Overview of changes to the ORIGEN family of codes from SCALE 6.1 to 6.2

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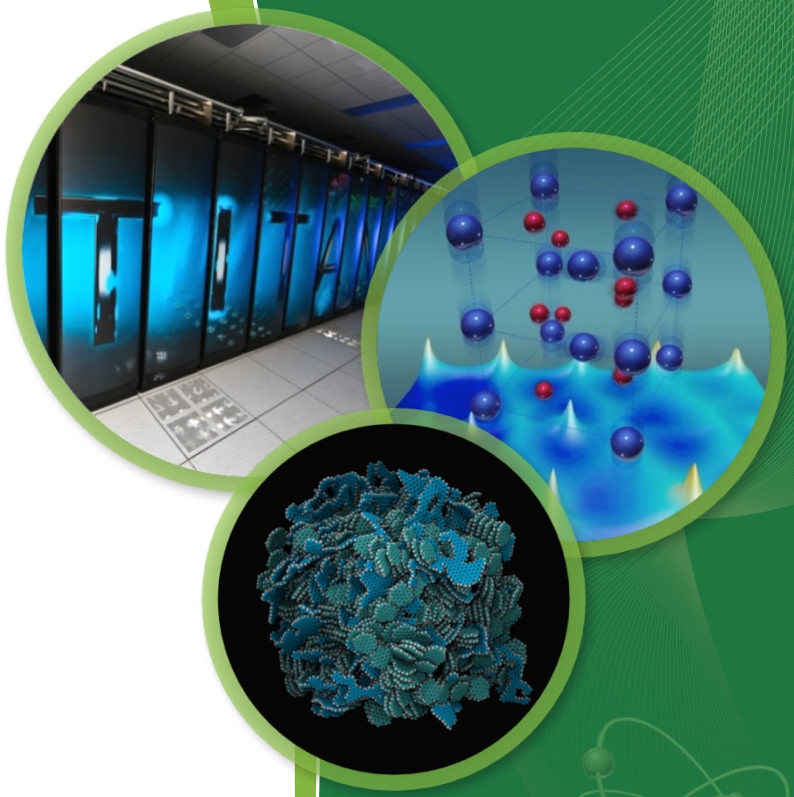

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OAK RIDGE National Laboratory

ORIGEN

- **O**ak **R**idge **I**sotope **Gen**eration calculates time-dependent concentrations, activities, and radiation source terms for a large number of isotopes generated by neutron transmutation, fission, and radioactive decay
- Used internally with TRITON and Polaris sequences in SCALE for depletion/decay

- ORIGEN stand-alone has unique capabilities
  - Simulates continuous nuclide feed and chemical removal (for liquid fuel or reprocessing systems)
  - Generates alpha, beta, gamma, and neutron decay emission spectra
- The guiding principle is to use current nuclear data without approximation
  - 2,200 nuclides
  - 54,000 transitions
  - Single-step calculation time <1s

ORIGEN family and friends

- Family
  - **ORIGEN**: main isotopics solver ($dN/dt = \boldsymbol{A}N$) and emission calculator [changed]
  - **COUPLE**: transition matrix management (creates ***A***)
  - **ARP**: transition matrix interpolation (interpolates ***A*** from reactor library)
  - **OPUS**: post-processor (outputs *N(t)* in various units)
- Friends
  - **ORIGAMI**: rapid spent fuel isotopics [new]
  - **ORIGAMI Automator**: graphical user interface (GUI) for managing many ORIGAMI calculations [new]
  - **ORIGEN Reactor Libraries**: set of parametrized ***A*** for various reactor types [updated]

Evolution of ORIGEN capabilities

- **SCALE 5.1 (2006):** includes GUI, new ORIGEN libraries for different reactor types
- **SCALE 6.0 (2009):** includes new base cross section libraries (ENDF/B-VI) and updated gamma ray libraries; retains all previous reactor libraries
- **SCALE 6.1 (2011)**
  - Includes ENDF/B-VII decay data, expanded nuclides, and energy-dependent fission yields
  - Replaces the old 3-group libraries with 238-group data from JEFF/A-3.0
- **SCALE 6.2 (2016)**
  - **Completely rewritten modular ORIGEN source code, dynamic memory allocations**
  - **New CRAM solver**
  - **Rewritten, streamlined input format**
  - **Endian-agnostic binary f71 and f33 formats**
  - **Integrated alpha and beta sources and spectra**
  - **ORIGEN application programming interface (API) to allow embedding depletion calculation in other codes**

Changes from SCALE 6.1 → SCALE 6.2

- **Refactored manual**
  - Dropped "-S" in "ORIGEN-S" ☺
  - An ORIGEN .f33 file is the only "library" disambiguated from
    - Fundamental data components which are now "resources"
    - Nuclide categories (light, actinide, or fission product) are now "sublibs"
    - Reactor-specific collections of .f33 files are "ORIGEN Reactor Libraries"
- **Changed file formats**
  - text output file (.out)
  - binary output files (.f71, .f33)
- **Default ARP interpolation method**
  - Lagrange→Cubic Spline, better but slower
- **Changed user interfaces**
  - ORIGEN text input redesigned using SCALE Object Notation (SON); also can read SCALE 6.1 FIDO, but may not work for all inputs
  - GUI with Fulcrum
- **Changes to nuclide ids**
  - Default is SCALE-standard **IZZZAAA**, e.g., **u235m** → **1092235** (instead of **922350**)
  - Also accepts symbolic IDs "u235m"
  - Introduced character sublibs 1→LT, 2→AC, 3→FP
- **Changed defaults for emission spectra**

Added/updated from SCALE 6.1 → SCALE 6.2

Added

- ORIGAMI: rapid spent fuel isotopics user interface for light water reactor (LWR) UO_2 systems
- ORIGAMI Automator: GUI component in Fulcrum for managing many ORIGAMI calculations
- CRAM solver (will be default in 6.3)

Updated

- ORIGEN reactor libraries
  - Updated using ENDF/B-VII.1 data
  - Included new reactor types
  - Generated using consistent, traceable methodology (SLIG)

Refactored manual

SCALE 6.1

- Organization
  - Each chapter was an ORNL TM document
  - Chapters
    - **D1** ORIGEN-ARP
    - **F6** COUPLE
    - **F7** ORIGEN-S
    - **F15** OPUS
    - **M6** ORIGEN-S Data Libraries
- Attribution
  - ORNL TM authors
  - Acknowledgments included to recognize past contributors and those from outside ORNL

SCALE 6.2

- Organization
  - Single Chapter 5 for Depletion, Activation, and Source Terms
  - Sections
    - **5.1** ORIGEN, COUPLE, ARP, OPUS
    - **5.2** Data Resources
    - **5.3** ORIGEN Reactor Libraries
    - **5.4** ORIGAMI
- Attribution
  - Introduction by code manager
  - All contributions to 6.2 acknowledged in author list
  - New section on version history will acknowledge previous contributors

Aside: the ORIGEN species

ORIGEN (1973)

ORIGEN-SANDIA

ORIGEN-RA (ANL)

RATAF (NRC)

KORIGEN (Karlsruhe)

ORIGEN-JR (JAEA)

