OAK RIDGE National Laboratory

ORIGEN Reactor Libraries in SCALE

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Oak Ridge National Laboratory

SCALE Users' Group Workshop

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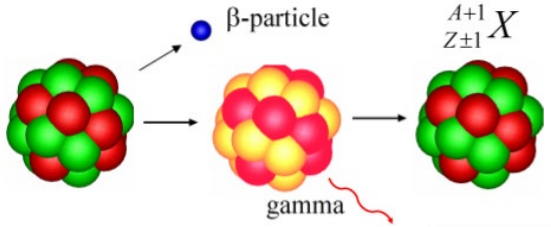
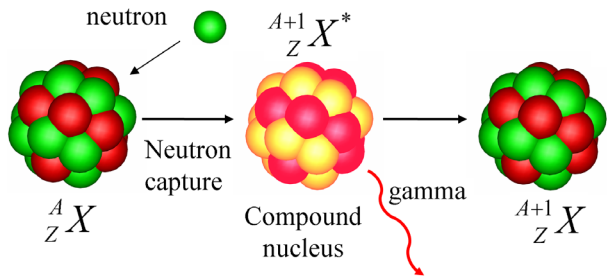
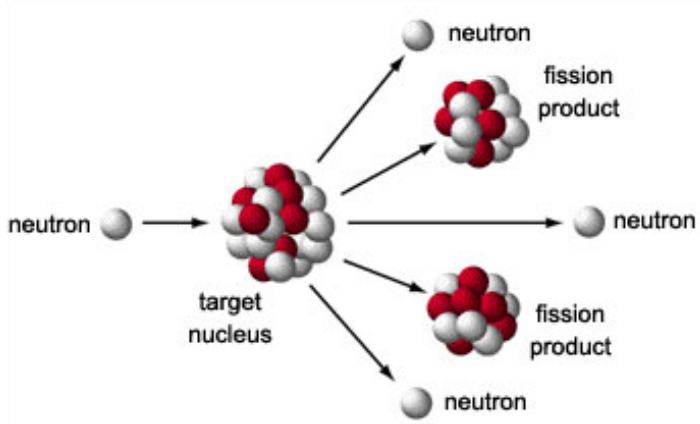
U.S. DEPARTMENT OF ENERGY

What is ORIGEN ?

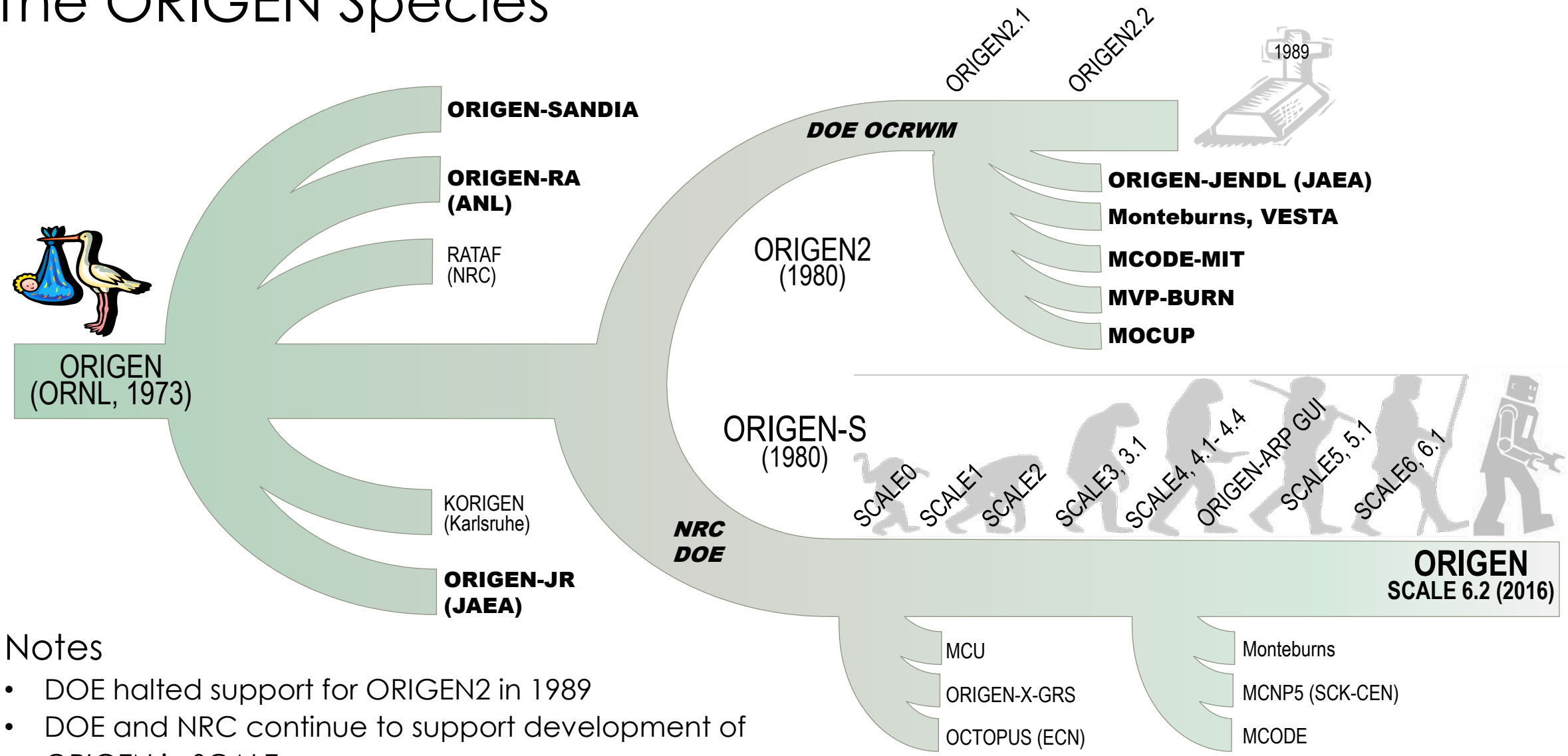
- **O**ak **R**idge **I**sotope **Gen**eration code in SCALE
- Irradiation and decay simulation code
- Explicit simulation of all pathways from neutron transmutation, fission, and decay
- ORIGEN tracks 2,237 isotopes
  - 176 actinides
  - 1,151 fission products
  - 910 structural activation nuclides







