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Overview of Depletion/Decay Sequences and Relevant Files

SCALE 6.3.1

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U.S. DEPARTMENT OF ENERGY

Learning goals

- **Introduce** users to the SCALE sequences used for depletion and decay workflows
- **Illustrate** how SCALE modules/sequences are used together to perform depletion and decay calculations

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Nomenclature refresher



Irradiated nuclear fuel

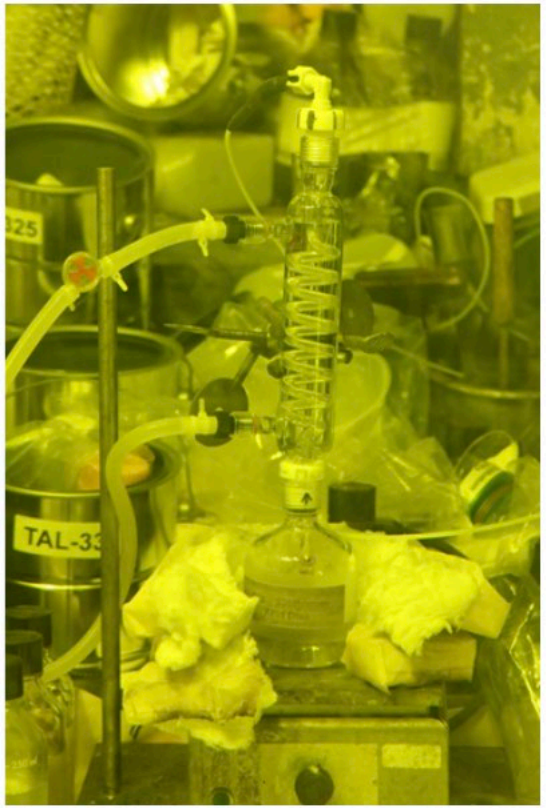
- Fresh fuel inserted in a reactor (e.g., U-based) undergoes nuclear transmutations, leading to production of higher actinides (e.g., Pu) and fission products (FPs)
- **What happens to the fuel material irradiated in the reactor?**
  - Irradiation changes the fuel material composition
  - U is lost through transmutation (mostly fission)
  - Pu is produced through neutron interactions (transmutation) of U
  - FPs are generated by fission of U, Pu
- **Relevant metrics for spent fuel characterization**
  - Nuclide inventories
  - Decay heat
  - Radioactivity
  - Radiation emissions (neutron, gamma sources)

Primary parameters for irradiated nuclear fuel

- **Burnup**
  - Measure of the integral number of fission events occurring in fuel during irradiation
  - Quantifies the amount of energy produced during irradiation
  - Unit: MWd/t or %FIMA
  - Burnup (MWd/t) = power (MW) × irradiation time (days)/initial heavy metal mass (metric ton)
  - %FIMA = (number of) fissions per initial metal atom, in percent
- **Cooling time**
  - Duration between the date the irradiated fuel is discharged from the reactor and a reference time of interest
  - Units: years, days
  - Highly relevant for decay heat and radiation emissions calculations
- **Initial enrichment**
  - Measure of the fissile mass in fresh fuel
  - Units: % ^{235}U/ U total for U-based fuel

Primary irradiated fuel parameters: Burnup

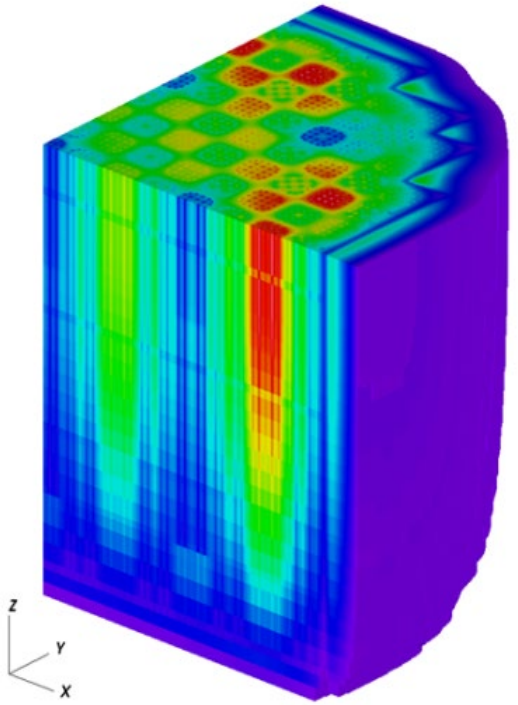
- **Burnup estimates by destructive assay (DA) experiments**
  - Based on burnup indicator fission products (e.g., ^{148}Nd) as a measure of total number of fissions in fuel
  - Requires cutting and dissolving fuel for radiochemical analysis (RCA)
  - Burnup $\propto$ ^{148}Nd (nuclide concentration)
  - Accuracy in burnup estimation based on ^{148}Nd generally $< 3\%$
- **Burnup estimates by non-destructive assay (NDA) experiments**
  - Based on neutrons and/or gamma measurements
  - Burnup $\propto$ ^{137}Cs (gamma)
  - $Burnup^4 \propto$ ^{244}Cm (neutron)
  - Requires knowledge of enrichment, cooling time, and reactor operating history
  - Codes are generally used to correlate NDA with burnup
  - Accuracy in burnup estimation based on NDA ~10%