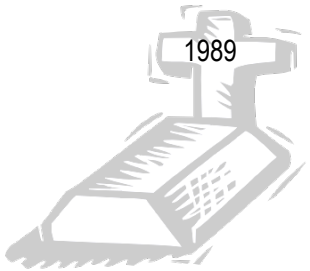
NRC DOE

DOE OCRWM

ORIGEN2 (1980)

ORIGEN2.1

ORIGEN2.2



ORIGEN-JENDL (JAEA)

Monteburns, VESTA

MCODE-MIT

MVP-BURN

MOCUP

ORIGEN-S (1980)

SCALE0

SCALE1

SCALE2

SCALE3, 3.1

SCALE4, 4.1- 4.4

ORIGEN-ARP GUI

SCALE5, 5.1

SCALE6, 6.1

ORIGEN
SCALE 6.2 (2016)

MCU

ORIGEN-X-GRS

OCTOPUS (ECN)

Monteburns

MCNP5 (SCK-CEN)

MCODE

Notes

- DOE halted support for ORIGEN2 in 1989
- DOE and NRC continue to support development of ORIGEN in SCALE

Library (.f33) and solution (.f71) file formats

SCALE 6.1

- Simple (Fortran) binary reading/writing
- Record-based storage
  - Header records
  - NBU burnup records
- Same Fortran I/O in many places throughout SCALE
- Difficult to introduce new data or remove old data without breaking formats
- Required using special compiler endianness flags to ensure that read/write worked across all platforms

SCALE 6.2

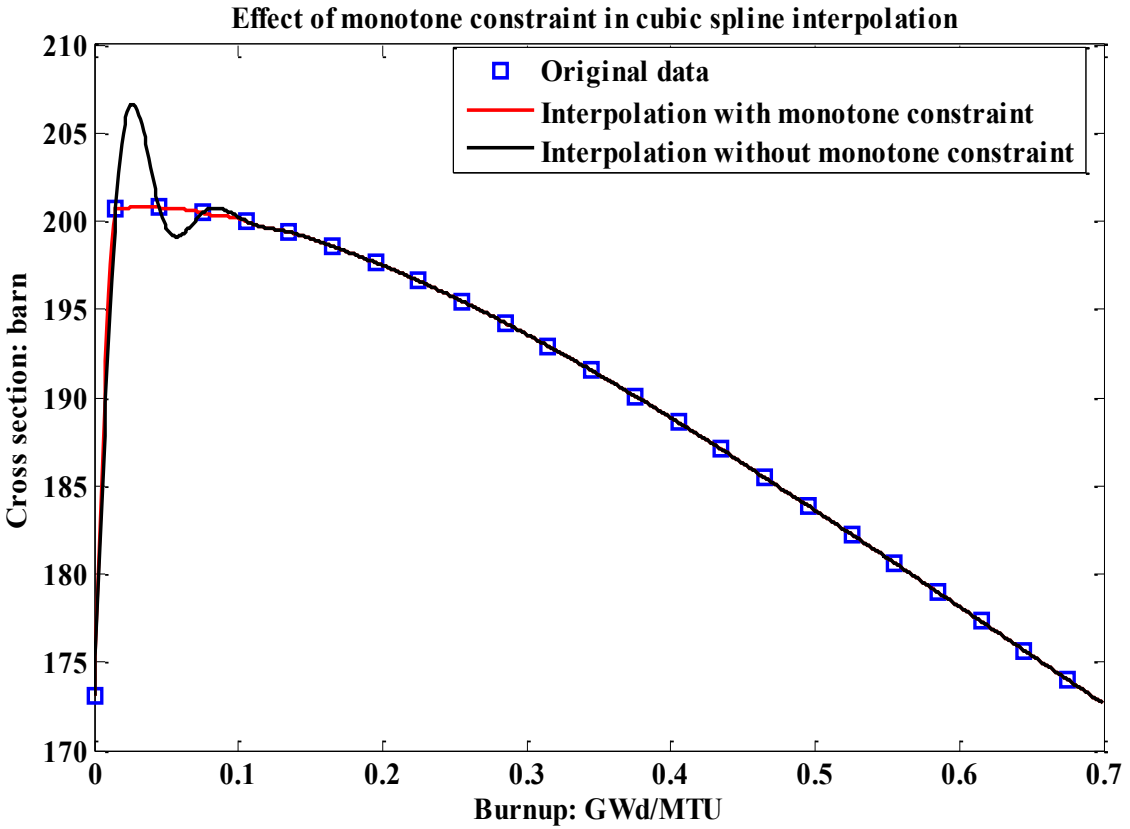
- New Binary Object File Format (BOFF)
- Keyword-based storage
  - Arbitrary hierarchy
  - Compartmentalized data
- Centralized I/O callable from C++/Fortran
- Easy to introduce new data, reorganize, recognize different versions of a particular file
- Automatic byte reversal for endianness → easy cross-platform
- Downside: can no longer read binaries with simple Fortran

Aside: coping with new binary formats (BOFF)

- Users require access to binaries usually just to read them into a post-process, e.g., to link an ORIGEN solution as input to another calculation
  - Do not need library (.f33) manipulation
  - Need solution (.f71) manipulation
- How to link in SCALE 6.2
  - Use OPUS post-processing .f71→.plt and process the (ASCII) .plt file
  - Build the C/C++ application against ORIGEN API
  - Experimental: use command line `f71tocsv` in SCALE install's `bin` directory to dump isotopic contents to CSV

Changed ARP interpolation

- More interpolation methods and change in default
  - Nearest
  - Linear
  - 4th order Lagrange poly **[6.1 default]**
  - Cubic spline
  - Monotonic cubic spline **[6.2 default]**
- Overcomes oscillation problem that can impact accuracy; for small xs (10^{-10} barns), interpolating near slight oscillations can result in a small negative xs



New ORIGEN user interface

- Simple decay problem
  - 2 Ci ^{60}Co
  - 1 Ci ^{137m}Ba
- Photon (gamma) emission spectra
- User-defined group structure

SCALE 6.1 FIDO

```
=origens
0$$ a11 71 e t
Outlet Term
3$$  2 1 1 27 a16 4 a33 47 e t
35$$ 0 t
54$$ a8 1 a11 0 e
56$$ 0 1 a6 1 a10 0 a13 98 3 3 0 2 0 e
57** 0  a3 1e-16 e
95$$ 0 t
Release End
Ci
60** 0
61** f0.05
65$$
'GRAM-ATOMS   GRAMS    CURIES     WATTS-ALL  WATTS-GAMMA
     3Z     1  0  0     3z    3z    3Z     6Z
     3Z     1  0  0     3z    3z    3Z     6Z
     3Z     1  0  0     3z    3z    3Z     6Z
81$$ 2 0 23 1 e
82$$ 2 e
83** 2.00E+07 1.40E+07 1.20E+07 1.00E+07 8.00E+06 7.50E+06 7.00E+06
     6.50E+06 6.00E+06 5.50E+06 5.00E+06 4.50E+06 4.00E+06 3.50E+06
     3.00E+06 2.75E+06 2.50E+06 2.35E+06 2.15E+06 2.00E+06 1.80E+06
     1.66E+06 1.57E+06 1.50E+06 1.44E+06 1.33E+06 1.20E+06 1.00E+06
     9.00E+05 8.00E+05 7.00E+05 6.00E+05 5.12E+05 5.10E+05 4.50E+05
     4.00E+05 3.00E+05 2.60E+05 2.00E+05 1.50E+05 1.00E+05 7.50E+04
     7.00E+04 6.00E+04 4.50E+04 3.00E+04 2.00E+04 1.00E+04 e
73$$
270600 561371 e
74**
2.00E+00  1.00E+00
75$$
1 3
t
56$$ 0 0 a10  1 e t
56$$ f0 t
end
```

