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New Features of the ORIGEN Transmutation Code in SCALE 6.2

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1. INTRODUCTION

This paper will serve to summarize the major features/enhancements of the ORIGEN isotope transmutation (decay/depletion/activation) code in the upcoming release of SCALE 6.2 and demonstrate some of the key features with comparisons to SCALE 6.1. Many of these features have been discussed individually in other recent papers [1–3]. This paper provides a comprehensive overview of all major features and presents the new ORIGEN input format for the first time.

- Basic data enhancements include
  - ENDF/B-VII.0-based fission yields that have been modified to address inconsistencies between ENDF/B independent and cumulative yields and decay data; and
  - a new decay beta emission data;
  - a single 999-group multi-group cross section library based on JEFF-3.0/A; and
  - using SCALE nuclide mass resources, instead of mass number, for unit conversions.
- Code enhancements include
  - an extensive testing framework including unit and regression testing and
  - a complete reworking of code structure into a well-defined API for high-performance transmutation calculations, with both C++ and Fortran bindings.
- The major calculation enhancement is the addition of a fast and accurate Chebyshev Rational Approximation Method (CRAM) solver.
- The major user interface enhancement is a new input format for stand-alone ORIGEN calculations.

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2. DESCRIPTION OF MAJOR FEATURES/ENHANCEMENTS

2.1. Basic Data Enhancements

The first category of enhancements involves the basic data resources of ORIGEN. The following is a complete list of basic data resources:

1. fission product yields,
2. decay emission data (alpha, beta, gamma, neutron),
3. reaction cross section data in the form of infinitely dilute and self shielded multigroup libraries ,
4. mass data,
5. energy per fission/capture, and
6. radioactive decay data (decay constants, branching ratios).

The first four data resources in the above list have been updated from SCALE 6.1 to SCALE 6.2.

The fission product yields used by ORIGEN have been updated to include modifications to make the independent (direct) yields more consistent with current decay chains and the cumulative yields [4]. Because ORIGEN tracks the full set of ~1100 fission products, it must use independent yields. The updates were motivated by inconsistencies between the fission yield data and decay data in ENDF/B-VII.

The decay emission data has been augmented with beta emission spectra for 716 nuclides, based on beta decay data from ENSDF [6]. This capability can be used, for example, to provide source terms for charged particle transport calculations. An example of a beta emission spectrum for Sr-90 as a function of decay time is shown in Figure 1, illustrating the change in beta spectrum with buildup of daughter Y-90.

ORIGEN uses an extensive multigroup reaction cross-section library based on JEFF-3.0/A, which contains neutron data for 98 elements and 774 different target nuclei, including first (m) or second (n) isomeric states, from H-1 to Fm-257, and 12617 neutron-induced reactions below 20 MeV. Available reactions include the following: (n,2n); (n,3n); (n,f); (n,nα); (n,n3α); (n,2nα); (n,3n α); (n,np); (n,n2α); (n,2n2α); (n,nd); (n,nt); (n,n3He); (n,nd2α); (n,nt2α); (n,4n); (n,γ); (n,p); (n,d); (n,t); (n,3He); (n,α); (n,2α); (n,3α); (n,2p); (n,pα); (n,t2α); (n,d2α); and (n,n').

The primary purpose of this JEFF-3.0/A multi-group library is to provide cross sections for target nuclides not included in the smaller set of ENDF/B-VII.1 multi-group library. The JEFF-3.0/A library may also be used for activiation problems where self shielding is not important. In SCALE 6.1, a multi-group JEFF/3.0-A library was created for *each* SCALE library group structure; i.e., a 44-group, 49-group, 200-group, and 238-group library for ORIGEN. In SCALE 6.2, there is now a single 999-group JEFF-3.0/A-based library, and the cross section data is collapsed on the fly to the user's group structure. The runtime for collapsing is less than one second and only needs to be performed once at the beginning of the calculation.

Mass data for ORIGEN has also been updated to access the SCALE StdCompLib resource for mass data,

which draws from the NIST database [5]. In SCALE 6.1 and earlier, ORIGEN performed unit conversions based on the mass number; e.g., Xe-135 mass-to-mole conversions were based on 135 g/mol instead of 134.907219 g/mol. Although unlikely to significantly impact most calculations, there are isotopes that may show a ~1% change in content due to this update. This change also provides consistency between ORIGEN and other SCALE modules.