The ORIGEN Species



Notes

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

Key Capabilities of ORIGEN in SCALE

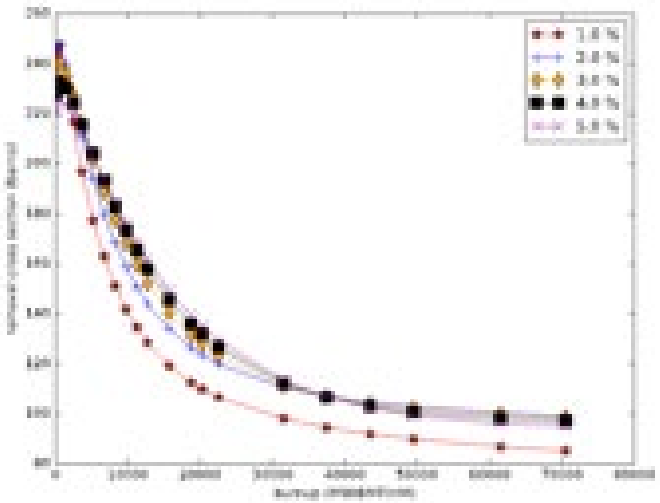
- **Comprehensive spent nuclear fuel characterization over large time scales**
  - Nuclide concentrations
  - Activities
  - Decay heat
  - Radiation emission rates and spectra (neutron, gamma)
- **Source terms for accident analyses** (operating reactors, spent fuel handling, storage
- **Structural material activation** (in-core, ex-core)
- **Fuel cycle analysis** (material feed and removal processing)
- **Maintained, up-to-date, nuclear data libraries**
- **Short run time (seconds)**

Nuclear Data Libraries for ORIGEN Simulations

- **Decay data**
  - Half-lives, decay modes and branching fractions, recoverable energy per disintegration
- **Cross sections** for neutron-induced reactions
- **Fission product yields**
  - Energy-dependent data for 30 actinides
- **Gamma ray production** data
- **Neutron production** data

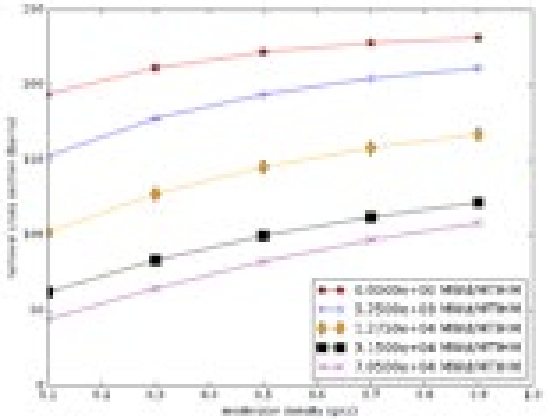
Accurate Cross Section Libraries are Key to Accurate ORIGEN Depletion Simulations

- Cross sections libraries are **problem dependent** and must be determined for the system being analyzed, as they depend on:
  - Fuel type
  - Enrichment
  - Burnup
  - Assembly design
  - Fuel temperatures
  - Moderator properties
  - Control rod/blade exposure



Pu-240 removal cross section vs. burnup and enrichment for BWR 10x10

Pu-240 removal cross section vs. burnup and coolant density for BWR 10x10



What are ORIGEN Reactor Libraries ?

