Learning Objectives

• How to calculate isotopic inventories, neutron and gamma sources using fast depletion capabilities in SCALE
  – Using available ORIGEN reactor libraries for fast irradiation and decay simulations under ORIGAMI
  – Using available nuclide concentration (f71) files for decay simulations with ORIGEN

• Refresher: clarify upon the involved approaches, files, and “jargon”

• Provide hands-on example for a BWR spent fuel application
Spent Nuclear Fuel

• Fresh fuel inserted in a nuclear reactor (usually U) undergoes nuclear transmutations, leading to production of higher actinides and fission products “spent” or “used” nuclear fuel

• What happens to fuels and other materials irradiated in reactor?
  – Irradiation changes the nuclear material composition
  – Uranium is lost through transmutation (mostly fission)
  – Higher actinides (Pu, Cm, etc.) are produced through neutron interactions (transmutation) of uranium
  – Fission products are generated by fission of U and Pu (primarily)

• Spent fuel “memorable” characteristics:
  – Burnup (measure of the integral number of fissions occurring in fuel during irradiation and consequently a measure of the associated energy released)
  – Cooling time (duration from discharge from reactor to a time of interest)
  – Enrichment (initial fuel enrichment in %U)
SCALE Capabilities for Fuel Depletion Simulations

- **Lattice physics computational tools (2D or 3D)**
  - Can simulate a fuel element (assembly) to calculate the spatial distribution of power (and burnup) of each fuel pin in an assembly (e.g., for LWR)
  - May also simulate a set of fuel assemblies or even the entire reactor, for small configurations (e.g., small research reactors), depending on the problem
  - Used generally to generate burnup-dependent lattice physics parameters for use in core simulators (e.g., nodal cross sections)
  - Requires usually 2D or 3D modeling capabilities, moderate computing power, and longer computing time (compared to 0D burnup codes)
  - Iteratively couples a 1D, 2D, or 3D neutron transport solver with a 0D depletion/burnup solver (e.g., ORIGEN)
  - Examples: SCALE/TRITON, SCALE/Polaris
ORIGEN is the foundation of depletion capabilities in SCALE
What is ORIGEN?

- **Oak Ridge Isotope Generation** code in SCALE
- Irradiation and decay simulation code
- Explicit simulation of all pathways from neutron transmutation, fission, and decay
ORIGEN Highlights

• How does it work
  – Solves the time-dependent transmutation equations over large time scales
  – Does not directly treat space and energy variables
  – Primary nuclear data needed: 1-group cross section, fission yield data, decay data
  – Accurate problem-dependent cross-section generation and accurate nuclear data is the secret
  – Based on state-of-the-art nuclear data and cross section processing methodologies
  – Fast computing time (seconds)

• Where is ORIGEN present in SCALE
  – Standalone depletion/decay code
  – ORIGAMI sequence
  – Depletion solver in SCALE lattice physics codes (TRITON, Polaris)

\[ \dot{N}(t) = \overline{A} \cdot N(t) \]
ORIGEN Family of Modules in SCALE

- **ORIGEN**
  - main engine: solves depletion, decay, activation, and feed problems, as well as the decay emission calculations (0D code)

- **OPUS**
  - performs post processing and analysis of ORIGEN results contained in ORIGEN concentrations files, including sorting, ranking, and unit conversion

- **COUPLE**
  - library management module for ORIGEN

- **ARP**
  - cross-section interpolator - interpolates on a set of pre-generated ORIGEN libraries to create a new ORIGEN library at different values of the interpolation parameters (e.g., burnup)

- **ORIGAMI (ORIGEN Assembly Isotopes)**
  - provides the capability to easily performing isotopic depletion and decay calculations with ORIGEN for LWR fuel assemblies (extensively expanded for SCALE 7.0)
Special F71 and F33 Files

• **ORIGEN Concentrations file (F71)**
  - Stores all nuclide inventory (always present) and neutron/photon sources (optional)
  - Content can be visualized with Fulcrum
  - Consistent usage across the ORIGEN family of modules