Hot cell used for DA
ORNL/TM-2022/2788

Computer codes for fuel irradiation simulations

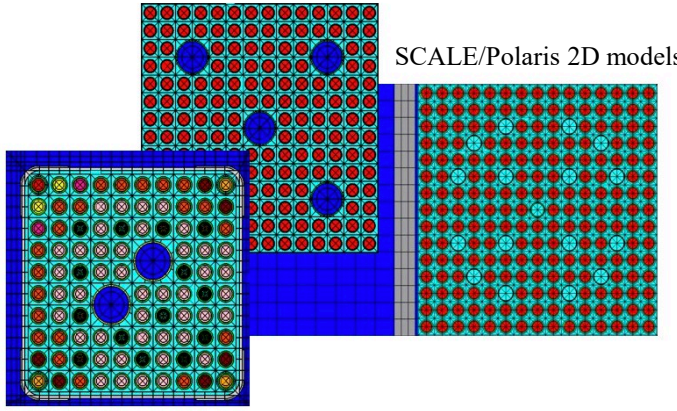
- **Reactor core simulators (3D)**
  - Simulate the entire reactor core to calculate the spatial distribution of power (and burnup) of each fuel element in the reactor
  - Used by reactor operators for operation and fuel management
  - Generally, require 3D modeling capabilities, significant computing power, and long computing time
  - Examples: VERA, CASMO/SIMULATE
- **Depletion/burnup and decay codes (0D)**
  - Simulate a single fuel element
  - Can calculate the complete set of nuclide contents in irradiated fuel
  - Can calculate radiation emissions used in spent fuel verification
  - Do not directly consider the spatial and energy dependence in the neutronic environment (however, this can be accounted for using the approach for generating cross section data)
  - Are very fast (seconds) compared to core simulators
  - Examples: ORIGEN, CINDER, FISPIN



CASLU-2015-0206-000, CASL (June 2016)

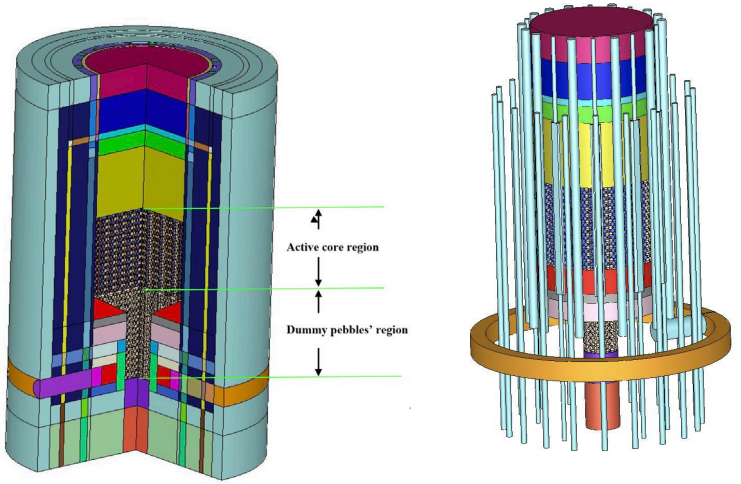
Computer codes for fuel irradiation simulations (cont.)