SCALE 6.2 SON

```
=origen
bounds{
    gamma=[
     2.00E+07 1.40E+07 1.20E+07 1.00E+07 8.00E+06 7.50E+06 7.00E+06
     6.50E+06 6.00E+06 5.50E+06 5.00E+06 4.50E+06 4.00E+06 3.50E+06
     3.00E+06 2.75E+06 2.50E+06 2.35E+06 2.15E+06 2.00E+06 1.80E+06
     1.66E+06 1.57E+06 1.50E+06 1.44E+06 1.33E+06 1.20E+06 1.00E+06
     9.00E+05 8.00E+05 7.00E+05 6.00E+05 5.12E+05 5.10E+05 4.50E+05
     4.00E+05 3.00E+05 2.60E+05 2.00E+05 1.50E+05 1.00E+05 7.50E+04
     7.00E+04 6.00E+04 4.50E+04 3.00E+04 2.00E+04 1.00E+04]
}
case
{
    title='DBST End of Release 6.4 hrs'
    lib{
        file="end7dec"
    }
    mat{
        iso=[
           co60(LT)=2
           ba137m(FP)=1
        ]
        units=CURIES
    }
    time{
        t=[6.4]
        units=HOURS
    }
    gamma{
        brem_medium=NONE
        conserve_line_energy=NO
        split_near_boundary=YES
    }
    print{
        gamma{
            summary=YES
            spectra=YES
        }
    }
}
end

```

Output file format (.out)

SCALE 6.1

```
no neutron source nuclides found, not printed
     ..............................................................
                                  (neutron spectra for problem specific
matrix)
1                      * gamma sources determined *
0case applies the following photon data base
                     master photon library
                     in binary mode
0    the sources include photons for the following nuclide groups

       light elements
       actinides
       fission products
1
page   4
                               gamma source intensity as a function of
time

0                               DBST End of Release
                                            gamma spectra,
photons/sec/basis
                                       basis = Ci

 grp   boundaries, mev       0.0 h
   1 1.00E-02 - 2.00E-02 0.000E+00
   2 2.00E-02 - 3.00E-02 0.000E+00
   3 3.00E-02 - 4.50E-02 2.348E+09
   4 4.50E-02 - 6.00E-02 0.000E+00
   5 6.00E-02 - 7.00E-02 0.000E+00
   6 7.00E-02 - 7.50E-02 0.000E+00
   7 7.50E-02 - 1.00E-01 0.000E+00
   8 1.00E-01 - 1.50E-01 0.000E+00
   9 1.50E-01 - 2.00E-01 0.000E+00
  10 2.00E-01 - 2.60E-01 0.000E+00
  11 2.60E-01 - 3.00E-01 0.000E+00
  12 3.00E-01 - 4.00E-01 5.503E+06
  13 4.00E-01 - 4.50E-01 0.000E+00
  14 4.50E-01 - 5.10E-01 0.000E+00
  15 5.10E-01 - 5.12E-01 0.000E+00
  16 5.12E-01 - 6.00E-01 0.000E+00
  17 6.00E-01 - 7.00E-01 3.385E+10
```

SCALE 6.2

```
================================================================================
Gamma source intensity (1/s) as a function of time for case '1' (#1/1)
=
=   DBST End of Release 6.4 hrs
=
--------------------------------------------------------------------------------
     boundaries (MeV)          0.0hr       6.4hr
      --- groups     1 through    15 are zero ---
 2.750E+00 - 2.500E+00    7.4000E+02  7.3993E+02
 2.500E+00 - 2.350E+00    7.4000E+02  7.3993E+02
 2.350E+00 - 2.150E+00    8.8800E+05  8.8791E+05
      --- groups    19 through    24 are zero ---
 1.440E+00 - 1.330E+00    3.6994E+10  3.6990E+10
 1.330E+00 - 1.200E+00    3.6994E+10  3.6990E+10
 1.200E+00 - 1.000E+00    7.3889E+10  7.3882E+10
 1.000E+00 - 9.000E-01    0.0000E+00  0.0000E+00
 9.000E-01 - 8.000E-01    5.6240E+06  5.6235E+06
 8.000E-01 - 7.000E-01    0.0000E+00  0.0000E+00
 7.000E-01 - 6.000E-01    3.3263E+10  0.0000E+00
      --- groups    32 through    35 are zero ---
 4.000E-01 - 3.000E-01    5.5500E+06  5.5495E+06
      --- groups    37 through    44 are zero ---
 4.500E-02 - 3.000E-02    2.6804E+09  0.0000E+00
      --- groups    46 through    47 are zero ---
  --------------------
                 total    1.8383E+11  1.4787E+11
================================================================================
.
```

More flexible nuclide identifiers

SCALE 6.1

- Old isotopics initialization handled by 3 arrays
  - ZZAAAI nuclide id (73$$)
  - amount (74**)
  - sublib (75$$)

```
73$$
270600 561371 e
74**
2.00E+00  1.00E+00
75$$
1 3
```

- For long lists (10+ nuclides), it was difficult to ensure that the id/sublib/amount matched up

SCALE 6.2

- New isotopics initialization uses a "triplet" `id(sublib)=amount`

```
mat{
    iso=[
        co60(LT)=2
        ba137m(FP)=1
    ]
    units=CURIES
}
```

- `sublib` is optional
  - "Light nuclide": 1 or LT
  - "Actinide": 2 or AC
  - "Fission product": 3 or FP
- `id` is either IZZZAAA or EAm by default
- `idform=ZAI` to use old ZZAAAI form

