ORIGEN Isotopic Depletion and Decay

Presented to:
VERA Workshop

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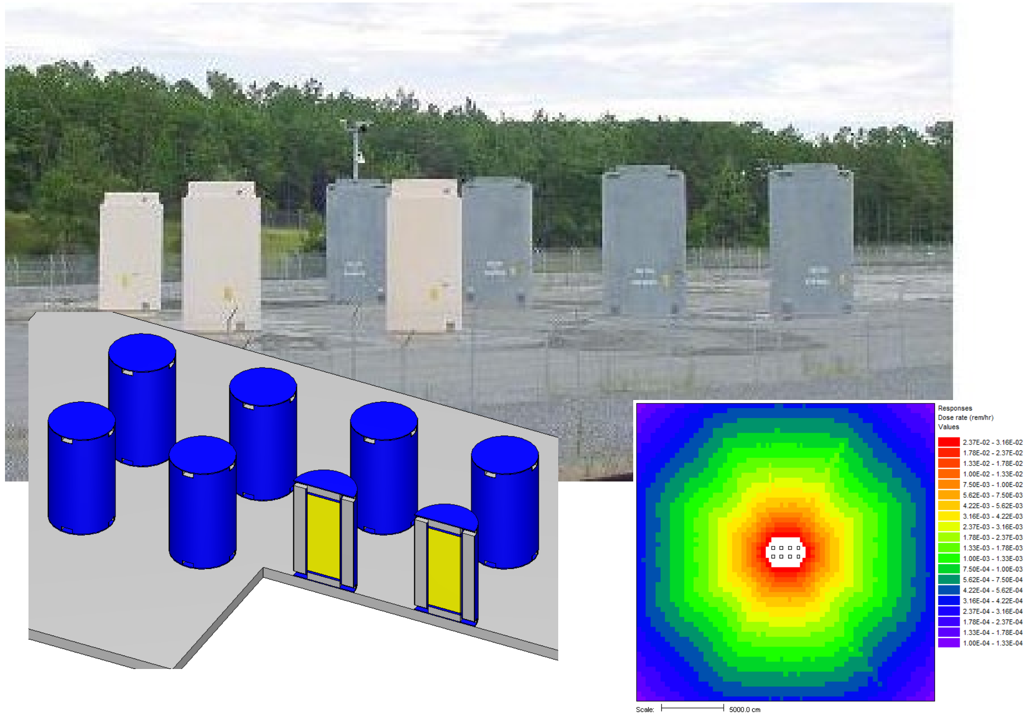
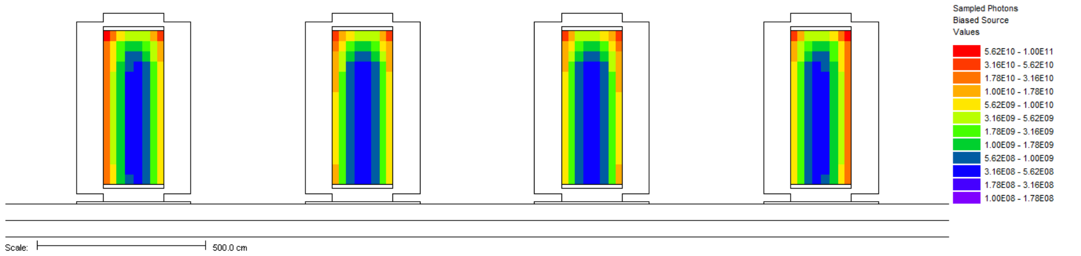
Key ORIGEN Capabilities

- Calculation of isotopics and source terms
  - Nuclide concentrations (atoms and mass)
  - Activities
  - Decay heat
  - Radiation emission rates and spectra (neutron and gamma)
  - Radiotoxicity
- Application Environments
  - Depletion/decay in operating reactors
  - Spent fuel storage/handling
  - Structural material activation (in-core, ex-core)
  - Fuel cycle analysis (Material feed and removal processing)





Within SCALE: ORIGEN calculates spent fuel gamma emissions and links to MAVRIC to calculate dose at pad or site boundary.