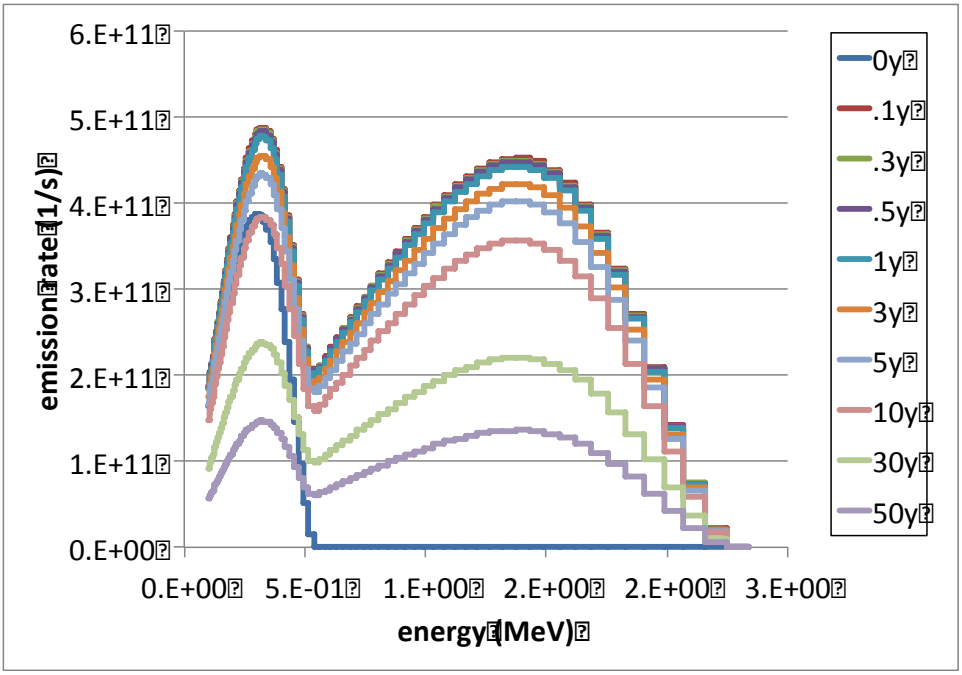

Figure 1. Beta emission spectra at various decay times.

2.2. Code Enhancements

ORIGEN has been extensively modernized from SCALE 6.1 to 6.2, with the main goals being to first refactor the code to improve organization, readability, and maintainability and then to create an API layer that can be used to perform ORIGEN calculations (depletion/decay/emission) without file I/O [1,3]. Basic statistics for the ORIGEN API in SCALE 6.2 are shown in Table 1.

Table 1. SCALE 6.2 ORIGEN API statistics

language	files	lines			
		blank	comment	code	unit tests
Fortran90	103	3260	7661	27011	7408
C++	156	5854	5255	26397	11492
C/C++ header	182	2486	3018	7804	27

One of the major efforts in SCALE 6.2 has been the implementation of a suite of *unit tests* designed to test

the proper functionality of the code at the lowest level. This type of testing does not use input files but actual source code to initialize classes, loads them with data, and performs a variety of checks. For C++ unit tests, the Google Testing (gtest) framework is used [7]. The new C++ code is well tested with over 11,000 lines of unit tests compared to 26,000 lines of source.

The ORIGEN API has been discussed in [1] and [3]. SCALE 6.2 users will be able to link to the ORIGEN API libraries from a SCALE 6.2 installation and integrate ORIGEN directly into their application. For the common use case of fuel depletion inside an existing transport code, the in-memory SCALE 6.2 ORIGEN API improves performance by a factor of 2 to 30 over the disk I/O-bound SCALE 6.1/ORIGEN [1]. This has enabled the ORIGEN API to be used as the depletion engine in the Consortium for Advanced Simulation of Light Water Reactors (CASL) core simulator, VERA-CS.