- **Lattice physics computational tools (1D, 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 simulate a set of fuel assemblies or even the entire reactor for small configurations (e.g., small research reactors), depending on the problem
  - Generally used to obtain burnup-dependent lattice physics parameters for use in core simulators (e.g., nodal cross sections)
  - Generally require 2D or 3D modeling capabilities, moderate computing power, and longer computing time (compared to 0D depletion codes)
  - Iteratively couple a 1D, 2D, or 3D neutron transport solver with a 0D depletion/burnup solver (e.g., ORIGEN)
  - Examples: SCALE/TRITON, SCALE/Polaris, Serpent



SCALE/Polaris 2D models

Wide range of LWR geometry support



SCALE/KENO-VI 3D model for HTR-10 pebble bed reactor

(ORNL/TM-2020/1500/v3)

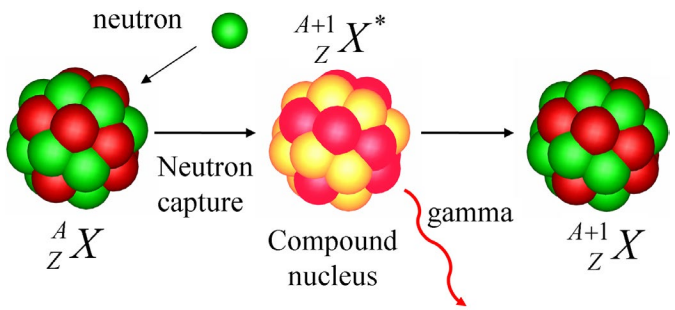
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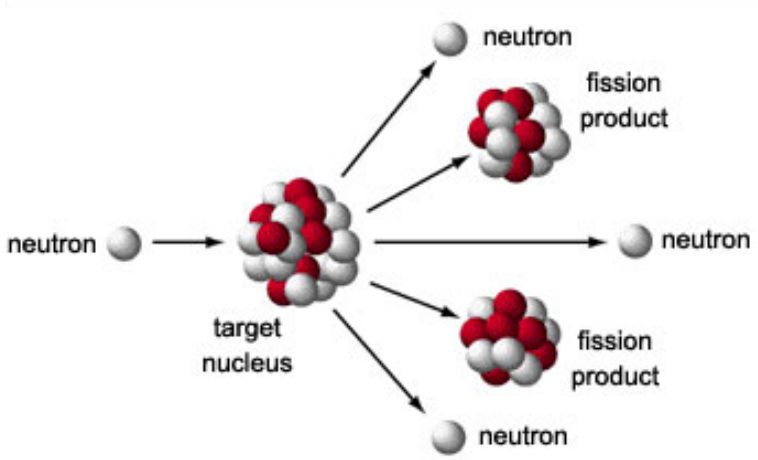
ORIGEN is the foundation of depletion capabilities in SCALE

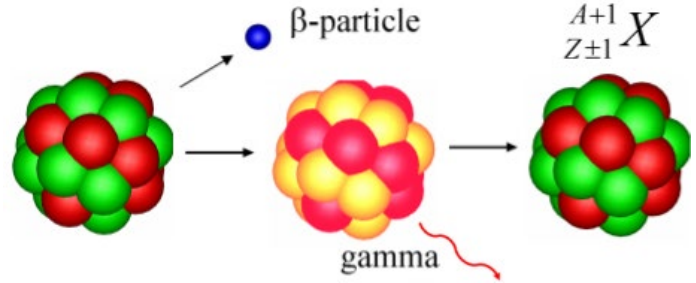


What is ORIGEN ?

- **O**ak **R**idge **I**sotope **Gen**eration code in SCALE
- Irradiation and decay simulation code
- Explicit simulation of all pathways from neutron transmutation, fission, and decay



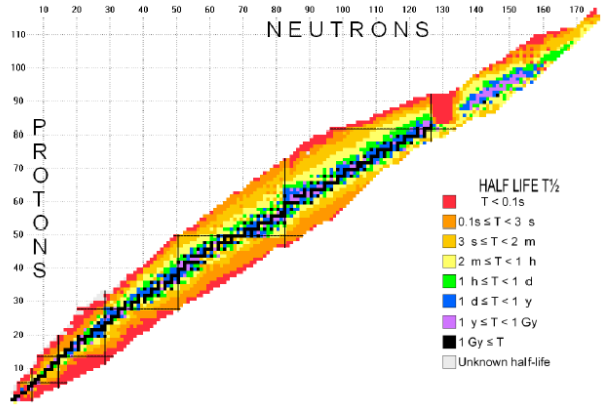




ORIGEN highlights

$$\dot{\boldsymbol{N}}(t) = \overline{\overline{\boldsymbol{A}}} \cdot \boldsymbol{N}(t)$$

- **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 sections**, fission yield data, decay data
  - Accurate problem-dependent cross section generation and accurate nuclear data are 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
  - Engine of ORIGAMI tool
  - Depletion solver in SCALE lattice physics codes (TRITON, Polaris)