ORIGEN Strategy

SCALE

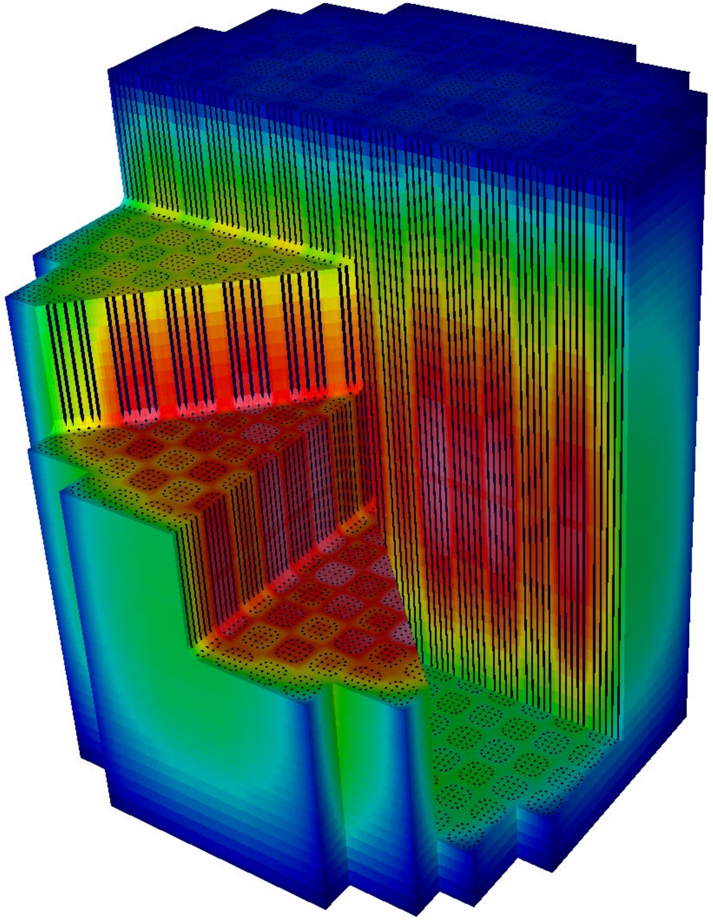
- general applications
  - 2237 isotopes
  - 54000 transitions between isotopes
    - all pathways in modern nuclear data for neutron transmutation, fission, and decay
    - all nuclides with half-lives > 1 ms
- Runtime **50-100 ms** per time step solve

VERA

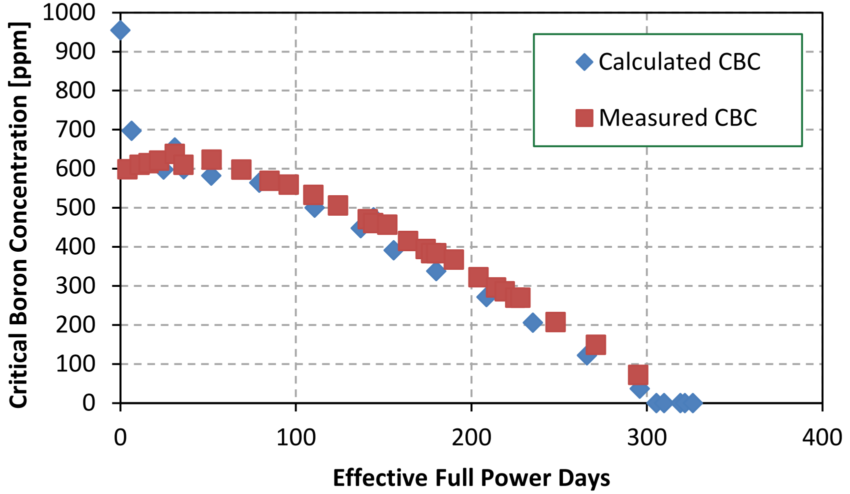
- LWR-specific applications
  - ~300 isotopes
  - ~8000 transitions between isotopes
  - Significant factor of ~8 memory savings (2237->300)
- Runtime **~10 ms** per time step solve
- Millions of depletion zones in VERA full core simulations
  - 3 radial zones * 50 axial zones per fuel rod
  - ~50,000 rods in core