2.3. Calculation Enhancements

One of the major enhancements, enabled by the API, has been the addition of a high-performance CRAM solver as a second solver kernel [2]. The CRAM solver outperforms the original solver kernel (MATREX) in both speed and accuracy for most problems. The example shown in Figure 2 includes a comparison of relative error for these two solvers for all ~2200 nuclides (based on atomic fraction). Errors are relative to a high-precision, numerical reference solution generated by the TTA method [2]. As shown, CRAM improved the relative error by orders of magnitudes. Also of note, is that the CRAM solver can perform adjoint calculations.

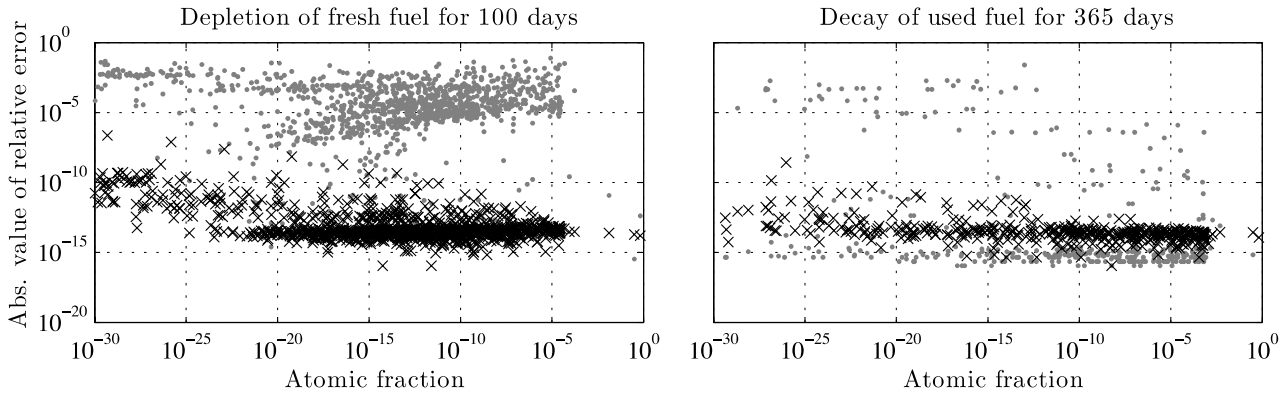

Figure 2. Relative errors for individual nuclides with MATREX (dots) and CRAM (x's) for a typical depletion and decay calculation. In both cases MATREX used 16 time steps while CRAM used 4 [2].

2.4. User Interface Enhancements

The user experience has been enhanced with SCALE 6.2 ORIGEN by moving from the FIDO-array style input to a derivative of Java Script Object Notation (JSON) called Standard Object Notation (SON). The SCALE 6.1 FIDO input is shown on the left in Figure 3, and the equivalent SCALE 6.2 SON input is shown on the right. The SON input uses braces "{}" to organize blocks of data and brackets "[]" to denote arrays. All other input is a simple "key=value" pair.

The final paper will include more detailed descriptions of the new capabilities and more demonstrations of

performance of the new ORIGEN compared to that of previous versions.

```
=origen
3$$ 1 1 e
4$$ 1 e t
end7dec
56$$ 18 a4 1 -1 a9 0 1 0 4 1 e t
Sr-91 decay
60** 0.25 0.5 0.75 1 2 3 4
     5 6 7 8 9 10 20 30 40 50 100
61** f1e-5
67$$ a41 1 0 1 0 1 e
73$$ 380910
74** 1
75$$ 3
83$$ a4 2 e
t
end
```

```
=origen
case{
    title="Sr-91 decay"
    lib{ file="end7dec" }
    time{
        units=days
        t=[0.25 0.5 0.75 1 2 3 4
            5 6 7 8 9 10 20 30 40 50 100]
    }
    mat{
        units="gram-atoms"
        comp=[380910(3)=1]
    }
    neutron{ medium=2 }
}
end
```

Figure 3. ORIGEN input in SCALE 6.1 using FIDO (left) and SCALE 6.2 using SON (right). This simple calculation is a single decay case with a neutron emission calculation. Root level keywords are shown in bold.

REFERENCES

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