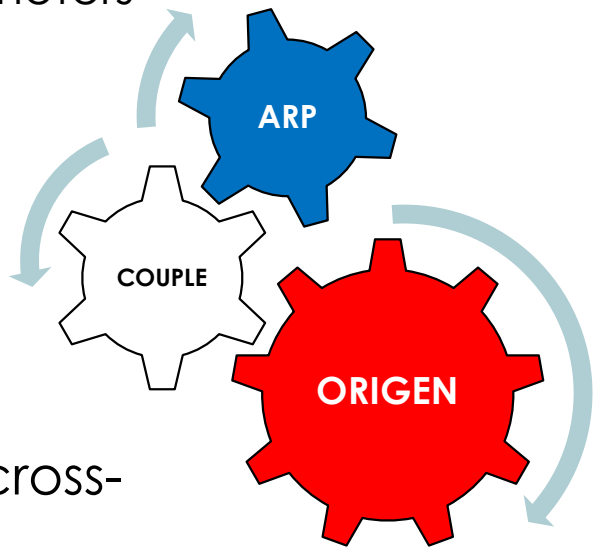
- ORIGEN Reactor Library = One set of pre-generated library files with burnup-dependent, 1-group, cross sections and other data ORIGEN needs for depletion simulations (decay data, fission yields) for a specific reactor type and fuel assembly configuration
  - e.g. BWR GE 10x10 library
- There is one library file containing burnup-dependent cross sections for a set of discrete values of parameters for the considered assembly design
  - e.g. file corresponding to enrichment 4.0wt% U-235 and 0.4 g/cm3 coolant density for GE 10X10
- Fuel/reactor specific ORIGEN libraries reside in directory SCALE-6.2\data\arplibs\
- Library information is provided in SCALE-6.2\data\arpdata.txt file for all reactor libraries
  - Fuel type (name of the reactor library)
  - Number of values for each variable parameter
  - Parameter values
  - Burnup values for each library position
  - Filenames for parameter-dependent libraries

ORIGEN Family of Codes in SCALE 6.2

- **ORIGEN**
  - main engine: solves depletion, decay, activation, and feed problems, as well as the decay emission calculations
- **COUPLE**
  - library management code for ORIGEN
- **ARP**
  - interpolates on a set of pre-generated ORIGEN libraries to create a new ORIGEN library at specific values of interpolation parameters (e.g., burnup, enrichment, coolant density)
- **ORIGAMI** (**ORIG**EN **A**sse**m**bly **I**sotopics) Graphical User Interface for ORIGEN
  - provides the capability to easily perform fast depletion and decay calculations with ORIGEN for LWR fuel assemblies
- **OPUS**
  - performs post processing and analysis of ORIGEN results contained in ORIGEN concentrations files, including sorting, ranking, and unit conversion

ORIGEN-ARP Methodology in SCALE 6.2

- **ORIGEN-ARP** = Innovative approach in SCALE
  - Enables fast and accurate depletion simulations with ORIGEN for a given assembly design and user-defined burnup and assembly discrete parameters (e.g. enrichment) using pre-generated ORIGEN reactor library files
- **ARP** (Automated Rapid Processing) utility code
  - Interpolates pre-generated cross-sections to user-defined burnup and enrichment
  - Interpolation parameters for uranium fuels are burnup, enrichment and moderator density
- **ORIGEN** can perform depletion calculations with ARP-interpolated cross-section data
- **ORIGAMI** combines ARP and ORIGEN to simplify the input and to perform calculations for axially or radially varying burnup and moderator density
- Accuracy of assembly models that were used to generate the ORIGEN reactor libraries are maintained

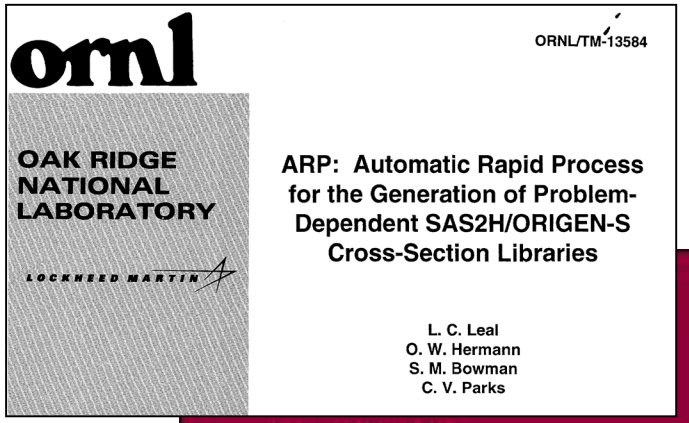


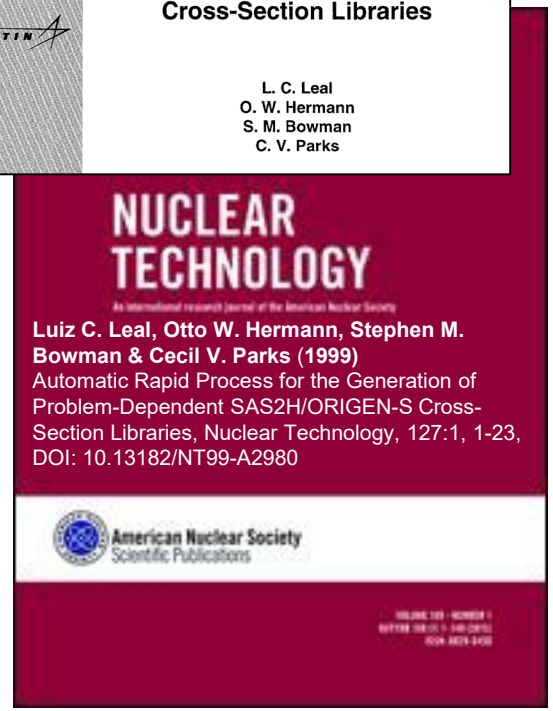
ORIGEN Reactor Libraries – the Forefathers