VERA Full Core Depletion

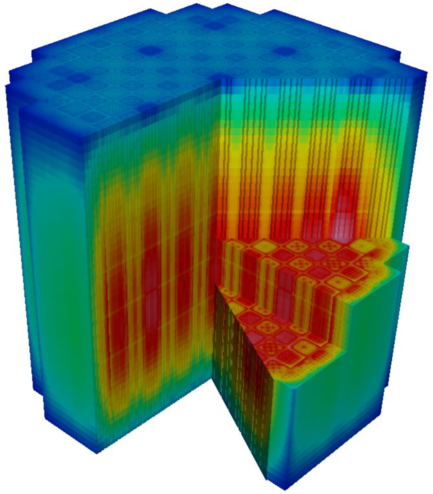
^{239}Pu Distribution



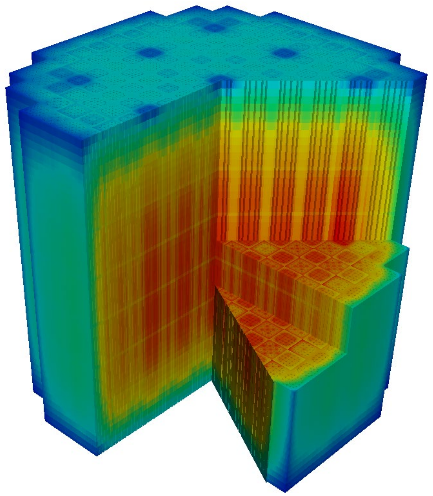
Critical Boron Comparisons



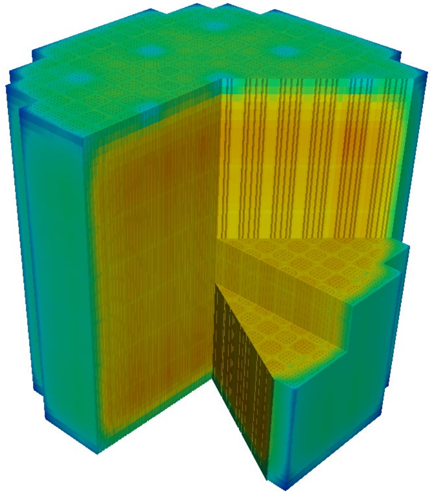
Power Shape During Cycle Depletion



Beginning of Cycle



Middle of Cycle



End of Cycle

ORIGEN Methods (1/4)

Mathematical Model

- General expression solved for production and loss rate of a nuclide

Rate of Change in Nuclide Concentration = Production Rate of Nuclide − Loss Rate of Nuclide

- Translated into a system of Ordinary Differential Equations (ODEs)

Rate of Change in Nuclide **i** Concentration = Decay into Nuclide **i** by other Nuclides **j** + Production of Nuclide **i** from Irradiation − Loss of Nuclide **i** through Decay, Irradiation, or Other Means

$$\frac{dN_i}{dt} = \sum_{j=1}^{m} l_{ij}\lambda_j N_j + \bar{\Phi}\sum_{k=1}^{m} f_{ik}\sigma_k N_k - (\lambda_i + \bar{\Phi}\sigma_i + r_i)N_i + F_i, \qquad (i = 1,\ldots,m) \ ,$$

ORIGEN Methods (2/4)

Matrix Exponential Form of the Solution

- The transmutation equation can be written in matrix form as

$$\frac{\mathrm{d}\vec{N}}{dt} = \boldsymbol{A}\vec{N}(t), \quad \text{with given initial condition } \vec{N}(0)$$

- The matrix exponential solution is given as

$$\vec{N}(t) = \exp(\boldsymbol{A}t)\vec{N}(0)$$

where

$\vec{N}(0)$ is a vector of initial isotopics

$\boldsymbol{A}$ *is an m x m* transition matrix containing rate coefficients for radioactive decay, neutron capture, fission, etc.

ORIGEN Methods (3/4)

Solver Kernel 1: Hybrid Matrix Exponential/Linear chains

- Exponential matrix $\exp(\boldsymbol{A}t)$ can be represented as a series expansion

$$\exp(\boldsymbol{A}t) = \sum_{n=0}^{\infty} \frac{(\boldsymbol{A}t)^n}{n!}$$

- But short lived transitions (e.g. large decay constant) are difficult to solve due to round off

  e.g. $e^{-100} = 1 - 100 + 100^2/2! - 100^3/3! + \ldots = 3.72 \times 10^{-44}$

- To prevent loss of numerical accuracy, short-lived nuclides for a specific time step are removed from the exponential matrix treatment and resolved using Bateman linear chains

$$N_i = N_i(0)e^{-d_i t} + \sum_{k=1}^{i-1} N_k(0) \prod_{n=k}^{i-1} \frac{a_{n+1,n}}{d_n} \left[\sum_{j=k}^{i-1} d_j \frac{e^{-d_j t} - e^{-d_i t}}{(d_i - d_j)} \prod_{\substack{n=k \\ n \neq j}}^{i-1} \frac{d_n}{d_n - d_j} \right],$$

ORIGEN Methods (4/4)

Solver Kernel 2: Chebyshev Rational Approximation Method

- Matrix exponential method based on Chebyshev rational approximation of the exponential function

$$\exp(\boldsymbol{A}t) = a_0 + 2Re\left[\sum_{i=1}^{k/2} a_i(At + \theta_i I)^{-1}\right] \qquad \vec{N}(t) = \exp(\boldsymbol{A}t)\vec{N}(0)$$