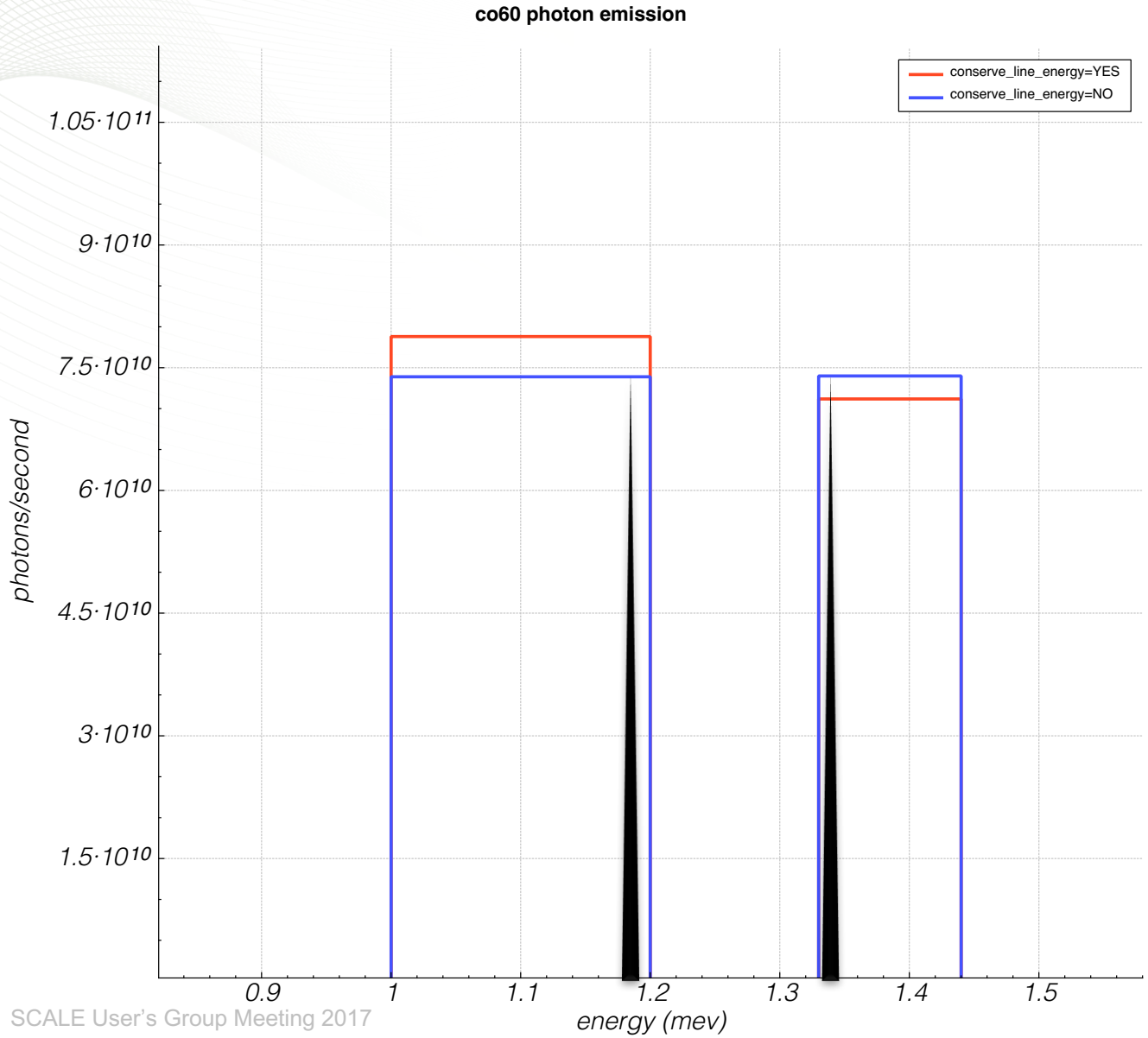
```
mat{
    iso=[
        270600(LT)=2
        561371(FP)=1
    ]
    idform=ZAI
    units=CURIES
}
```

Change to gamma emission spectra defaults

- Two interesting options for binning photon line data
  - `split_near_boundary`
    If a line is within 3% of a bin boundary→add 50% to both adjacent bins
  - `conserve_line_energy`
    If a line energy does not coincide with the bin middle energy→adjust photon emission rate so that energy emission rate is conserved
- `conserve_line_energy` can significantly change results for ***coarse energy grids***

- We must choose to conserve **particles or energy** when binning line data
  - *Once binned, the energy distribution within the bin is lost*
  - *It becomes the energy of the midpoint of the bin*
- 6.1 (cannot change through input)
  - `split_near_boundary=YES`
  - `conserve_line_energy=YES`
- 6.2 defaults
  - `split_near_boundary=NO` **[changed]**
  - `conserve_line_energy=YES`

Understanding conserve_line_energy



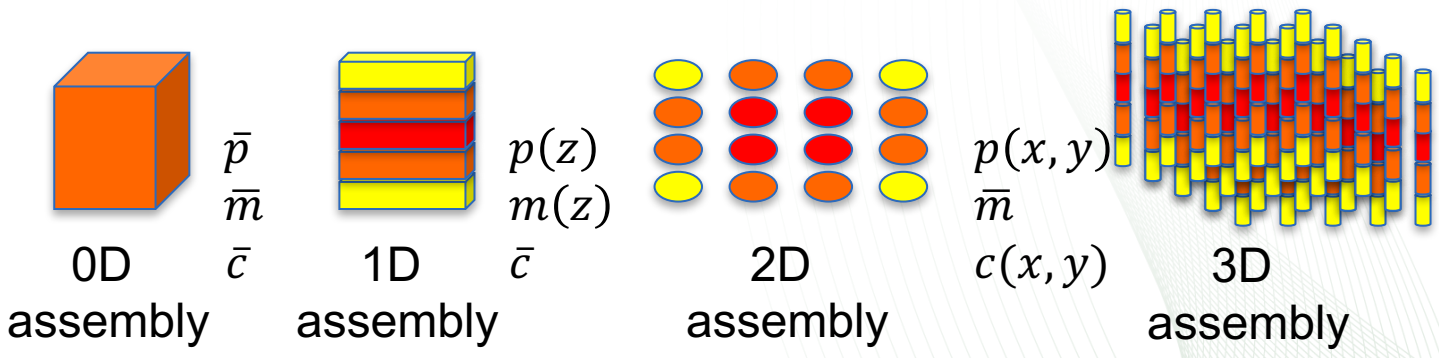
- ^{60}Co lines
  - 1.173 MeV at 7.4E10 photons/sec
  - 1.332 MeV at 7.4E10 photons/sec
- `conserve_line_energy=NO`
  - Emission is binned as expected
- `conserve_line_energy=YES`
  - For 1.173 MeV, because bin middle energy is ***below*** line energy, photons/sec are scaled UP to preserve line energy
  - For 1.332 MeV, because bin middle energy is ***above*** line energy, photons/sec are scaled DOWN to preserve line energy

- NOTE: If we were looking at energy emission (MeV/second) instead, `conserve_line_energy=YES` would look "better"
- The effect of the choice disappears for "fine" grids