- 1-group cross section libraries were released with ORIGEN 2 in the 1980's using 1D transport models for 3 PWR and 3 BWR state points (1 burnup and 1 enrichment for each model), using a mixture of ENDF/B-IV and ENDF/B-V data
- 36 sets of ORIGEN-S reactor libraries for 2 reactor types (one PWR, one BWR) and 18 individual combinations (burnup, enrichment, specific power) for each configuration were released in the 1980s
- ORIGEN-S reactor libraries had a 3-group structure (therm, res, and fast) and were based on ENDF/B-IV and ENDF/B-V data
- **ARP** was developed by L. Leal in 1992-1995
- **ORIGEN-ARP methodology** was first implemented in 1990s in SCALE 4.3, with reactor libraries generated using SAS2H (1D assembly models)
- **ORIGEN-ARP GUI 1.0** with reactor libraries for 4 LWR designs was released in 2001

L. C. LEAL, O.W. HERMANN, and C. V. PARKS, "Automatic Rapid Processing SCALE SAS2H-Produced Parameter-Dependent Cross Section for ORIGEN-S," Trans. Am. Nucl. Soc., 70, 356, **1994**

C. V. PARKS, "Overview of ORIGEN2 and ORIGEN-S: Capabilities and limitations, IHLRWM, Las Vegas, NV, **1992**

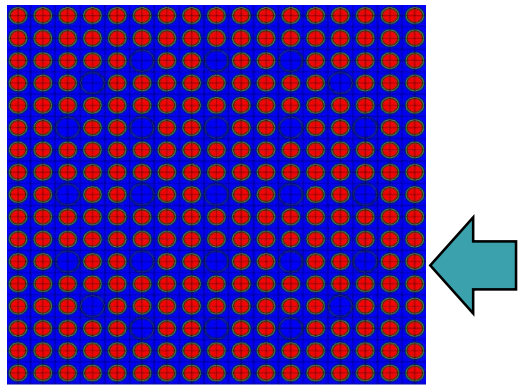




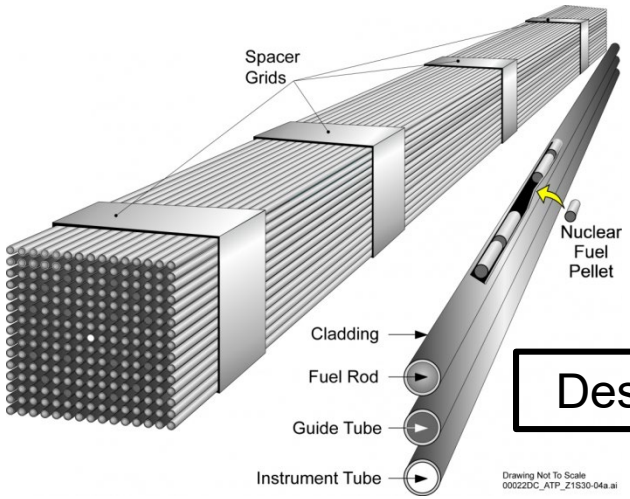
ORIGEN Reactor Libraries Major Releases

- SCALE 4.3 (2001)
  - 3 PWR (15x14, 15x15, 17x17) and 1 BWR (8x8)
- SCALE 5.1 (2006)
  - Libraries generated using 2D assembly models and ENDF/B-V cross sections for
    - 7 PWR UO2 (CE14x14, CE16x16, W14x14, S14x14, W15x15, W17x17, W17x17 OFA)
    - 9 BWR UO2 (GE 7x7, GE 8x8, ABB8x8, GE9x9, GE10x10, ATRIUM-9, ATRIUM-10, SVEA-64, SVEA-100)
    - 6 PWR MOX (14x14, 15x15, 16x16, 17x17, 18x18)
    - 4 BWR MOX (8x8, 9x9-1, ATRIUM 9, 10x10)
    - 5 VVER (VVER-100, VVER440 flat enrichment, VVER440-3.82, VVER440-4.25, VVER440-4.38)
    - 1 RBMK
  - MGNOX, CANDU, and AGR libraries ported from 5.0, generated with 1D models and ENDF/B-V cross sections
- SCALE 6.1 (2011)
  - All libraries ported from 5.1
- SCALE 6.2 (2016)
  - Major update
  - Libraries generated with 2D models end ENDF/B-VII.1 cross sections

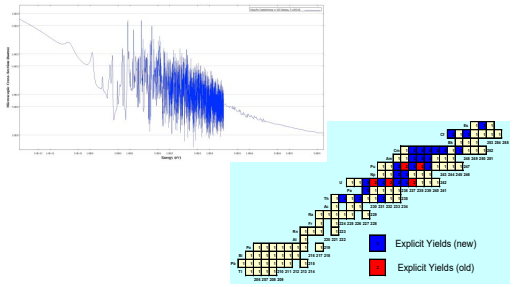
How to Generate ORIGEN Reactor Libraries in SCALE 6.2



TRITON Model



Design Data



Depletion Calc.

