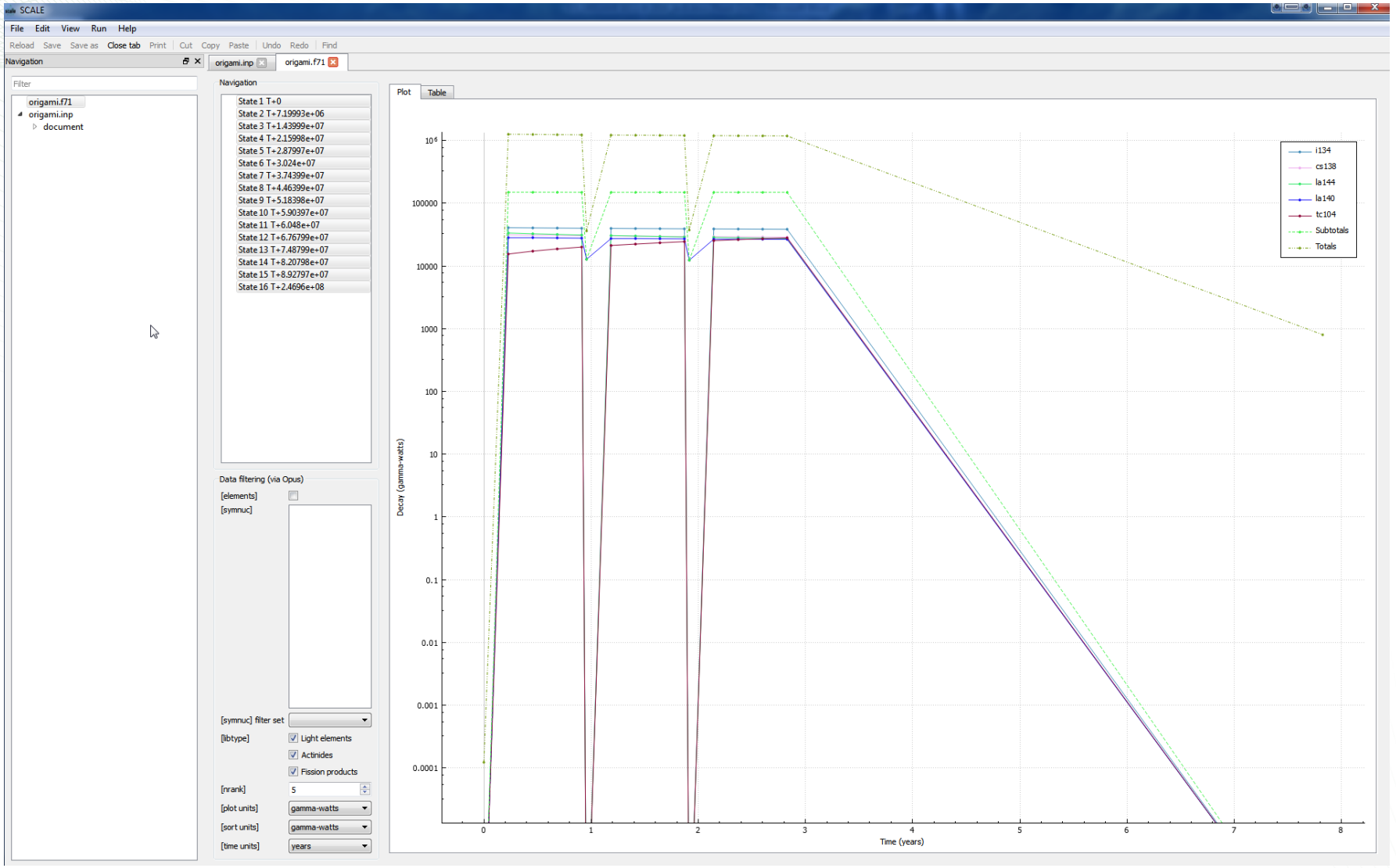
- performs by default 10 substeps
  - depletion equal length
  - decay rule of 3s
- nlib=4 would require 4 cases in ORIGEN
- the input to the left is (4+4+4+1)*10=130 depletion solves

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*

document | SCALE 6.2 | Run

```
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    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

end
```

- **`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*

document | SCALE 6.2 | Run

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    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