- Fast and accurate, able to handle large systems of nuclides
- Overall accuracy almost independent of step lengths
- Adjoint solution implemented (Annals of Nuclear Energy 85, p.68, 2015)

ORIGEN Nuclear Data

- **Decay data (ENDF/B-VII.1)**
  - ~2600 decay transitions allowed with T ½ (> 1 ms)
  - Decay branching fractions β^-, β^+, EC, a, IT, $\beta^-\beta^-$, β^-n, SF, n, β^-a
  - Transitions to ground and excited states
  - Recoverable energy from decay (a, β, γ)
- **Neutron reaction cross section data (JEFF-3.1/A)**
  - ~800 nuclides (ENDF/B has ~400)
  - ~13000 neutron-induced reactions
  - Expanded reaction types supported (ENDF/B in red)

    (n,2n), (n,3n), (n,f), (n,na), (n,n3a), (n,2na), (n,3n a), (n,np), (n,n2a), (n,2n2a), (n,nd), (n,nt), (n,n ^{3}He), (n,nd2a), (n,nt2a), (n,4n), (n,g), (n,p), (n,d), (n,t), (n,^{3}He), (n,a), (n,2a), (n,3a), (n,2p), (n,pa), (n,t2a), (n,d2a), (n,n')
  - Isomeric transitions, e.g. Am-241 -> Am-242m

- **Fission product yields (ENDF/B-VII.0)**
  - 30 actinides: ^{227,228,232}Th, ^{231}Pa, $^{232\text{-}238}$U, $^{238\text{-}242}$Pu, ^{241,242m,243}Am, ^{237,238}Np, $^{242\text{-}246,248}$Cm, ^{249,252}Cf, and ^{254}Es
  - Data are from England and Rider compilations
  - Energy-dependent yields tabulated at
    - Thermal fission: 0.0253 eV
    - Fast fission: 500 keV
    - High energy fission: 14 MeV
  - Actual yields are interpolated using the mean energy of neutrons causing fission

SCALE/ORIGEN team evaluates new nuclear data and corrects/reports errors for downstream users
Example from ENDF/B-VII.0

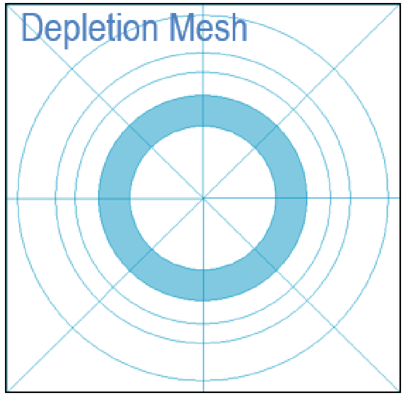
***Issue:** ^{234}Th beta decay daughter incorrectly assigned as ^{234}Pa instead of isomer ^{234m}Pa*

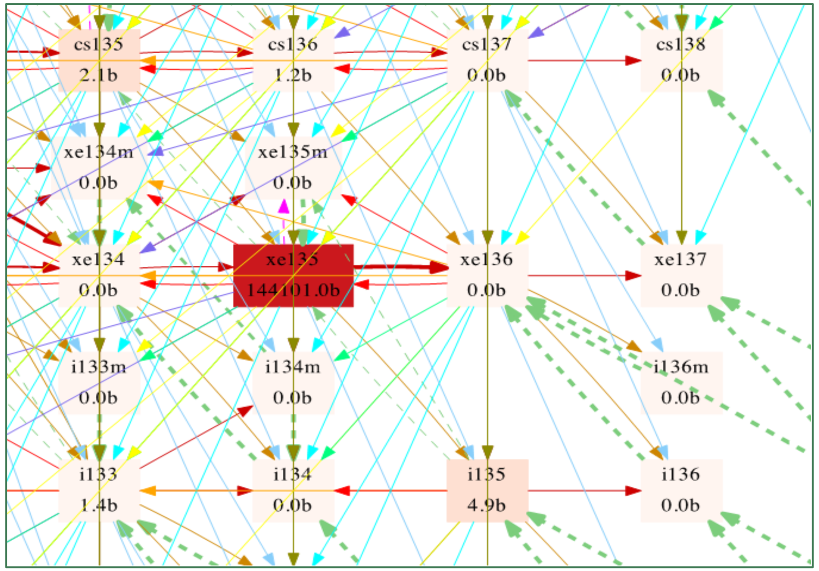
***Impact:** order of magnitude difference in gamma spectra for ^{238}U decay*

ORIGEN API (Fortran/C++)