ORIGEN family in SCALE

- **ORIGEN**
  - Main engine: solves depletion, decay, activation, and feed/removal problems, as well as radiation emission calculations (0D code)
- **ORIGAMI** (ORIGEN Assembly Isotopics)
  - Provides the capability to easily perform depletion and decay calculations with ORIGEN for LWR fuel assemblies
- **OPUS** (ORIGEN Post-processing Utility for SCALE)
  - Utility to perform post-processing and analysis of ORIGEN results contained in ORIGEN concentrations files, including sorting, ranking, and unit conversion
- **ARP** (Automatic Rapid Processing)
  - Cross section interpolator – interpolates on a set of pre-generated ORIGEN libraries (see next slide) to create a new ORIGEN library at different values of the interpolation parameters (e.g., burnup)
- **OBIWAN** (ORIGEN Binary Interrogation Without a SCALE Input)
  - Command-line utility for viewing, manipulating, and converting ORIGEN binary files F71, F33 (see next slide)

Special files: F71 and F33

- **ORIGEN concentration file (F71)**
  - Stores all nuclide inventory (always present) and neutron/gamma sources (optional)
  - Content can be visualized with Fulcrum and interrogated with OBIWAN
  - Consistent usage across the ORIGEN family
- **ORIGEN library file (F33)**
  - Special "library" that contains all the information needed to "reconstruct" a depletion calculation (details to be presented later this week)
  - Can be generated with TRITON or Polaris
  - Integral part of the ORNL ORIGEN-ARP method (more details in ORIGAMI presentation)
  - Consistent usage across ORIGEN, ORIGAMI, and ARP
  - Content can be interrogated with OBIWAN (see Section 5.2 of SCALE manual)

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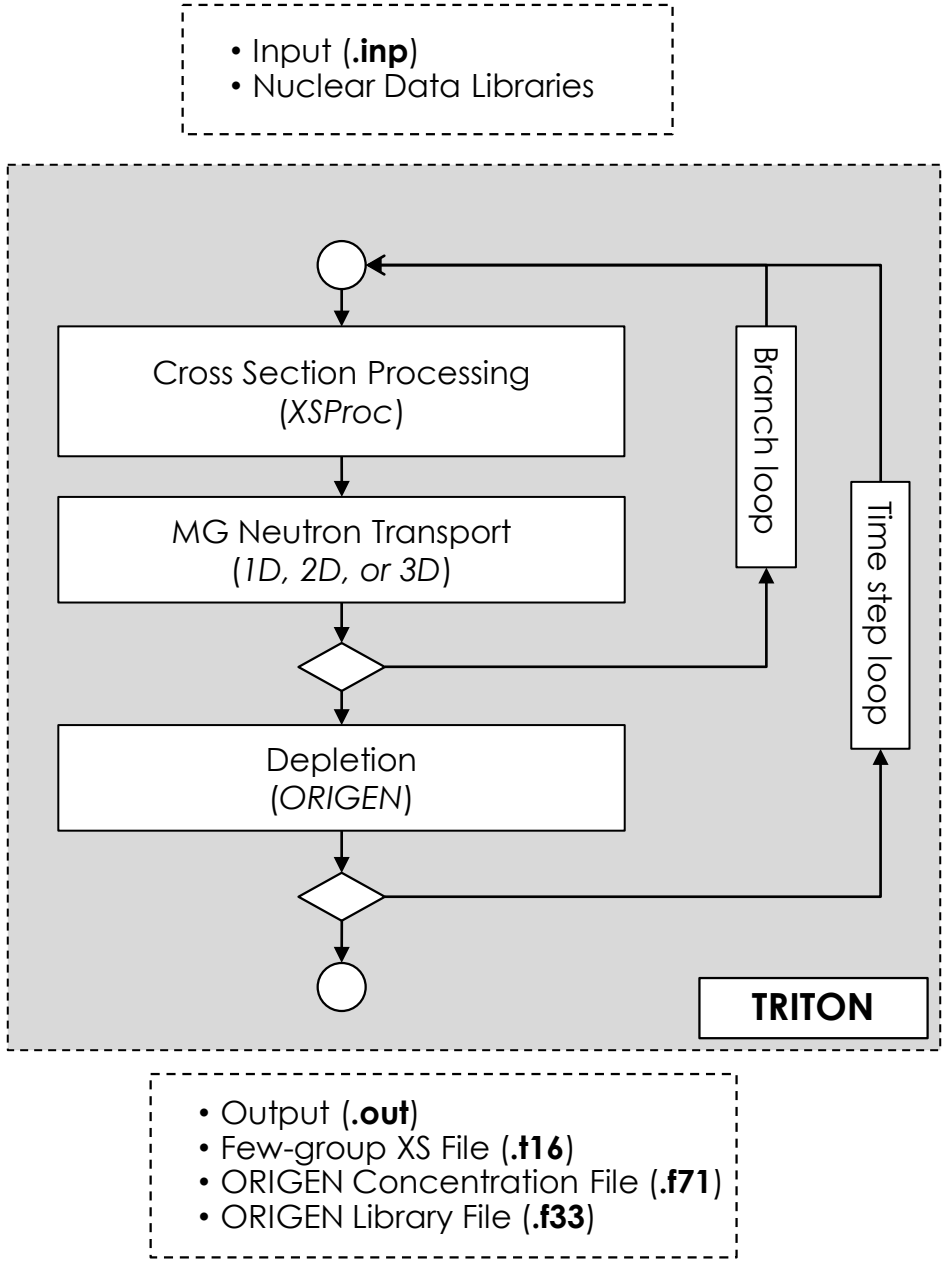
Depletion sequences in SCALE