• **ORIGEN Library file (F33)**
  - Special "library" contains all the information needed to "reconstruct" a depletion calculation
  - Integral part of the ORNL ORIGEN-ARP method (more details in ORIGAMI presentation)
  - Consistent usage across ORIGEN, ORIGAMI, COUPLE, ARP
TRITON and Polaris Nuclide Inventory Calculation Capabilities
1. Fresh fuel compositions/designs are specified in the SCALE input file
   - TRITON (any general geometry)
   - Polaris (simple LWR geometry)
   - ORIGAMI (geometry assumed based on loaded ORIGEN reactor library aka F33)

2. Irradiation history specified in the SCALE input file
   - Power vs. time
   - State (void, temperature) vs. time

3. Decay with ORIGEN to calculate neutron/gamma sources
   - read discharge nuclide inventory from F71 file and decay to a cooling time of interest
   - generate new nuclide inventory neutron/gamma emission sources in a new F71 file
How to Enable Output from within TRITON & Polaris

- **ORIGEN Concentrations file (F71)**
  - TRITON, Polaris, and ORIGAMI depletion *automatically generates F71*
  - ORIGEN calculations
    - user must provide energy bins for neutron and gamma emissions sources and explicitly request the emission calculations
    - also must explicitly request saving information to F71

- **ORIGEN Library file (F33)**
  - TRITON F33 is automatically generated but must be copied from the temporary directory
    - one F33 per each depleted mixture
    - one "combined" F33 representing entire system
  - Polaris F33 generation automatically copies file back
    - new feature in SCALE 6.3
Basic Capabilities for TRITON and Polaris

- Both use ORIGEN as depletion/decay solver
- Calculate nuclide concentration during fuel depletion (irradiation)
  - TRITON
    - TRITON-NEWT: 2D general system depletion (Polaris ancestor)
    - TRITON-KENO: 3D general system depletion (available in SCALE 6.2 and later)
    - TRITON-Shift: 3D general system depletion (new in SCALE 6.3)
  - Polaris: easy-to-use interface for 2D LWR assembly depletion
- Calculate one-group cross sections for ORIGEN during depletion
  - integral part of special ORIGEN+ARP strategy for fast spent fuel nuclide inventory and source term calculations (ORIGAMI)

F71 File
- inventory (moles per isotope)
- gamma/neutron spectra (optional)

F33 File
- one group xs vs. burnup
- decay constants
- decay heat Q-values
New in SCALE 6.3

• Content of F71 and F33 files can be visualized with the OBIWAN utility (hidden in SCALE 6.2, documented in SCALE 6.3.0)

• F33 file save (changed from 6.2 to 6.3)
  – in SCALE 6.2, users can use the shell block to copy back from TMPDIR to current (or desired) directory
  – in SCALE 6.3, the F33 files are automatically copied back; instead of a file ".combined", there is now a "system.f33" file

• Additional dataset option for FT71 in SCALE 6.3
  – Weighted sum of concentrations of all depleted mixtures (case=0) (also in SCALE 6.2)
  – Weighted sum of concentrations for selected mixtures (case=-1) (also in SCALE 6.2)
  – Weighted sum of concentrations for fuel mixtures (case=-2)
ORIGEN Decay with F71 Input
What is Needed for ORIGEN Decay Calculations with F71 Input?

• ORIGEN decay calculation using as input existing F71 file is also called ORIGEN “restart” calculation

• The “F71” file is the key to transferring nuclide inventories from one part of SCALE to another

• What is needed
  – name and location of the F71 file
  – position (number) on the F71 file to use as input

• The F71 file can originate from
  – depletion simulation with TRITON
  – depletion simulation with Polaris
  – depletion simulation with Origami
  – other ORIGEN decay calculation
Why using ORIGEN Restart Calculations?