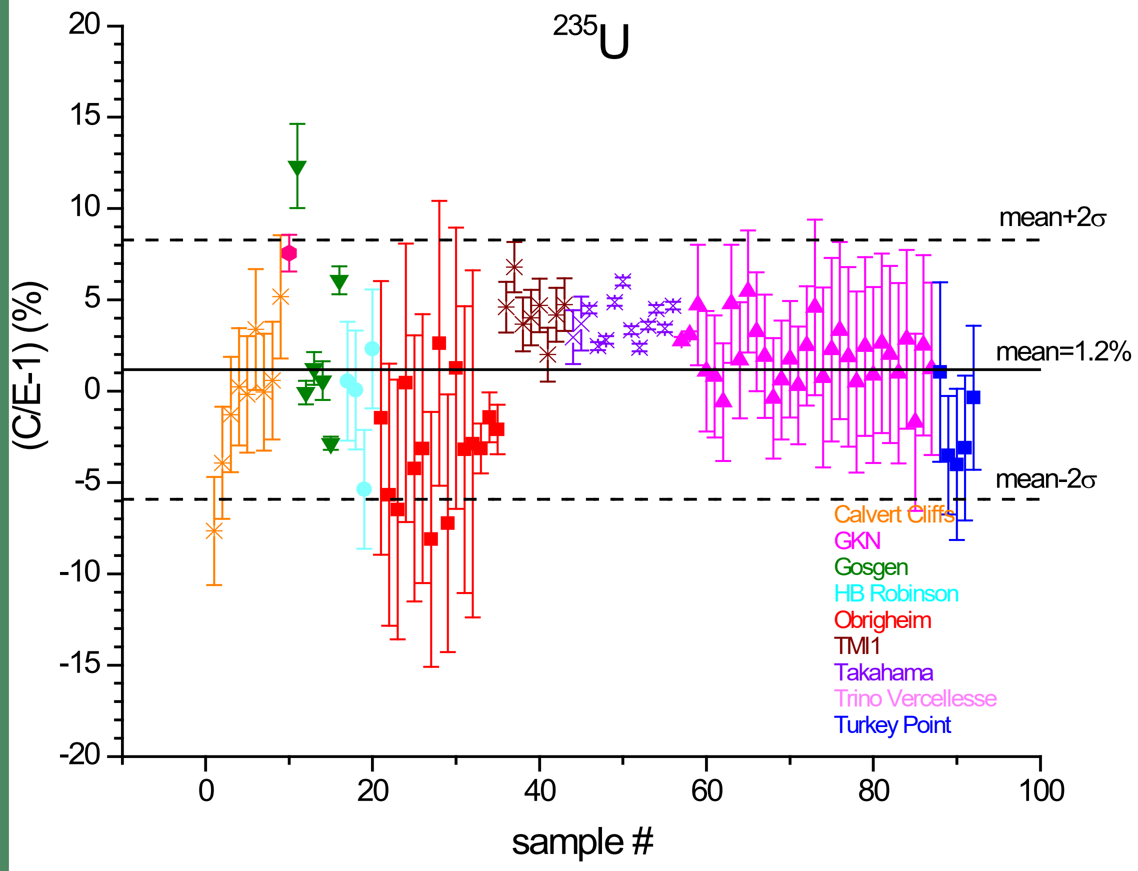
- API for depletion/decay
  - load data resources (decay, yields, etc.)
  - update transition data ***A*** in each depletable zone
    - multigroup flux spectrum from MPACT updates
      - energy-dependent fission yields, e.g. U-235 -> (n,f) -> Xe-135
      - energy-dependent isomeric transitions, e.g. Am-241 -> (n,g) -> Am-242m
    - update any 1-group xs known in transport (e.g. total absorption)
  - solve for end-of-step number densities $\vec{N}(t) = \exp(\boldsymbol{A}t)\vec{N}(0)$