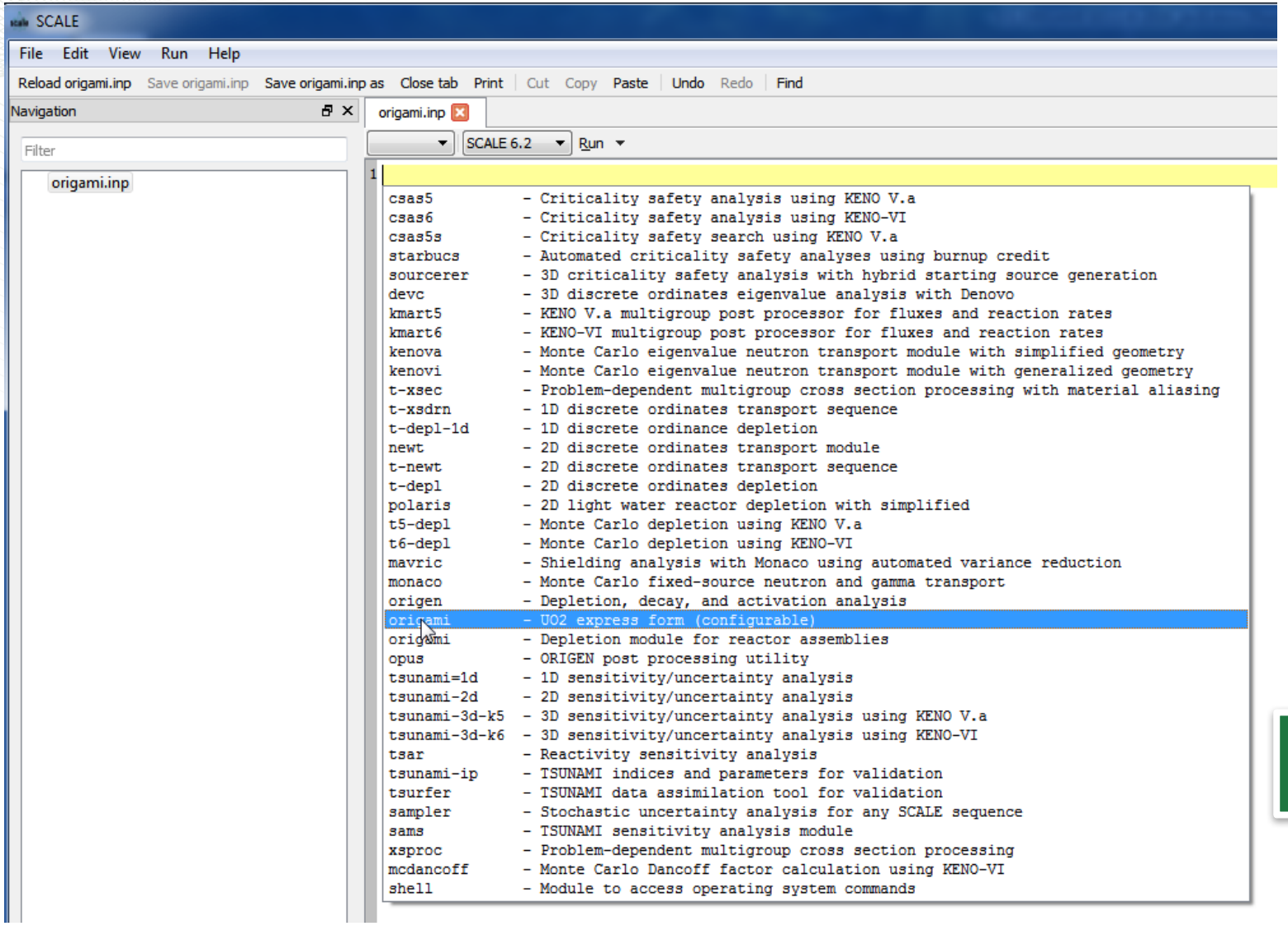
New sequence: ORIGEN Assembly Isotopics - ORIGAMI

- Motivation
  - Perform many spent fuel calculations
    - US fuel inventory analysis (200,000+ assemblies) for UNF Standards
    - NRC Level 3 probability risk assessment (3000+ assemblies)
  - Using SCALE 6.1 GUI impractical

- Power shape
  axial & radial → $p(z) \times p(x,y)$
- Moderator density
  axial only → $m(z)$
- Fuel composition
  radial only → $c(x,y)$



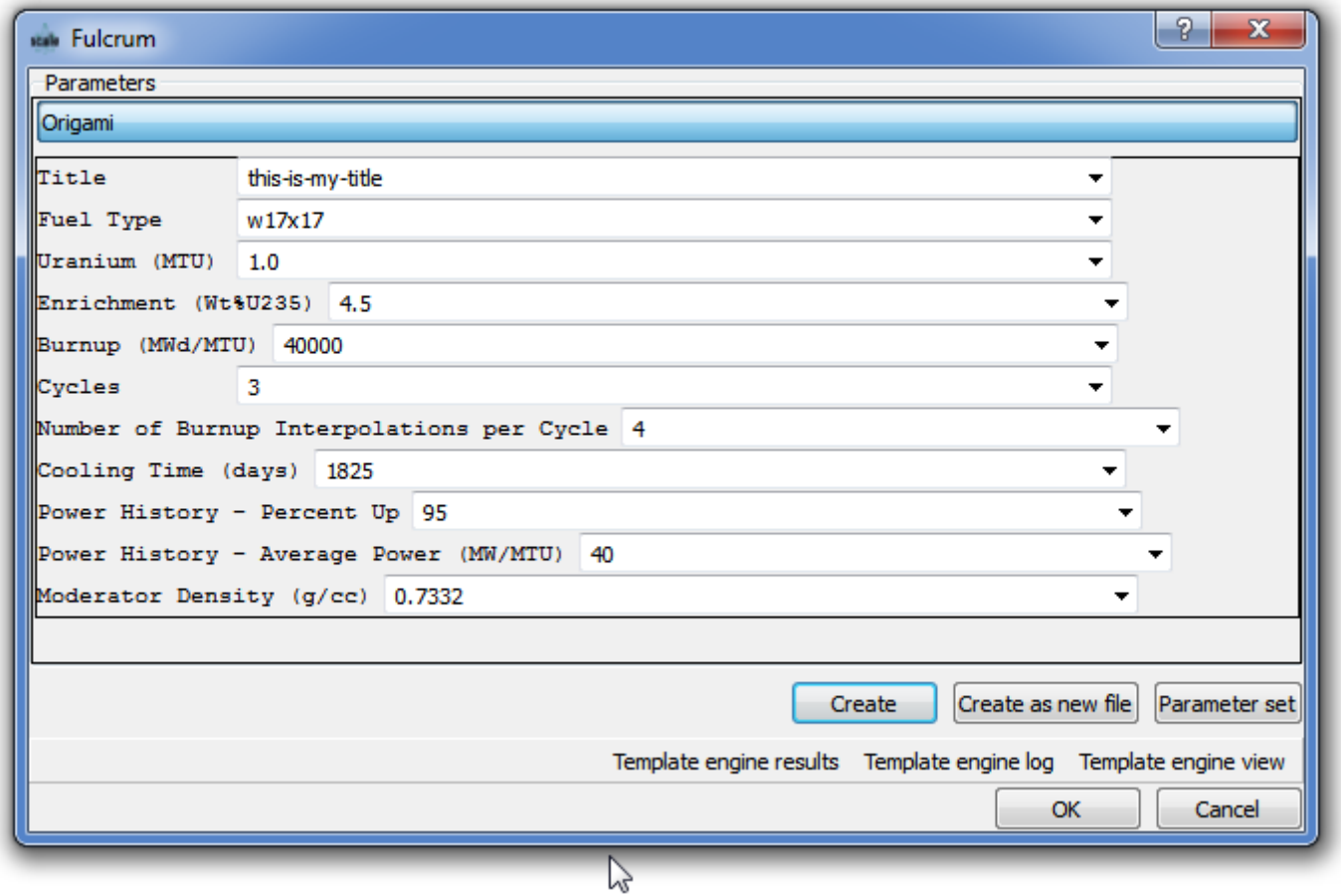
ORIGAMI Express Form In Fulcrum



- Quick start
  - Create empty file (origami.inp)
  - CTRL+SPACE inside empty file
  - Choose "origami – UO_2 express form (configurable)"