• ORIGEN can use as input for the mat card the nuclide inventory (all nuclides in the ORIGEN library) corresponding to a given position in available FT71 file

• Potential applications
  – calculate source terms (nuclide inventory, decay heat, neutron emission, gamma emission) at desired cooling times for an assembly burnup (burnup indicated by position) of interest for a fuel assembly already simulated with TRITON or Polaris over a burnup range from fresh fuel to X GWd/t
  – calculate at desired cooling times the source terms for a specific fuel rod in a fuel assembly already simulated with ORIGAMI
F71 File Structure for file Generated with TRITON

- Stores nuclide concentration for **every depleted mixture** \((1, 2, ..., N)\) in the problem and for **each timestep**, plus a weighted sum of all depletion materials or selected sets of depletion materials.

- Time corresponding to each time dump can be identified if opening the F71 file with Fulcrum.

- TRITON output file gives an overview (which position on the F71 belongs to which mixture at which depletion step)
ORIGEN Decay for Neutron and Gamma emission

```
=ORIGEN

%take 200-group neutron group structure from this SCALE library
%take 47-group gamma group structure from this SCALE library
bounds{
    neutron="scale.rev12.xn200g47v7.1"
    gamma="scale.rev12.xn200g47v7.1"
}

case(my_case){
    ...
    % request neutron emission and use problem-dependent matrix for
    (alpha,n) slowing down; request gamma emission, with no
    Bremsstrahlung
    neutron{alphan_medium=CASE}
    gamma{brem_medium=none}

    % print out neutron and gamma spectrum info in ORIGEN out file
    print{neutron{spectra=yes} gamma{spectra=yes}}

    % save binary results file for all steps
    save{file="my_decay_results.f71"steps=all}
}

' Post-process the resulting ORIGEN binary results
file with OPUS to generate a plot of the neutron
spectrum and gamma spectrum

=OPUS

data="my_decay_results.f71"
title="(alpha,n) neutron spectrum"
typarams=anspectrum
time=years
units=intensity
end

=OPUS

data="my_decay_results.f71"
title="gamma spectrum"
typarams=gspectrum
time=years
units=intensity
end

'end of ORIGEN decay calculation
```
Example of ORIGEN decay with F71 input

```bash
=shell
  cp "${INPDIR}/file_from_triton.f71" "${TMPDIR}/my_f71"
end

=origen
case{
  lib{file="end7dec"}
  mat{load{file="my_f71" pos=25}}
  time{units=YEARS t=[10 1 100]}
  print{nuc {units=[grams]}}
  save{ file="origen_restart_bu30.f71" steps=all}
}
end

=opus
data="origen_restart_bu30.f71"
typarams=nuclides
sort=no
symnuc=u-235 pu-239 end
units=grams
end
```
Recap: ORIGAMI express and detailed inputs
Example of ORIGAMI Express Input

```
=origami
  title="Nuclide inventory in typical PWR spent fuel"
  options{ mtu=1.0 ft71=all}  % Set 1 MTU mass basis & save all timesteps
  libs=[ "w17x17" ]           % Use the Westinghouse 17x17 assembly library
  fuelcomp{
    uox(fuel){ enrich=5 }     % Use 5 wt % enriched fuel
    mix(1){ comps=[ fuel=100 ] }
  }
  modz=[ 0.7332 ]            % Set moderator density to 0.7332 g/cc
  pz=[ 1.0 ]
  hist{
    cycle{ power=20 burn=540 nlib=2 down=30 }  % 3 active cycles @ 20, 19, & 18 MW/MTU
    cycle{ power=19 burn=540 nlib=2 down=30 }  % Followed by 10 years decay
    cycle{ power=18 burn=540 nlib=1 down=0 }
    cycle{ down=3652.5}
  }
end
```
Example of ORIGAMI Detailed Input

- `pz` - axial power shape (unitless)
  - renormalized by default

- `meshz` - used to evaluate non-uniform axial nodes.
  - `pz` +1 number of entries