TRITON depletion sequence

TRITON: SCALE's modular, general-geometry, reactor physics sequence

- Cross section processing: XSPROC
  - Wide range of self-shielding options
  - Same module used in criticality safety and shielding sequences
- Multigroup neutron transport:
  - 1D SN (XSDRNPM)
  - 2D ESC-SN (NEWT)
  - 3D Monte Carlo (KENO-V.a, KENO-VI, Shift)
- Transport-to-depletion coupling
  - Normalizes power/flux levels
  - Prepares transition matrices for ORIGEN
  - Manages time-stepping (predictor-corrector)
- Depletion (ORIGEN)
- TRITON in SCALE 6.2+ also supports 3D CE depletion



Basic capabilities for TRITON depletion

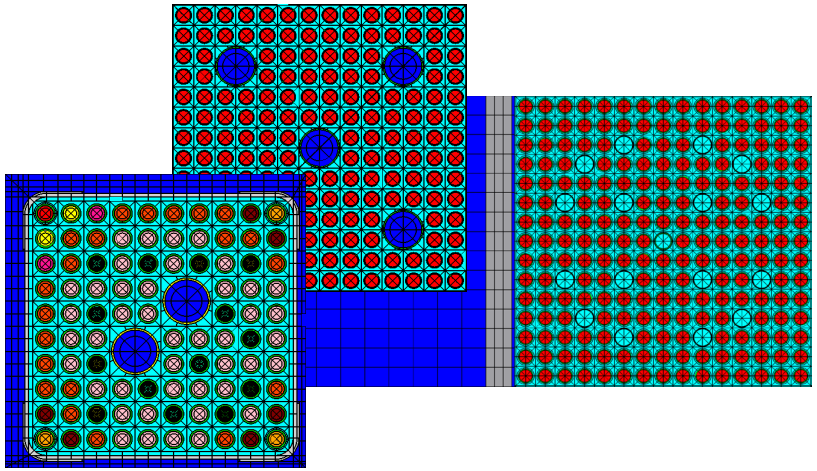
- **Calculates evolution of nuclide concentrations during fuel depletion (irradiation, decay)**
  - TRITON-NEWT: 2D general system depletion (available in SCALE 5.1 and later)
  - TRITON-KENO: 3D general system depletion (available in SCALE 5.1 and later)
  - TRITON-Shift: 3D general system depletion (new in SCALE 6.3)
- **Uses ORIGEN as depletion/decay solver**
- **Calculates 1-group cross sections for ORIGEN during the depletion simulation**
  - Integral part of special ORIGEN+ARP strategy for fast spent fuel nuclide inventory and source term calculations (in ORIGAMI)