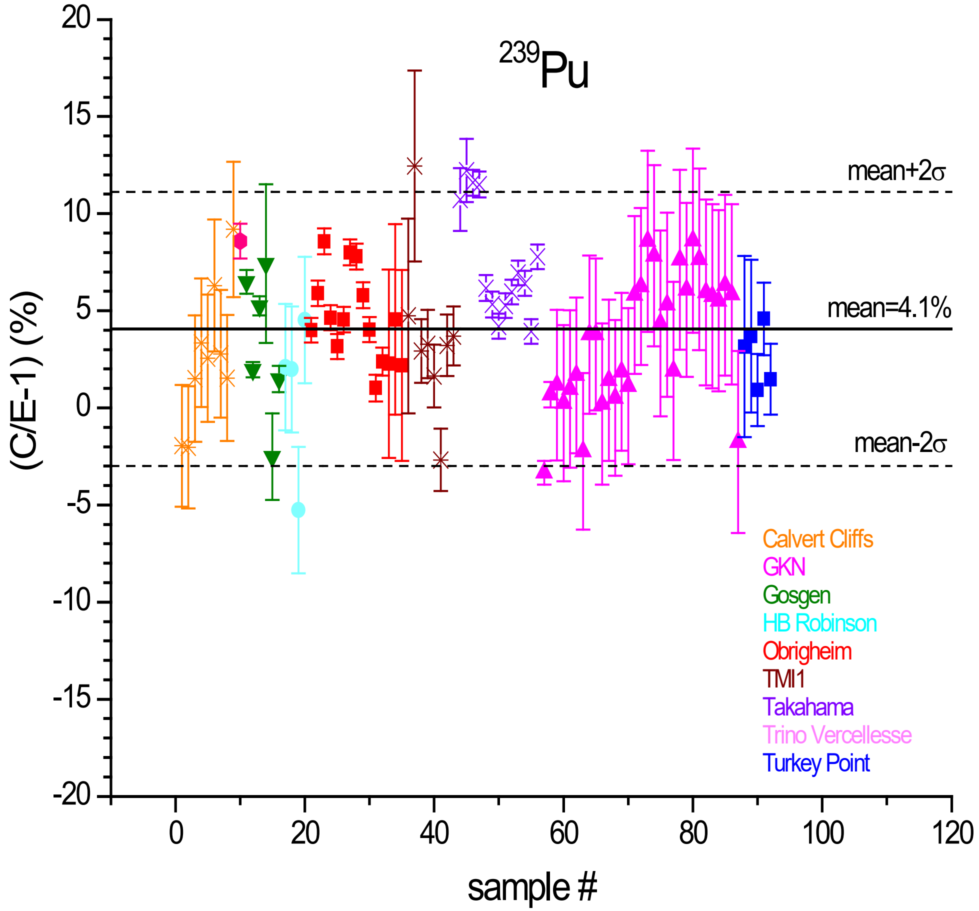
- (new) API for decay emissions
  - given isotopics: calculate decay heat, neutron and gamma emissions
  - can be used for secondary source modeling, shutdown doses/cooling