ORIGEN Library

Collection + Documentation

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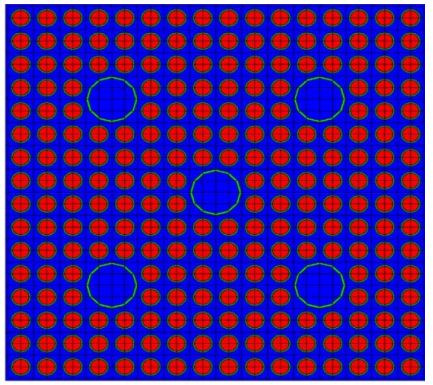
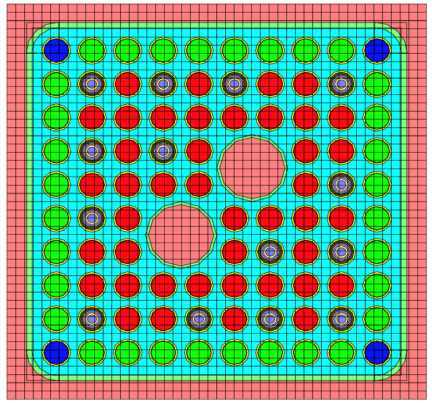
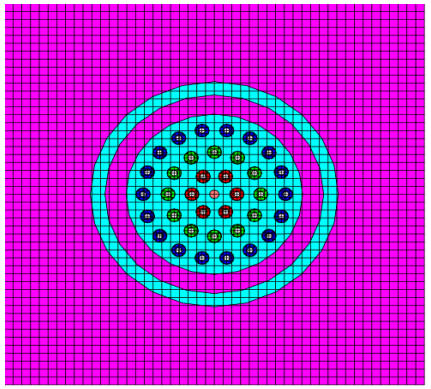
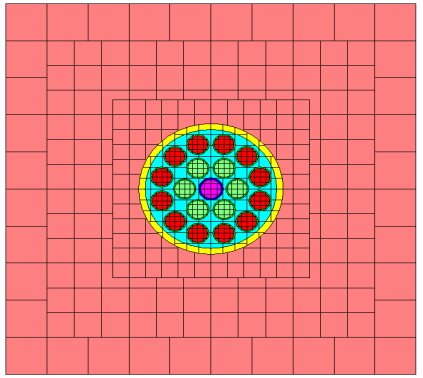
ORIGEN Reactor Libraries in SCALE 6.2 (2016)

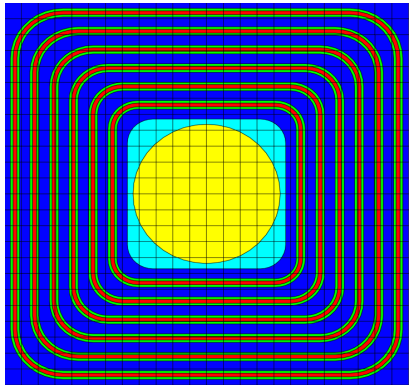
- Major update of all previous libraries and new additions included
- Generated using 2D TRITON assembly models and 252-group ENDF/B-VII.1 cross sections
- **All templates are available on C:\SCALE-6.2\etc\slig\testing\templates**
- Large variety of assembly designs
  - 8 PWRs, 10 BWRs, 4 VVER-440s, 1 VVER-1000, 1 RBMK (UO2 fuel)
  - 5 PWRs and 4 BWRs (MOX fuel)
  - CANDU (natural UO2)
  - MAGNOX (natural U metal)
  - Advanced Gas-Cooled Reactor (AGR)
  - IRT – research reactor fuel (HEU, LEU)





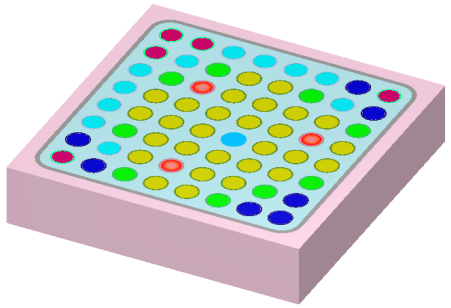






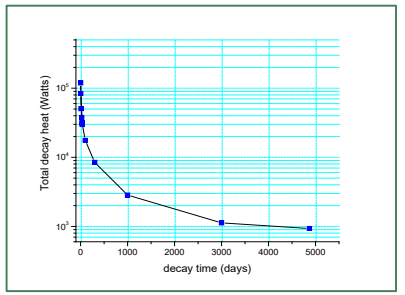
How to use ORIGEN Reactor Libraries in SCALE 6.2