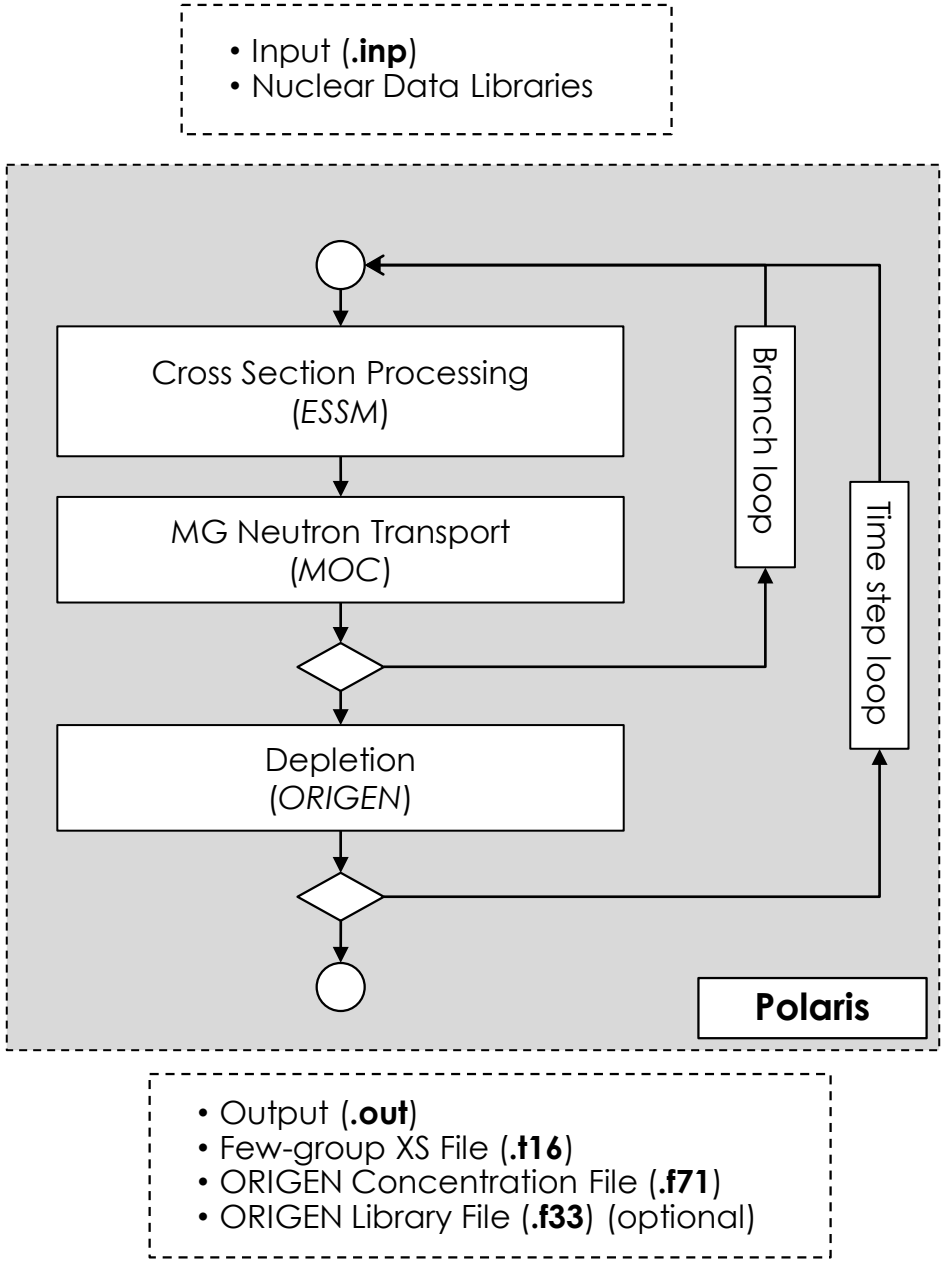
F33 File
- 1-group cross sections vs. burnup
- decay constants
- decay heat Q-values

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

Polaris lattice physics sequence

- SCALE's fast, easy-to-use 2D lattice physics capability for LWR analysis
- Simple input
  - Assembly geometry
  - Material definitions
  - Range of system conditions
- Wide range of LWR geometry support





Typical fuel depletion analysis with SCALE



1. Fresh fuel composition/design are specified in the SCALE input file
   - TRITON (any general geometry)
   - Polaris (LWR geometry only)
   - ORIGAMI (geometry assumed based on the pre-generated ORIGEN reactor library file, F33, that is specified in input)
2. Irradiation history is specified in the SCALE input file
   - Power vs. time
   - State (void, temperature) vs. time (in TRITON and Polaris)
3. Decay with ORIGEN to calculate inventories, decay heat, and neutron/gamma sources as a function of desired cooling time
   - Read discharge nuclide inventory from F71 file and decay to a cooling time of interest

Relevant output from within TRITON and Polaris

- **ORIGEN concentrations file (F71)**
  - TRITON, Polaris, and ORIGAMI depletion **automatically generates F71**
  - ORIGEN calculations
    - User must provide energy bins for neutron and gamma emission calculations and explicitly request the emission calculations; also, must explicitly request saving information to a new F71