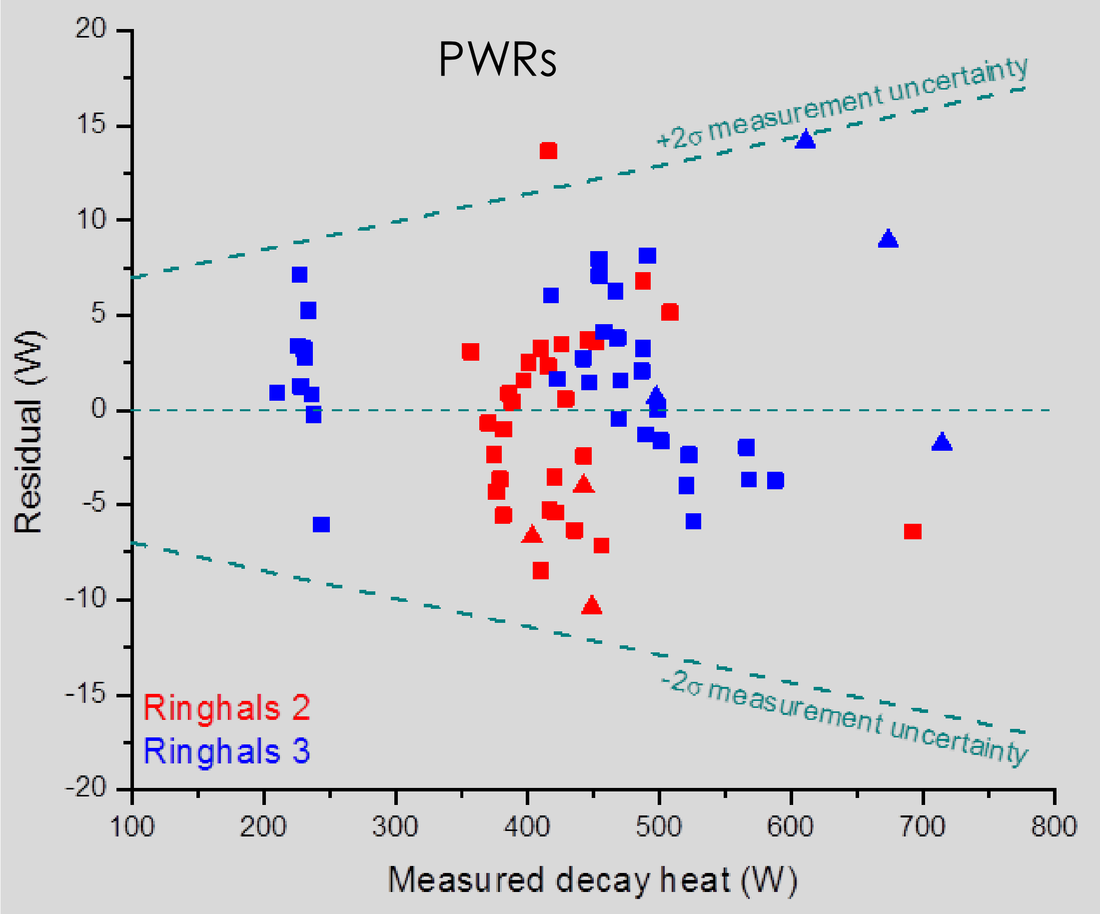


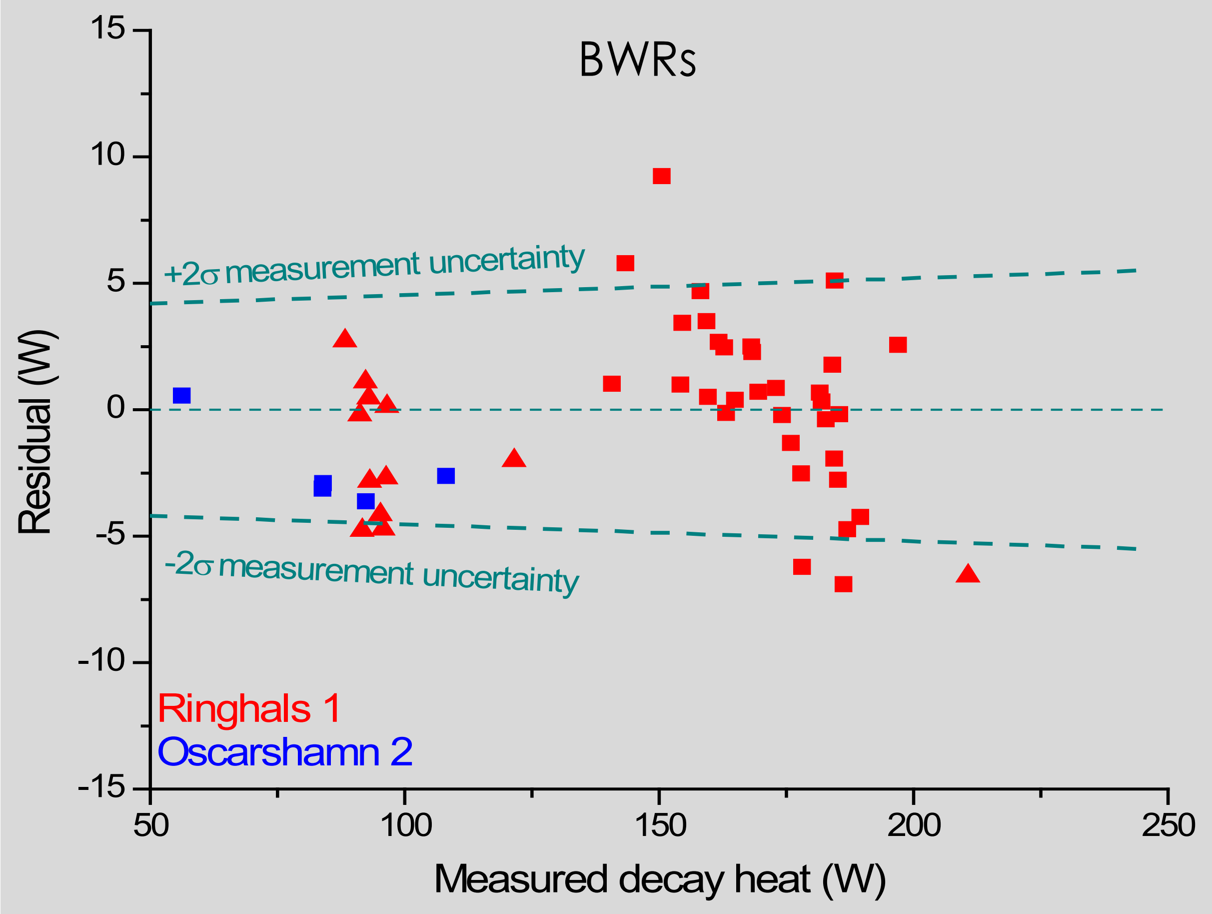
ORIGEN Validation Highlights (1/3)





