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SUBLIBRARIES IN ORIGEN

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CONTENTS

LIST OF TABLES

1. INTRODUCTION

Libraries produced for the ORIGEN depletion code [1] have the ability to label nuclides with a sublibrary integer tag. While this is useful for tracking different sources of the nuclides, it adds some complexity, increasing memory usage and computational effort. This report documents the effort of making the sublibraries optional in an ORIGEN calculation, with a focus on the creation of libraries using the `LibraryBuilder` application programming interface (API). ORIGEN will gain the ability to either use the normal sublibrary set, a reduced, unique, sublibrary set, or no sublibrary at all.

2. SUB-LIBRARIES

Isotopes in ORIGEN are internally identified using a SIZZZAAA number, where

- **S** is the sublibrary number,
- **I** is the isomeric state (0 for ground),
- **ZZZ** is the atomic number, and
- **AAA** is the atomic weight.

For example, 21092235 would be ^{235m}U in the second sublibrary, and 10006012 would be ^{12}C in the first sublibrary.

As a convention, the default sublibraries are given as follows:

- **1** are light elements,
- **2** are actinides, and
- **3** are fission products.

This allows the user to track fission products separately from other decay nuclides. The binary ORIGEN library labels the nuclides from different sublibraries as different materials. Therefore, the cross-section data are duplicated for each sublibrary in which the material is present. This causes additional memory use for the duplicated data and computational slow-down due to the extra duplicated data in the transition matrix.

2.1 CURRENT SUBLIBRARY USE

Currently, ORIGEN defaults to the three sublibraries discussed previously. These sublibraries are typically used when exporting nuclide concentrations at the end of a depletion calculation. While the transition coefficients are the same, having different sublibraries allows the user to know if daughter nuclides were created through fission or some other process. While this knowledge can be useful in some cases, it causes extra memory and computational effort to be used. For cases in which the user only wants to know the total nuclide concentrations, or if the user is coupling a depletion calculation with a transport calculation, much of this extra information is not needed.

3. REMOVAL OF SUBLIBRARY PROCESS

Several steps are needed to remove the sublibraries. It is desired to keep sublibraries available as an option for those who run ORIGEN standalone and wish to track nuclides as described above. Also, ORIGEN is designed to be run with sublibraries enabled. The input file provides a way to specify the sublibraries for which information is needed, and it allows the user to specify the sublibraries where a user-entered nuclide belongs. The output file is hard coded to present nuclide concentrations to the user in the three predefined sublibraries discussed in Section 2 on the preceding page.

The API within ORIGEN provides the user with the `LibraryBuilder` and various other supporting classes that allow the user to manipulate the `TransitionSystem`. The transition system as represented by the API does not store sublibrary information. Therefore, each nuclide is unique inside of the transition system. When a library is created, the appropriate sublibraries are assigned to each nuclide as they are written to the library file.

3.1 UNIQUE NUCLIDES

As a first step to removing dependence on the sublibraries, an option was created where the nuclides in the transition system can be assigned only one sublibrary when they are written to the library. In this method, all nuclides with an atomic number less than 90 are assigned to one sublibrary—sublibrary 1, and all others are assigned to another—sublibrary 2. This split allows the user to track filter by actinides and light nuclides if desired.

Keeping the sublibrary nomenclature and ensuring that every nuclide exists in at most one sublibrary provides many of the benefits of having no sublibraries with minimal effort. To implement this method, the ORIGEN API was modified to obtain all nuclides from the default SCALE 6.2 nuclide set and then sort them based on their atomic numbers. This results in a library that contains two sublibraries, with all nuclides with an atomic number below 90 in one, and all the remaining nuclides in the other sublibrary. As expected, this results in a smaller library, as nuclides that were previously present in multiple sublibraries have been culled. When ORIGEN is run, the total nu-

clide mass results are the same as with all the sublibraries, as expected. A summary of the timing and memory requirements is given in Table 1 for a simple decay library.

Table 1: Size and Timing for Libraries in Decay Case

Library	Number of Nuclides	Size on Disk [kb]	ORIGEN Time [s]
Complete	2237	128	0.53
Unique Nuclides	1675	104	0.39

3.2 NO SUBLIBRARIES

The next step is to create an option to set the sublibrary identifier to zero, effectively removing the sublibrary parameter from the library. This was performed in a manner similar to that used to create the unique nuclide library, as described above, with the additional step of removing the sublibrary identifier. This approach works because the internal transition system storage class does not store the information specifying the sublibraries to which a nuclide belongs. The sublibrary identification is based on the nuclide set, and the appropriate sublibraries are assigned to nuclides as the library is being written. If the nuclide set contains no sublibrary information, then nuclides will simply be written to the library file without a sublibrary number.

Currently, ORIGEN is designed to issue a fatal error when a library with no sublibraries is used. However, the library can still be used with the ORIGEN API instead of the stand-alone ORIGEN program directly. Ongoing work is being performed to explore removing this limitation from ORIGEN. This work is discussed briefly in the next section.

4. CONCLUSIONS AND FUTURE WORK

The sublibrary feature of the ORIGEN program allows for ease of tracking the source of fission products versus decay products, but it sometimes adds needless complexity. By maintaining several copies of a large number of transitions, the memory usage, library size, and run-time are all increased. However, in some cases, the user is only interested in the total concentrations of the nulcides in the depletion calculations. In these cases, the distinction between nuclide birth type is superfluous and can be removed.

Work has been performed to produce libraries that (1) either contain unique nuclides but still have sublibraries, or (2) that have no sublibrary information at all. ORIGEN can be run successfully with the first such library, but if no sublibraries are present, then ORIGEN will give a fatal error. Work is needed to update ORIGEN to work without sublibraries. Since all of the output tables of ORIGEN are formatted with the expectation that sublibraries will be used, it should be fairly straightforward to adjust the tables, but this must be done in multiple places. In addition, the solvers must be inspected to ensure that they can work without the sublibrary indentifiers.

REFERENCES

[1] B. T. Rearden and M. A. Jessee. *SCALE Code System, Version 6.2.1*. Technical Report ORNL/TM-2005/39, Oak Ridge National Laboratory, Oak Ridge, TN (2016).