ORIGEN library

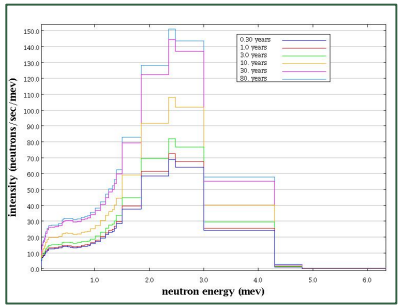


Assembly irradiation and decay history

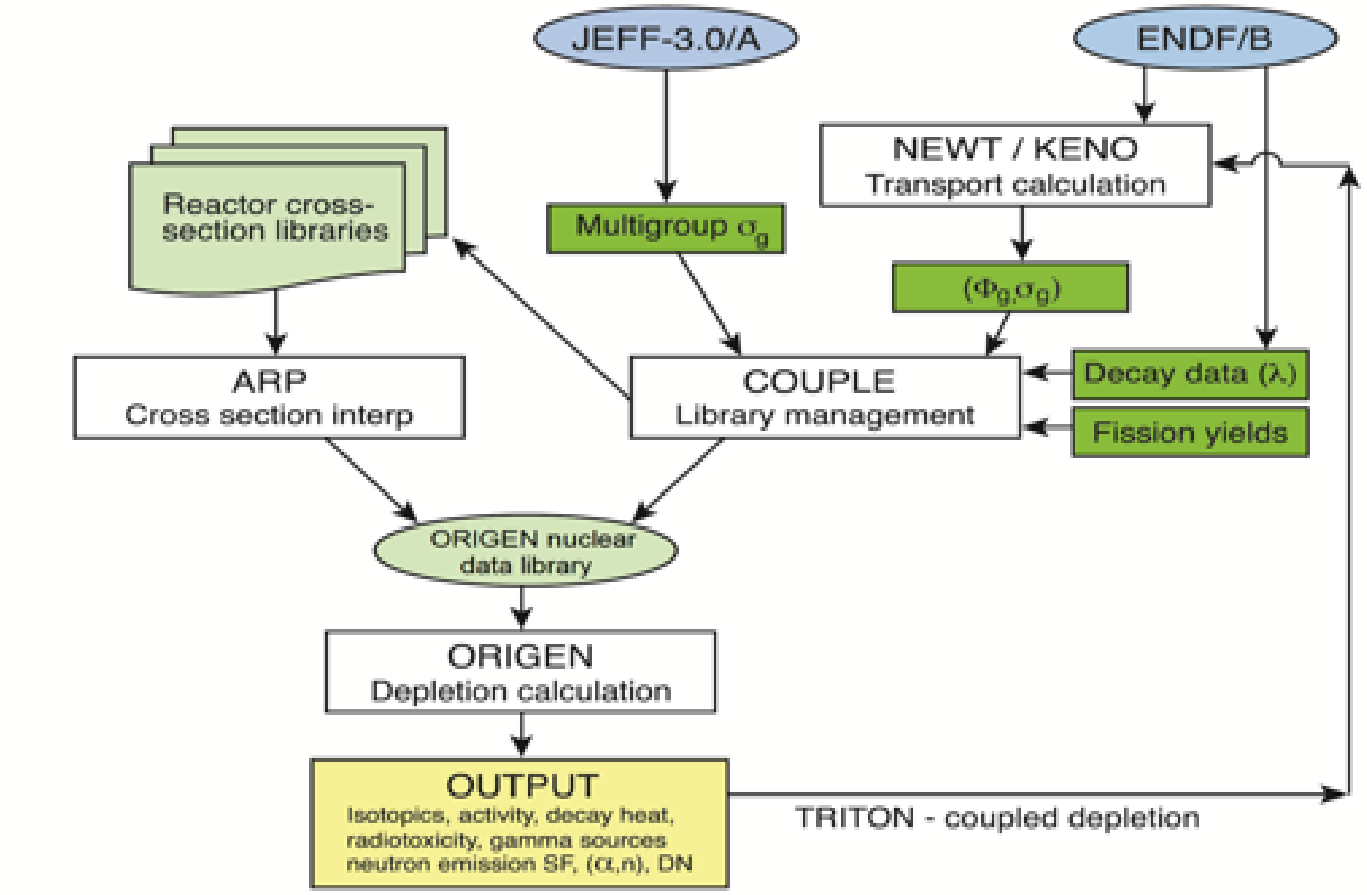
ORIGEN
ORIGAMI



Nuclide inventory
Decay heat
Radioactivity
Sources and spectra



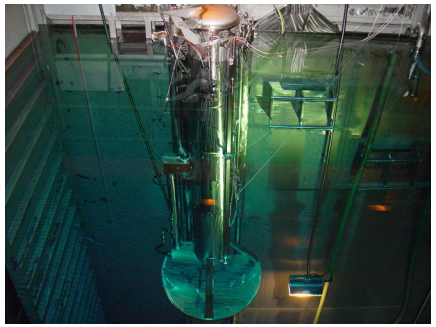
Generating ORIGEN Reactor Libraries with SCALE in a Nutshell