NOTE: ORIGAMI was ***intended*** to replace the need for ORIGEN-ARP GUI

ORIGAMI Express Form (continued)



- Window will appear
- Click "Create"
- Click "OK"

ORIGAMI input (in brief)

origami.inp*

document | SCALE 6.2 | Run

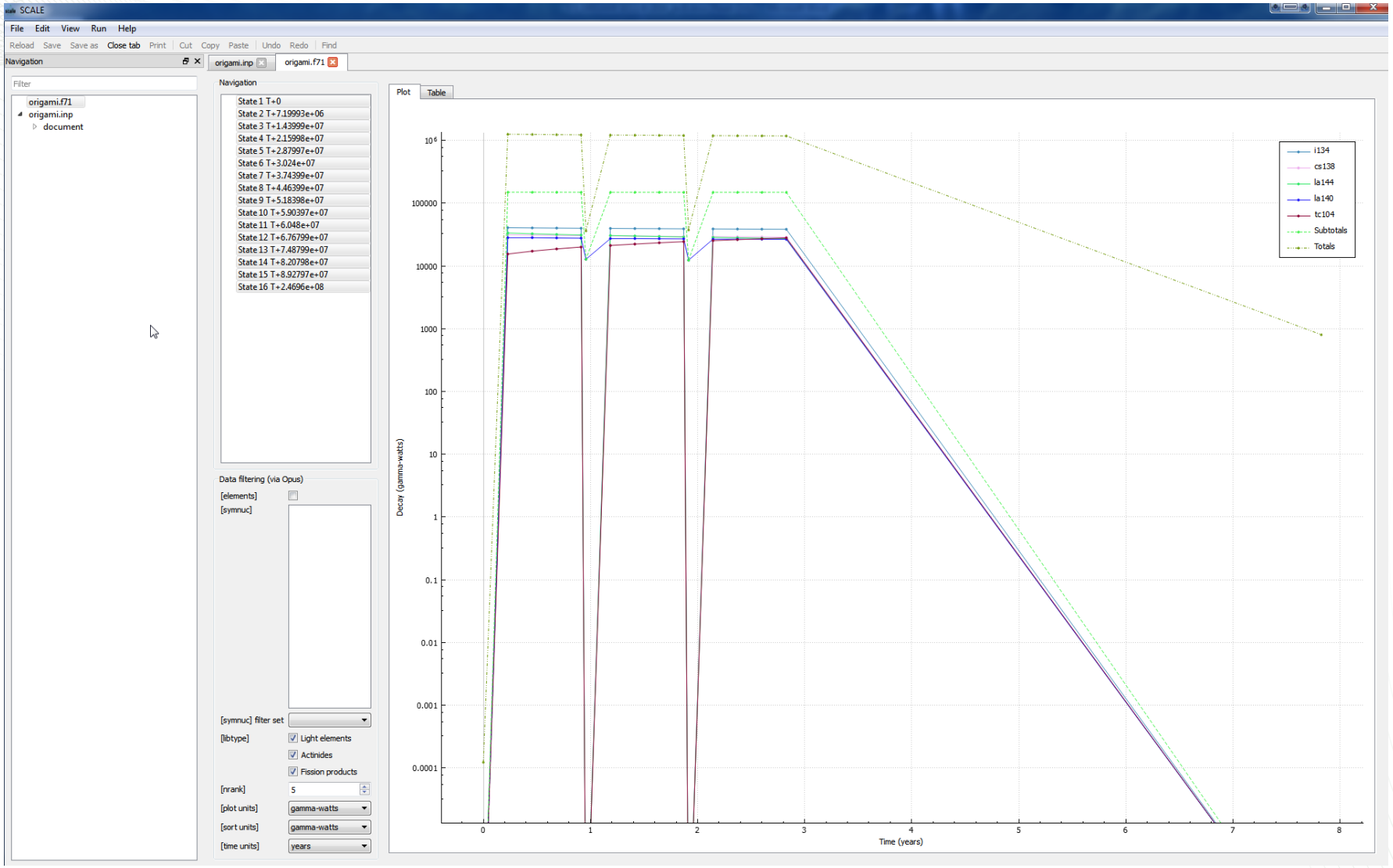
```
=origami

  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
```

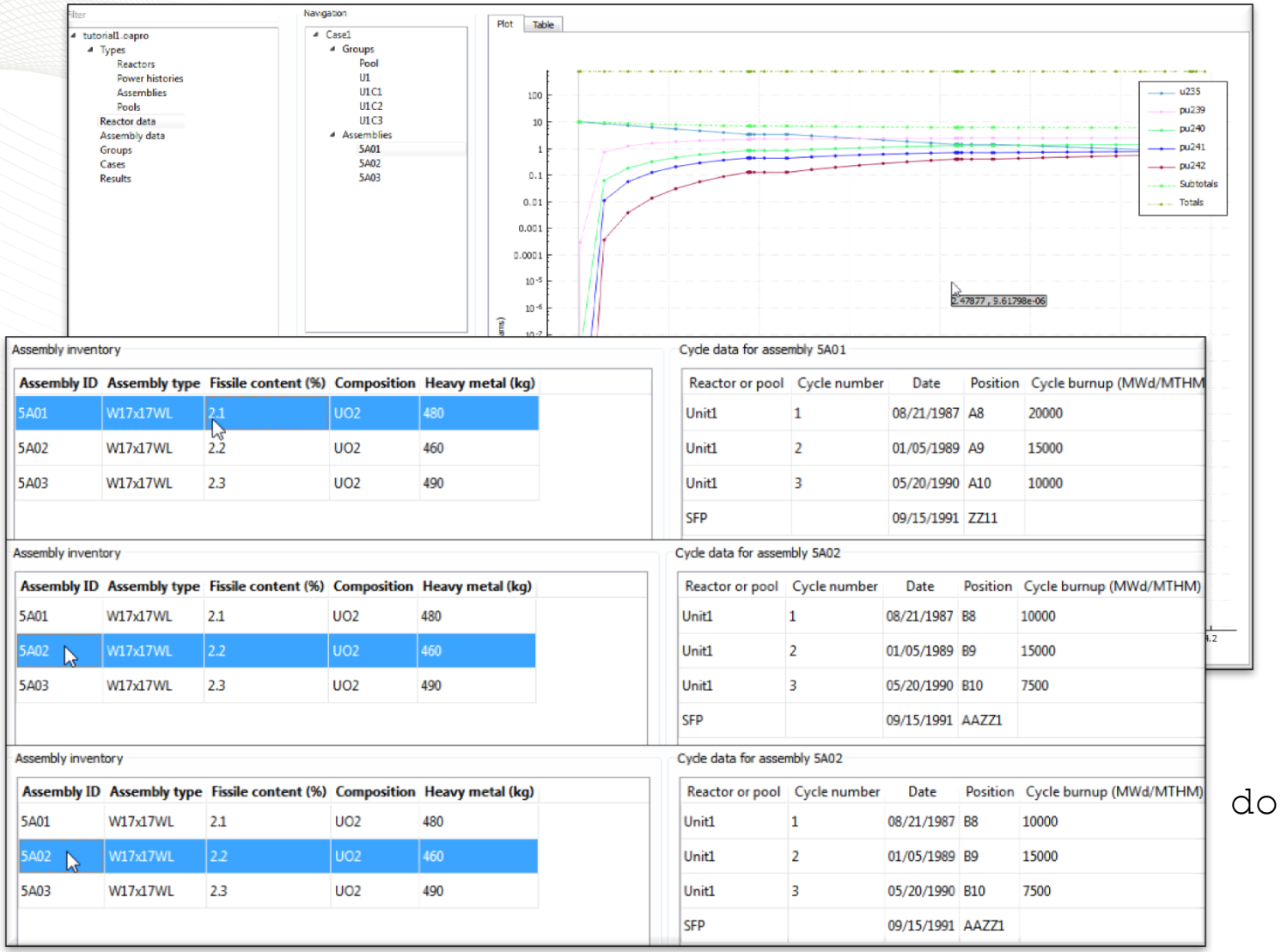
- **`title`** – set a descriptive title
- **`options`** – various global options
- **`fuelcomp`** – declare mixtures (single mixture problems use 1)
- **`modz`** – axial moderator density
- **`pz`** – axial power shape
- **`hist`** – operating history