- `modz` - used to evaluate changing moderator density
  - same number of entries as `pz`
  - requires moderator density interpolation in reactor library or will always use same value.

```plaintext
  =origami
  title="Origami depletion and decay 2x2 fuel array"
  options{ decayheat=yes stdcomp=yes }
  lib=[ w17x17 w15x15 ]
  libmap=[ 1 2
            2 1 ]
  fuelcomp{
    uox{fuel}{enrich=5.0}
    mix(1){ comp[ fuel=100.0 ] }
    uox(fuel2){enrich=4.0}
    mix(2){ comp[ fuel2=100.0 ] }
}
  compmap=[ 2 1
            1 2 ]
  hist[ cycle{ power=20 burn=2500 down=3650 }]
  pxy=[ 0.80 1.00
        1.00 0.80 ]
  pz=[ 0.20 0.50 0.80 1.00 1.10 1.15 1.20 0.90 0.60 0.30 ]
  modz=[ 0.75 0.74 0.73 0.72 0.71 0.70 0.69 0.68 0.67 0.66 ]
  meshz=[ 0 10 50 100 150 200 250 300 350 360 370 ]
  end
```
Effect on BWR source terms of modeling the axial variation in burnup and coolant density
Problem: Model a BWR assembly using 0D and 1D models

• Given a GE14 BWR assembly (ge10x10-8), what is the relative impact of assuming an assembly-average (0D) burnup and coolant density instead of axial burnup and coolant density profiles (1D) at discharge and 10-year cooling time on
  – assembly U-235, Pu-239, total Pu content
  – assembly decay heat
  – assembly total neutron source
  – assembly total gamma source

• Evaluate the impact using a typical 0D ORIGAMI calculation (UOX Express) and a 1D ORIGAMI detailed input calculation for simulating the fuel depletion

Void fraction and discharge burnup profile for a representative BWR assembly (from NUREG/CR-7240)
Part 1: 0D approximation

- **Irradiation history and assembly data**
  - discharge burnup: 45.2 GWd/MTU
    - assume uniform specific power (21.836 MW/MTU)
  - 3 irradiation cycles, 690 days per cycle, 30 days downtime between cycles
  - library: ge10x10-8
  - enrichment 4.5% $^{235}$U
  - assembly-average coolant density 0.3084 g/cm$^3$
  - use nlib=2

- Evaluate at 10 years cooling time

Start with the UOX express form!
Part 2: 1D approximation

- **Irradiation history and assembly data**
  - discharge burnup: 45.2 GWd/MTU
    - assume uniform specific power (21.836 MW/t)
  - 3 irradiation cycles, 690 days per cycle, 30 days downtime between cycles
  - library: ge10x10-8
  - enrichment: 4.5% $^{235}$U
  - axial power: use provided data
  - axial coolant density: use provided data
  - axial node height: use provided data
  - use nlib=2

- Evaluate at discharge and 10 years cooling time

<table>
<thead>
<tr>
<th>Axial node height (cm)</th>
<th>Axial node coolant density (g/cc)</th>
<th>Axial node power (relative)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.48</td>
<td>0.750</td>
<td>0.549</td>
</tr>
<tr>
<td>45.72</td>
<td>0.710</td>
<td>1.189</td>
</tr>
<tr>
<td>91.44</td>
<td>0.557</td>
<td>1.340</td>
</tr>
<tr>
<td>106.68</td>
<td>0.370</td>
<td>1.283</td>
</tr>
<tr>
<td>121.92</td>
<td>0.330</td>
<td>1.256</td>
</tr>
<tr>
<td>137.16</td>
<td>0.297</td>
<td>1.226</td>
</tr>
<tr>
<td>182.88</td>
<td>0.270</td>
<td>1.238</td>
</tr>
<tr>
<td>213.36</td>
<td>0.210</td>
<td>1.162</td>
</tr>
<tr>
<td>228.60</td>
<td>0.200</td>
<td>1.104</td>
</tr>
<tr>
<td>259.08</td>
<td>0.170</td>
<td>1.030</td>
</tr>
<tr>
<td>304.80</td>
<td>0.147</td>
<td>0.975</td>
</tr>
<tr>
<td>381.00</td>
<td>0.124</td>
<td>0.559</td>
</tr>
</tbody>
</table>