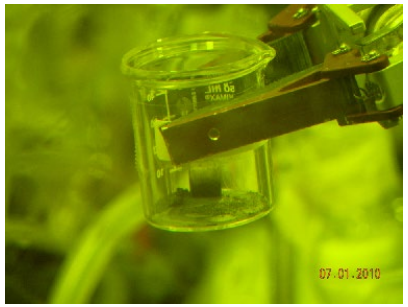


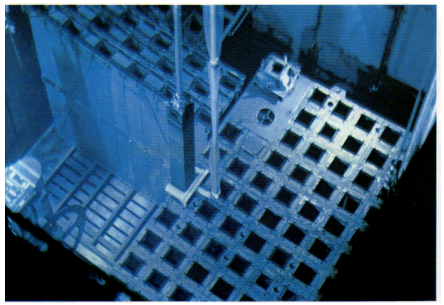
- ENDF/B-VII SCALE neutron transport libraries include ~420 materials
- Cross sections for additional materials obtained from JEFF-3.1/A activation file
  - 774 nuclides, 12,617 neutron-induced reactions
  - Binary datasets in /scale6.2/data/jeff252g, jeff238g, jeff200g, jeff56g, jeff49g
- Data has standard AMPX format and may be visualized in Fulcrum

Performance of ORIGEN Reactor Libraries

- ORIGEN reactor libraries can be used to provide adequate characterization of **assembly-averaged metrics** that are important for a variety of spent nuclear fuel applications
  - Nuclide inventory
  - Decay heat
  - Activity
  - Radiation emissions
- Pin-wise ORIGEN libraries can be generated and used for applications requiring within-assembly detailed information (and used with ORIGAMI)
  - e.g., source terms for NDA detector systems in safeguards