View ORIGAMI .f71 in Fulcrum



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

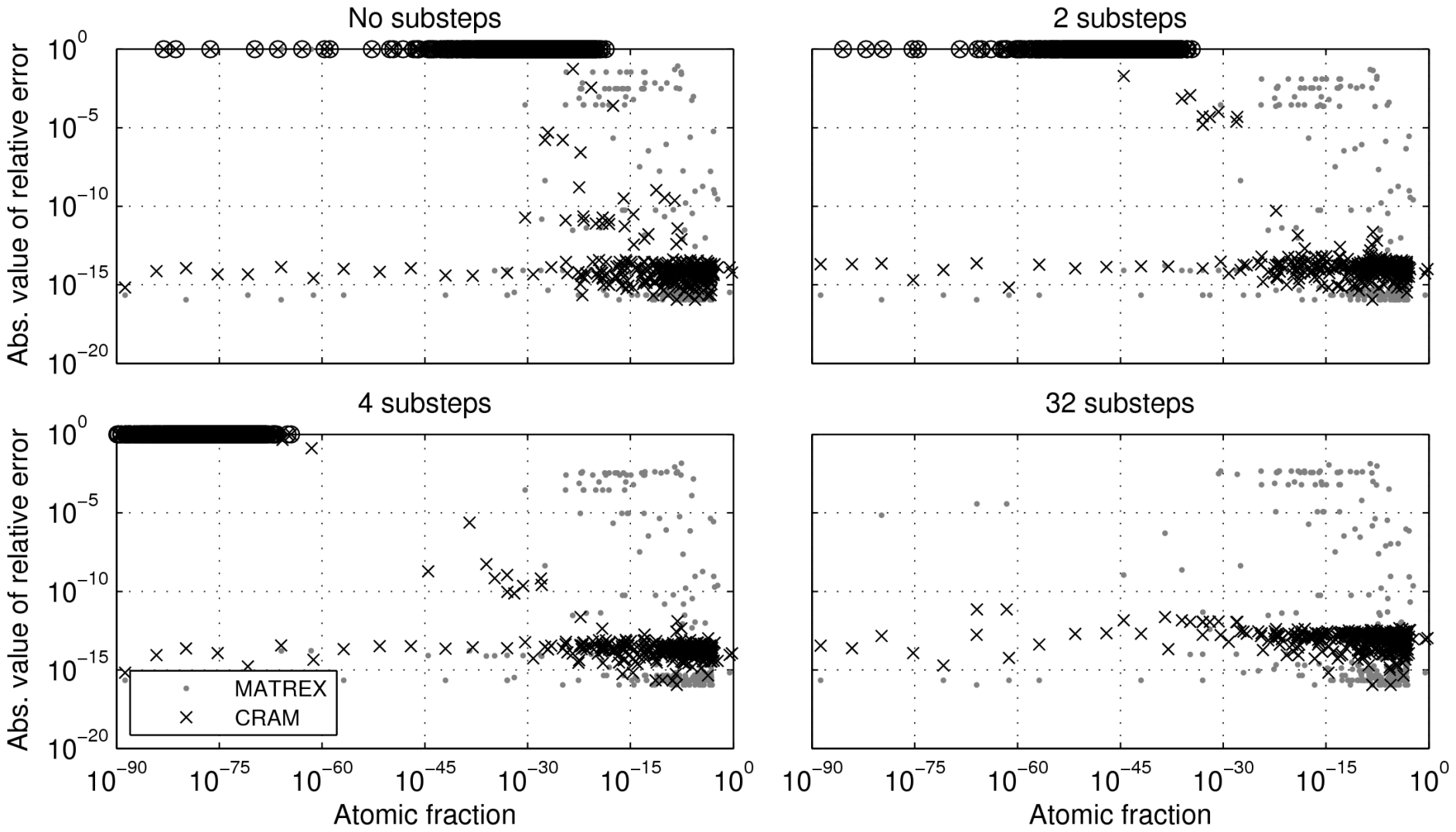
ORIGAMI Automator



- setup of assembly details
  - click through GUI
  - import via JSON or CSV
- simple time-dependent location declaration for assembly
  - Spent Fuel Pool
  - Dry Storage
- assembly grouping capability based on location, e.g. Decay Heat in SFP over time
- for more information see primer in SCALE install directory

`docs/Primers/ORIGAMI_Automator.pdf`

CRAM (new) vs. MATREX (old): 100-day decay of spent fuel



RUNTIMES (milliseconds)

Depletion substep

MATREX	40-150
CRAM	40-50

Decay substep

MATREX	5
CRAM	10

NOTE: *CRAM requires fewer substeps per step, so always faster in practice!*

Updated ORIGEN Reactor Libraries

SCALE 6.1

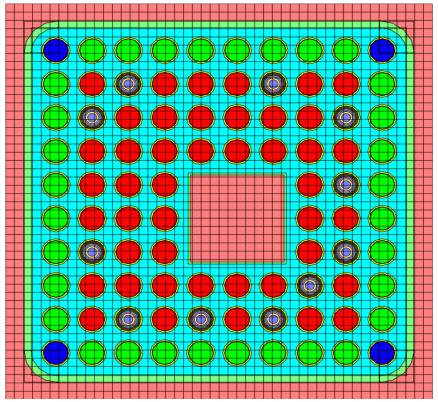
- most data was generated in SCALE 5.1
  - BWR and PWR libraries generated using TRITON 2-D models
  - some libraries were pre-SCALE-5.1, generated using SAS2H (1-D) models
  - based on ENDF/B-V, 44-group cross-section data for neutron transport
  - NITAWL cross-section processing used with TRITON
- Outdated modeling assumptions (not consistent with recent SCALE capabilities and nuclear data)
- Selected libraries have been generated under different projects since 2006, but not released with SCALE

SCALE 6.2

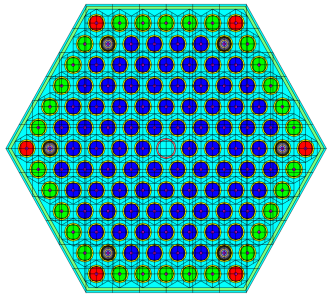
- Automation tool (SLIG) allow reactor libraries to be generated with each official release of SCALE
- New libraries are based on current ORNL modeling best practices
  - 252-group ENDF/B-VII.1 cross-section library for the neutron transport solution
  - CENTRM cross-section processing for the NEWT transport solver
  - Specialized Dancoff factors for BWR corner and edge pins
  - Finer spatial solution grid than previously used
  - Updated models with better assumptions and sources of information
  - Updated MOX data with radial zoning
- downside: now 6.9GB of data (was 2.4GB)

What do you get for 7GB?