ORIGEN Validation Highlights (2/3)





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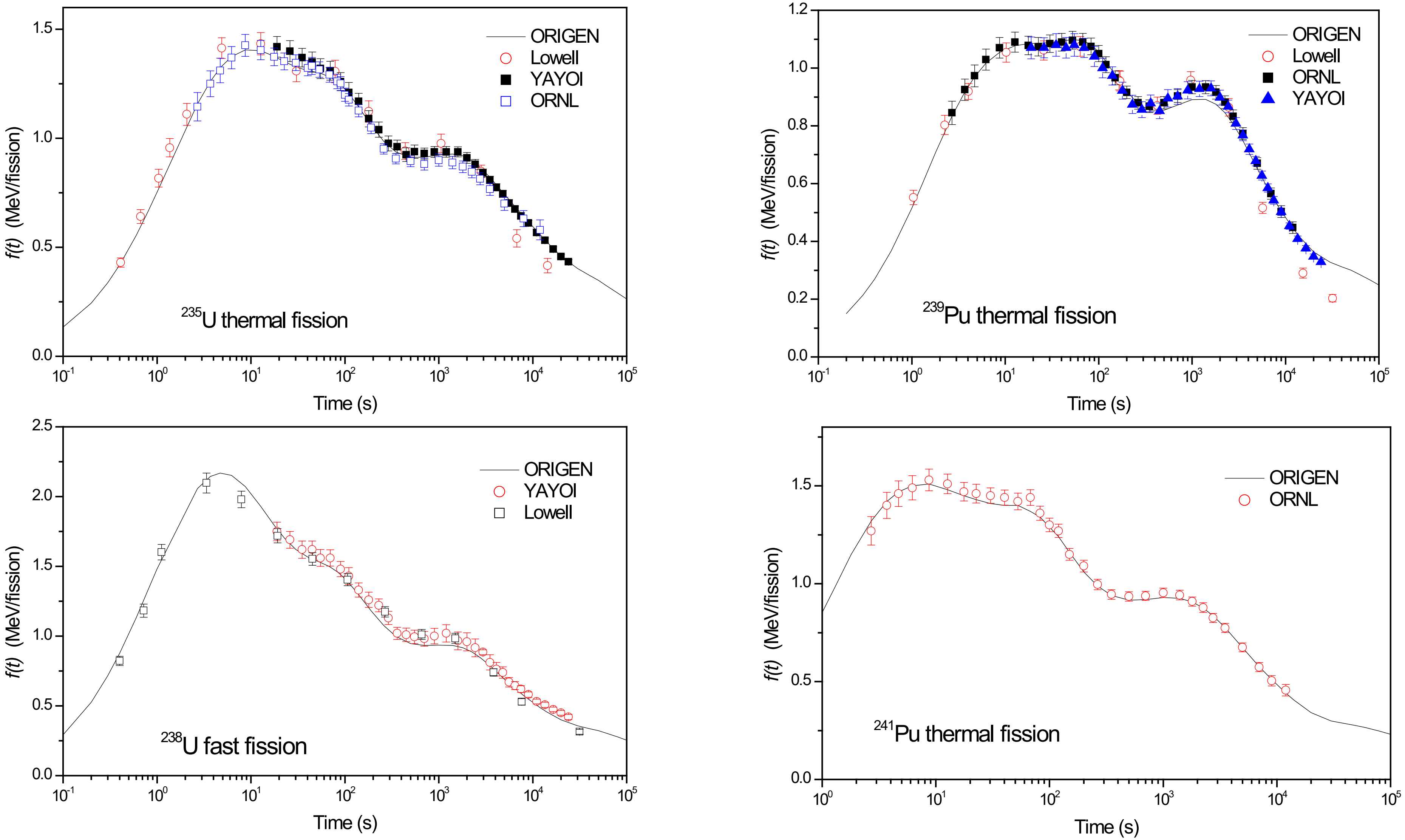
ORIGEN Validation Highlights (3/3)

Single Fission Decay Heat Measurements



Summary

- ORIGEN within VERA
  - Primary depletion/decay engine
  - Reduced number of nuclides/transitions for million-zone problems
  - Neutron emission capabilities (e.g. for secondary source modeling)
  - Use of fundamental data has allowed "out of the box" modeling of
    - MOX fuel depletion
    - Tritium production
    - Antimony activation
- ORIGEN within SCALE
  - Method improvements (CRAM, sensitivity capability in progress)
  - Nuclear data testing/evaluation
  - Validation against experiment-- ***CASL provides a whole new avenue for ORIGEN validation!***