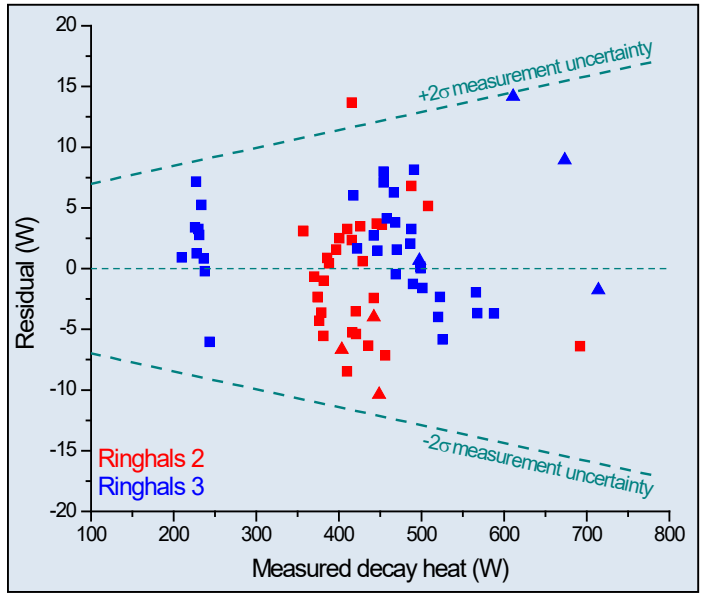


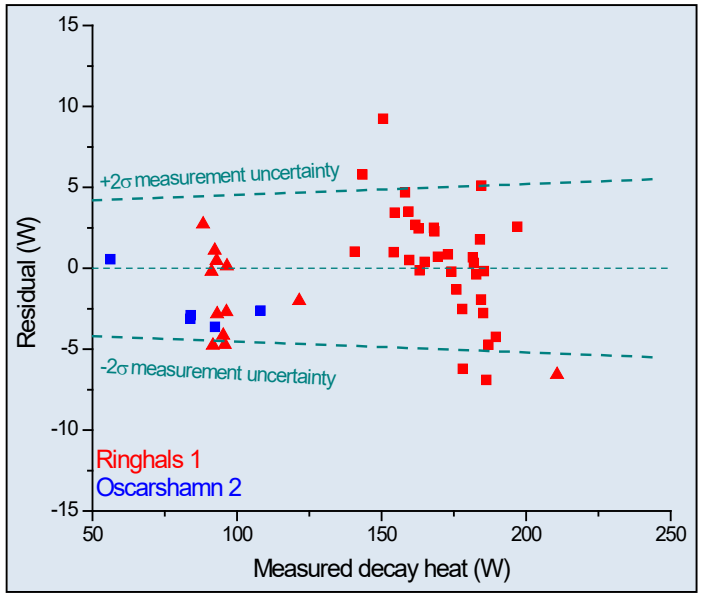




Performance of ORIGEN Reactor Libraries

ex: decay heat, long decay times



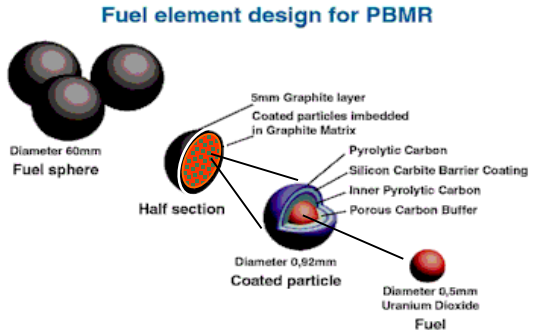


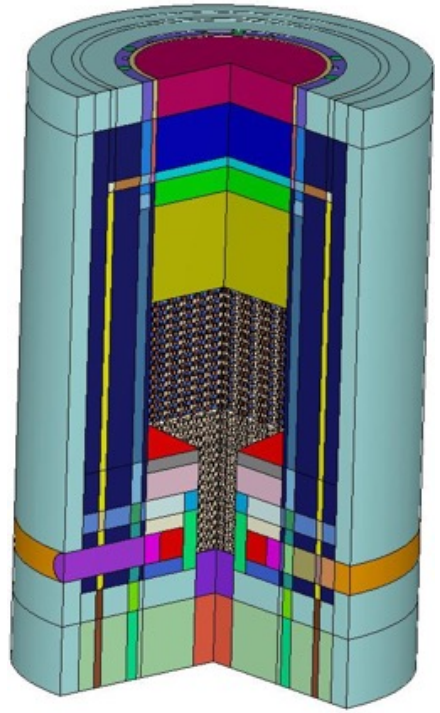
Data set	No. of measurements	C/E mean	C/E σ	Residual C-E (W) mean	Residual C-E (W) σ
PWR	71	1.002	0.012	0.57	4.91
BWR	50	0.997	0.024	-0.25	3.36

G. Ilas, I. C. Gauld, and H. Liljenfeldt, **Validation of ORIGEN for LWR used fuel decay heat analysis with SCALE**, Nuclear Engineering and Design, vol. 273, p. 58-67 (2014) https://doi.org/10.1016/j.nucengdes.2017.05.009

Coming up

- Validation report (multi-volume) for SCALE 6.2.4 with ENDF/B-VII.1 data is planned for 2020
  - Volume 3, dedicated to validation for reactor physics applications, include validation against nuclide inventories and decay heat experiments
- New with SCALE 6.3
  - ORIGEN reactor libraries will be re-generated with SCALE 6.3/TRITON, ENDF/B-VII.1 data, with extended enrichment (8wt%) and burnup (80GWd/MTU) for LWRs
  - ORIGEN reactor libraries can be generated with Polaris
- Planned for SCALE 7
  - ORIGEN reactor libraries for advanced reactors
  - ORIGAMI for non-LWRs





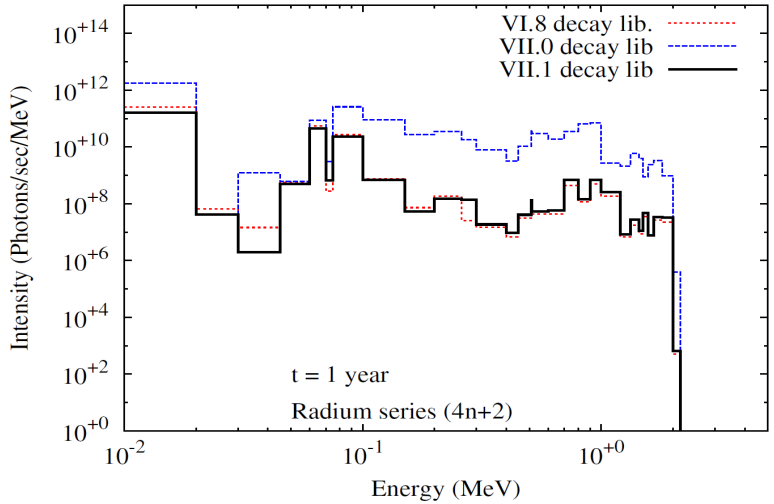
Questions ?

Backup slides, if needed

Nuclear Decay Data Are Also Important !

(Ex: Known ENDF/B-VII.0 Performance Issues)

- ^{234}Th beta decay daughter incorrectly assigned in ENDF/B-VII.0 as ^{234}Pa instead of isomer ^{234m}Pa
- Impact on gamma spectra: order of magnitude difference in gamma spectra for ^{238}U decay
- Small effect on assembly decay heat : **0.2%** for ENDF/B-VII.0 vs ENDF/B--VII.1 nuclear decay data libraries



I. C. Gauld, M. T. Pigni, and G. Ilas, "**Validation and testing of ENDF/B-VII decay data**", Nuclear Data Sheets 120, p.33-36 (2014)

Nuclide identifiers: sub-library search

- When you do not specify a sublib, e.g.

```
iso = [ gd155=1.0 ]
```

where does it go?

- If the sublib for a nuclide/element is not provided, it is guessed in the following manner:
  - if the nuclide is in fact an element, then it is placed in sublib=1/LT,
  - if the atomic number Z<26, an *attempt* is made to place it in sublib=1/LT,
  - otherwise (Z≥26 or attempt fails), sublibs are searched in reverse order, from 3/FP, 2/AC, then 1/LT.
- sublibs are used extensively throughout ORIGEN family for **output**, e.g. actinides only (AC)

iso=[gd=1] % →1/LT
(and split into nuclides based on nat. abund.)

iso=[o16=1] % →1/LT
iso=[gd155=1] % →3/FP