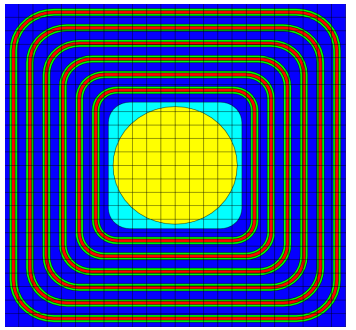
- Pressurized Water Reactors (PWRs)
- Boiling Water Reactors (BWRs)
- Mixed-oxide (MOX) libraries for typical BWRs and PWRs
- Russian VVER reactors
- Russian RBMK reactors
- Canadian CANDU reactors
- UK Advanced Gas Reactors (AGRs)
- MAGNOX Reactors
- IRT Reactors



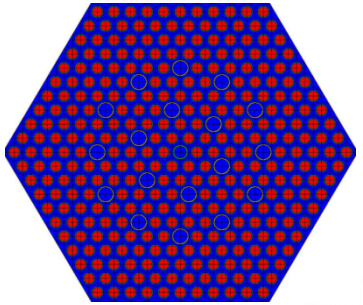
ATRIUM 10



VVER-440



IRT



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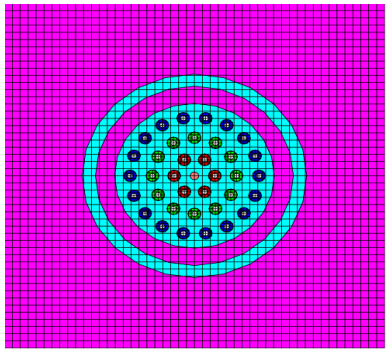
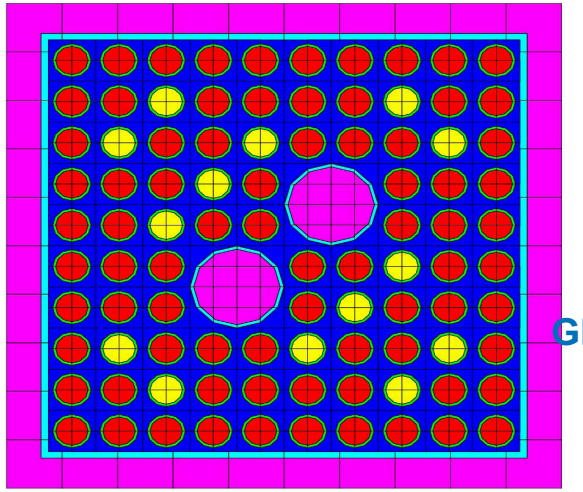


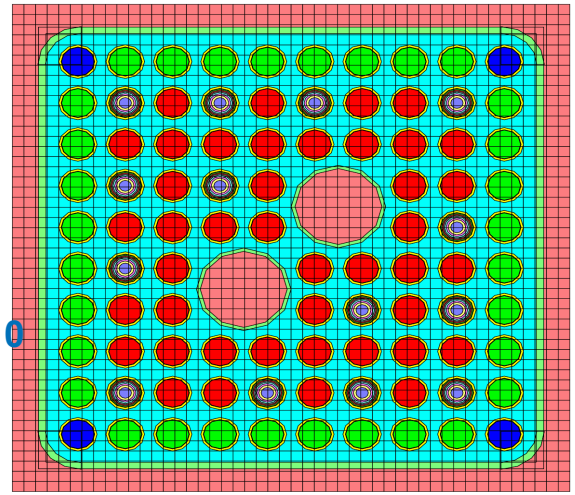
AGR

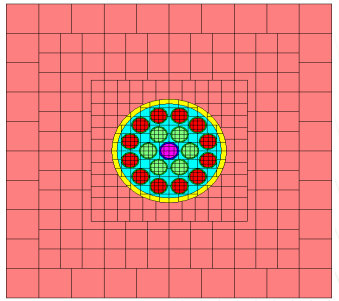
SCALE 6.1



GE 10x10

SCALE 6.2





RBMK

Summary ORIGEN-S 6.1 → ORIGEN 6.2

- **Refactored manual**
  - Reorganized
  - Refined terminology around “libraries”
- **Changed file formats**
  - Text output file (.out)
  - Binary output files (.f71, .f33)
- **New User Interfaces**
  - ORIGEN itself uses SON now
  - Main GUI is Fulcrum
  - New spent fuel isotopics interface, ORIGAMI
  - New ORIGAMI Automator GUI
- **New solver**
  - CRAM solver (will be default in 6.3)
- **Changes to nuclide ids**
  - Default is more SCALE-standard **IZZZAAA**
  - Also accept symbolic ids “u235m”
  - Introduced character sublibs 1→LT, 2→AC, 3→FP
- **Changed defaults for emission spectra**
  - pay attention to `conserve_line_energy`!
- **ORIGEN reactor libraries**
  - Updated using ENDF/B-VII.1 data
  - New reactor types
  - Generated using consistent, traceable methodology (SLIG)

ORIGEN API

- API for ORIGEN has been main funding source of all development

  NEAMS primary
  (also CASL, LDRD)

- Documentation: google “ORIGEN API”
- Main Capabilities
  - Avoid file I/O!
  - C/C++/Fortran interfaces to perform coupled depletion and transport
    - Collapse multi-group flux
    - Provide self-shielded one-group XS
    - Create transition matrix ***A***
    - Deplete over a step
  - Supports flux in arbitrary group structure (fast/thermal/etc. does not matter)
- Integrations
  - SCALE (ORIGEN, TRITON, Polaris)
  - CASL/MPACT full-core, pin-by-pin (almost pellet-by-pellet) depletion
  - SHIFT standalone
  - PROTEUS (ANL unstructured mesh transport)
  - BISON (INL fuel performance)
  - CYCLUS (fuel cycle)

SCALE 6.3

- **Main goal:** Grand Unification
  ARP+COUPLE+ORIGEN+OPUS→**ORIGEN**
  - Make ORIGEN a cohesive sequence for set up, calculation, and post-processing
  - Deprecate family members
    - ARP library interpolator
    - COUPLE library management
    - OPUS post-processor
  - Fold member capability into ORIGEN directly
- **SCALE-wide goal**: Update to ENDF/B-VIII data
  - Second metastable nuclides, e.g., $^{135m2}Xe$
  - revise “general” (2237) nuclide set