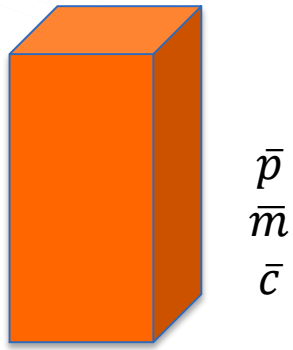
end
```

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

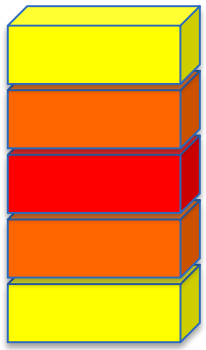
ORIGAMI spatial variation

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



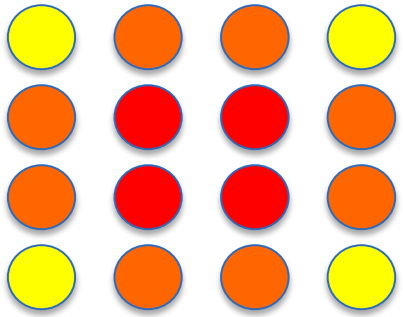
$\bar{p}$
$\bar{m}$
$\bar{c}$

0D assembly



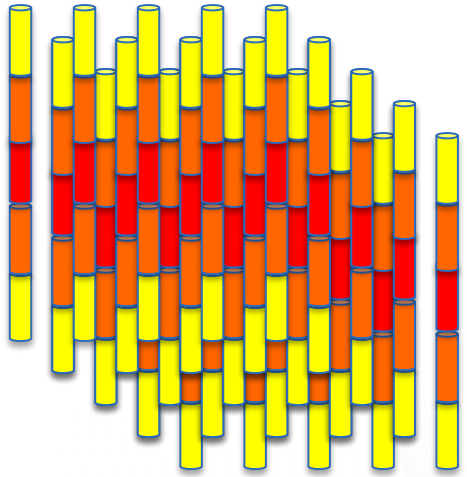
$p(z)$
$m(z)$
$\bar{c}$

1D assembly



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

2D assembly

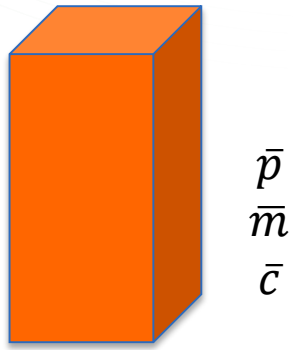


$p(x,y) \times p(z)$
$m(z)$
$c(x,y)$

3D assembly

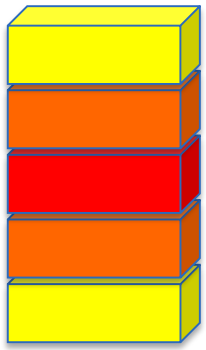
ORIGAMI spatial variation

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



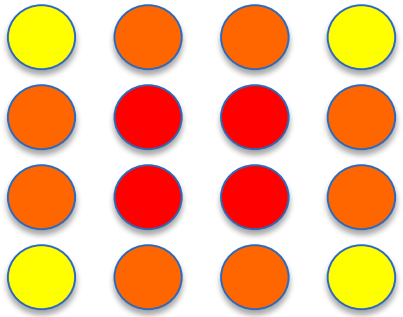
$\bar{p}$
$\bar{m}$
$\bar{c}$

0D assembly



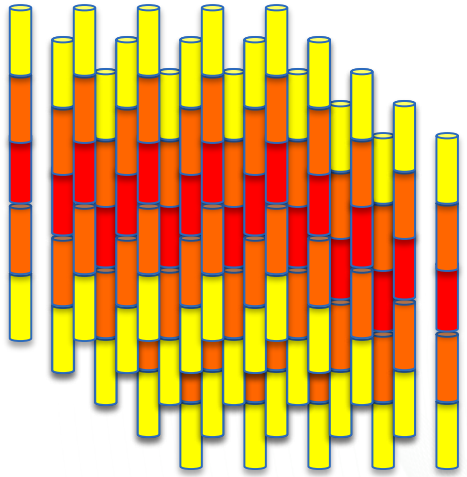
$p(z)$
$m(z)$
$\bar{c}$

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*

document | SCALE 6.2 | Run

```
=origami

  title="this-is-my-title"
  options{ mtu=1.0 ft71=all}
  libs=[ "w17x17" ]
  fuelcomp{
    uox(fuel){ enrich=4.5 }
    mix(1){ comps=[ fuel=100 ] }
  }
  modz=[ 0.7332 ]
  pz=[ 1.0 ]
  hist[
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

end
```

TRITON-inspired mixtures

- **`mix(N)`**
  - **`N`** mixture index
  - **`comps`** array of composition names and wt. %
- **`uox(name){…}`**
  - creates a SCALE StdComp UO_2 Mixture
- StdComp has everything (zirc4, gd2o3, etc.)

ORIGAMI Input: libs

origami.inp*

document | SCALE 6.2 | Run

```
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  options{ mtu=1.0 ft71=all}
  libs=[ "w17x17" ]
  fuelcomp{
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    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

end
```

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*

document | SCALE 6.2 | Run

```
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  title="this-is-my-title"
  options{ mtu=1.0 ft71=all}
  libs=[ "w17x17" ]
  fuelcomp{
    uox(fuel){ enrich=4.5 }
    mix(1){ comps=[ fuel=100 ] }
  }
  modz=[ 0.7332 ]
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  hist[
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

end
```

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*

document | SCALE 6.2 | Run

```
=origami

  title="this-is-my-title"
  options{ mtu=1.0 ft71=all}
  libs=[ "w17x17" ]
  fuelcomp{
    uox(fuel){ enrich=4.5 }
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    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

end
```

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

```
=origami

  title="W17x17 Assembly wtih Axial Distribution"
  options{ mtu=1.0 ft71=all }
  libs=[ "w17x17" ]
  fuelcomp{
    uox(fuel){ enrich=4.5 }
    mix(1){ comps=[ fuel=100 ] }
  }

  meshz=[0    50    100   200   300    350]
  modz =[ 0.73  0.72  0.71   0.70  0.69   ]
  pz   =[ 0.80  0.90  1.00   0.85  0.75   ]

  hist[
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

end
```

5 axial zones

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

Axial Distribution Uses

```
=origami

  title="W17x17 Assembly wtih Axial Distribution"
  options{ mtu=1.0 ft71=all }
  libs=[ "w17x17" ]
  fuelcomp{
    uox(fuel){ enrich=4.5 }
    mix(1){ comps=[ fuel=100 ] }
  }

  meshz=[0    50    100   200   300    350]
  modz =[ 0.73  0.72  0.71   0.70  0.69   ]
  pz   =[ 0.80  0.90  1.00   0.85  0.75   ]

  hist[
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
    cycle{ power=40 burn=333.33 nlib=4 down=0 }
    cycle{ down=1825 }
  ]

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 UO_2
- 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}Pu+^{241}Pu)/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)

  U-234 = 445

  U-235 = 50000

  U-236 = 230

  U-238 = 949325

  O = 1.34432e5

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	Cooling time (years)	
(GWd/MTU)	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