Tip: We can reuse (expand upon) our prior input!
Let’s work on this together!
Solution
ORIGAMI: 0D approximation

Decay heat:
• Discharge: 1.342 MW/MTU
• 10 years: 1.590 kW/MTU

Plutonium content (kg/MTU)

<table>
<thead>
<tr>
<th></th>
<th>Discharge</th>
<th>10 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{239}$Pu</td>
<td>6.19</td>
<td>6.24</td>
</tr>
<tr>
<td>$^{240}$Pu</td>
<td>2.78</td>
<td>2.79</td>
</tr>
<tr>
<td>$^{241}$Pu</td>
<td>1.52</td>
<td>0.93</td>
</tr>
<tr>
<td>$^{238}$Pu</td>
<td>0.31</td>
<td>0.30</td>
</tr>
<tr>
<td>$^{242}$Pu</td>
<td>0.64</td>
<td>0.64</td>
</tr>
<tr>
<td>Total Pu</td>
<td>11.44</td>
<td>10.92</td>
</tr>
</tbody>
</table>

Neutron source (n/s/MTU)

<table>
<thead>
<tr>
<th></th>
<th>10 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>(alpha,n)</td>
<td>1.019E+07</td>
</tr>
<tr>
<td>SF</td>
<td>4.813E+08</td>
</tr>
<tr>
<td>Total</td>
<td>4.915E+08</td>
</tr>
</tbody>
</table>

$^{244}$Cm (g/MTU)
• Discharge: 62.6
• 10 years: 42.7
ORIGAMI: 1D approximation

**Decay heat:**
- Discharge: 1.340 MW/MTU
- 10 years: 1.643 kW/MTU

**Plutonium content (kg/MTU)**

<table>
<thead>
<tr>
<th></th>
<th>Discharge</th>
<th>10 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{239}$Pu</td>
<td>6.22</td>
<td>6.27</td>
</tr>
<tr>
<td>$^{240}$Pu</td>
<td>2.70</td>
<td>2.73</td>
</tr>
<tr>
<td>$^{241}$Pu</td>
<td>1.43</td>
<td>0.88</td>
</tr>
<tr>
<td>$^{238}$Pu</td>
<td>0.33</td>
<td>0.32</td>
</tr>
<tr>
<td>$^{242}$Pu</td>
<td>0.69</td>
<td>0.69</td>
</tr>
</tbody>
</table>

**Total Pu**
- Discharge: 11.43 kg/MTU
- 10 years: 10.89 kg/MTU

**Neutron source (n/s/MTU)**

<table>
<thead>
<tr>
<th>Source</th>
<th>10 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>(alpha,n)</td>
<td>1.182E+07</td>
</tr>
<tr>
<td>SF</td>
<td>6.968E+08</td>
</tr>
<tr>
<td>Total</td>
<td>7.086E+08</td>
</tr>
</tbody>
</table>

**$^{244}$Cm (g/MTU)**
- Discharge: 90.2 g/MTU
- 10 years: 61.6 g/MTU
How large is the axial modeling effect for BWRs?

- You fill in the data for U-235 and Pu-239 😊
- 0.3% decrease in assembly total Pu @ 10 years
- 3.3% increase in assembly decay heat @ 10 years
- 30.6% increase in total neutron source @ 10 years
  (44% increase in $^{244}\text{Cm}$ content @ 10 years)
- You fill in the data for total gamma source 😊

Conclusion?
Best-estimate models for BWR neutron source calculations benefit from including axial information.
Impact on the neutron source of various modeling assumptions
Impact on the neutron source of various modeling assumptions added burnup and coolant density profiles