- **ORIGEN library file (F33)**
  - TRITON **automatically generates F33 files**
    - One F33 is generated per each depleted mixture in the problem; one combined F33 is also generated, representative of the entire system that is modeled

      basename.mixNNNNNN.f33, where NNNNNN is the material number and BASENAME is the root name of the input file (BASENAME.inp)

      basename.system.f33
  - Polaris **generates F33 per request** in the input file (*opt DEPL* card)
    - One F33 can be generated per each depleted mixture and for the entire system

      filename.hname.XXX.f33, where XXX is the name of the material (or system), filename is the root name of the input file, and hname is the name for the history

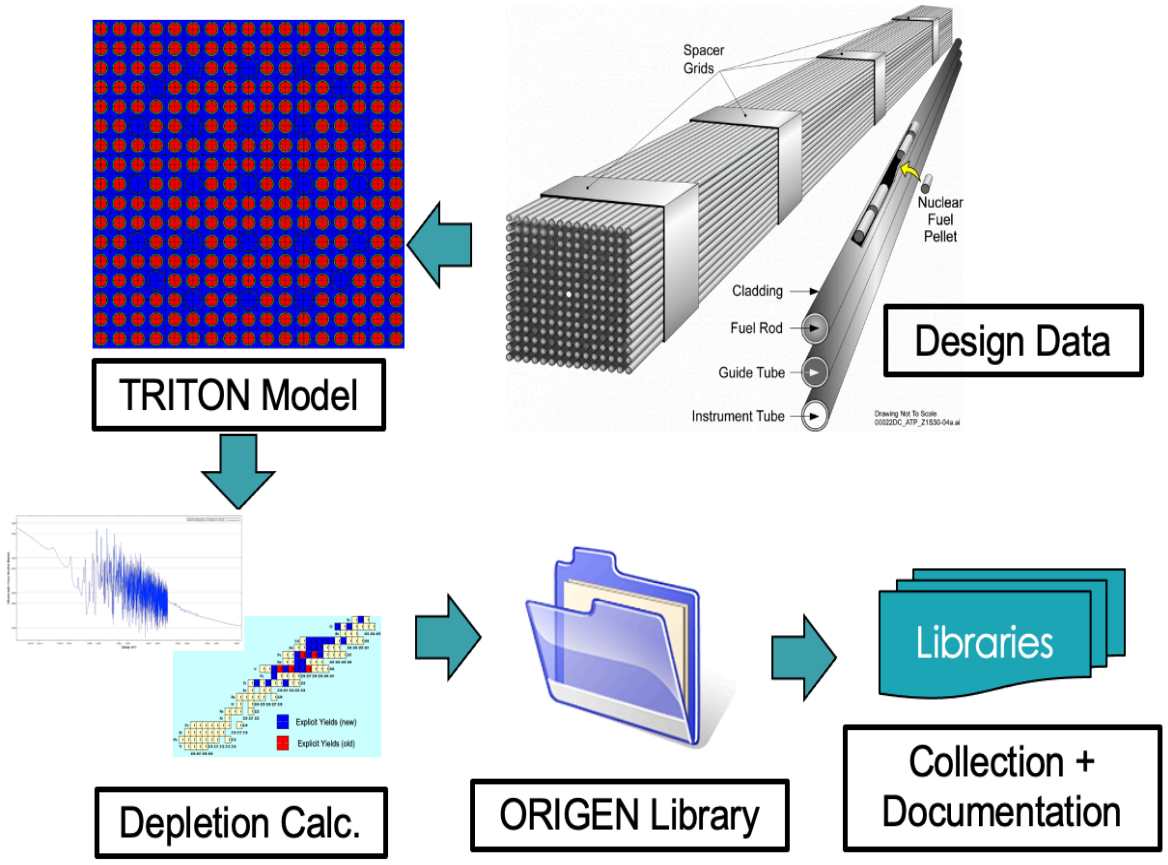
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Fast depletion calculations with SCALE

Typical approach in a nutshell



Generate ORIGEN reactor libraries (F33) with TRITON or Polaris



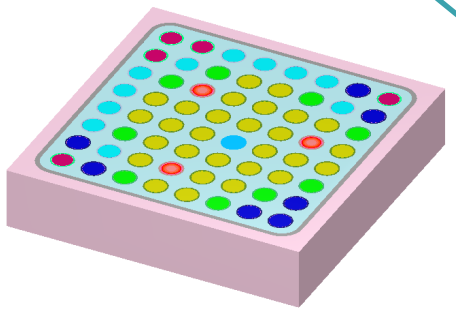
We'll learn how to generate reactor libraries later this week

Calculate source terms with ORIGAMI

using an ORIGEN reactor library and assembly data as input



ORIGEN reactor library

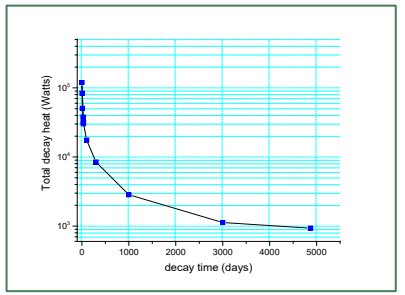


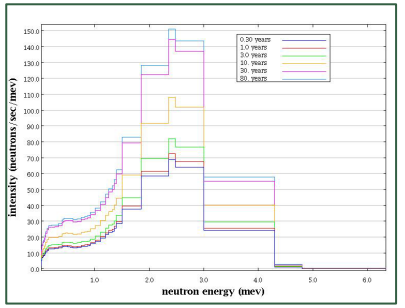
Assembly data
irradiation/decay
history data

ORIGAMI

(ORIGEN)

Nuclide inventories
Decay heat
Activities
Sources and spectra

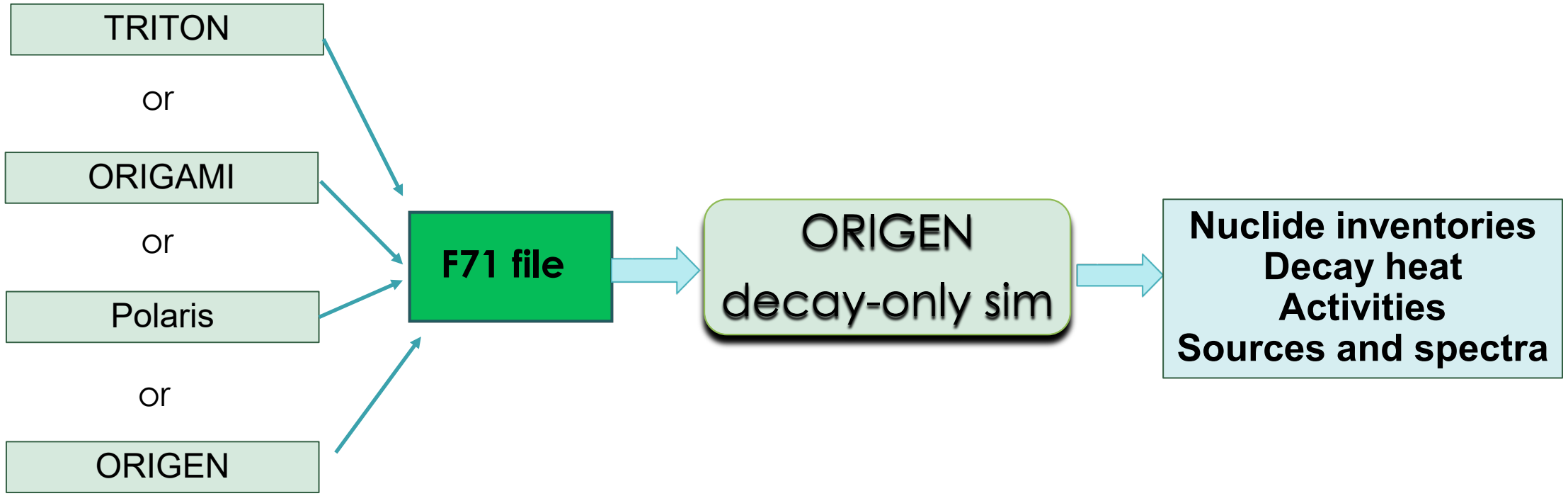




We'll learn hands-on how to use ORIGAMI later this week

Source terms calculation via ORIGEN decay

using available nuclide inventory from an F71 file as input



We'll learn hands-on how to perform ORIGEN decays later today and throughout this week

Summary

- ORIGEN is the foundation of all depletion capabilities in SCALE
  - Used as standalone or under the hood in ORIGAMI, TRITON, and Polaris sequences
- There are two highly relevant files for depletion, which are consistently used across all SCALE depletion sequences
  - ORIGEN nuclide concentration file (F71)
  - ORIGEN reactor library file (F33)
- Best approaches and practices on how to use the depletion capabilities may vary, depending on the application of interest
  - An example is presented for source term calculations (once the F71 file is available, the solution is only an ORIGEN-decay away)