THE SCALE 6.2 ORIGEN API FOR HIGH PERFORMANCE DEPLETION

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ABSTRACT

In recent years, the SCALE 6.2 development efforts have included modernization of key components of the modular SCALE code system. The ORIGEN depletion/decay module has received extensive improvements, including the addition of an application programming interface (API) for both C++ and Fortran with modern object-oriented design and various solver enhancements. This paper highlights the API capabilities that are currently available in beta release for embedding ORIGEN depletion calculations in other codes (e.g., for coupled transport/depletion calculations). The capabilities of the API are described and timing results are presented for both stand-alone depletion and coupled transport/depletion. The coupled timing was performed with the CASL full-core, pin-resolved deterministic transport code, MPACT, where memory and runtime constraints prompted use of an emerging capability to create small, specific-purpose burnup/decay chains.

Key Words: high-performance, depletion, ORIGEN, API

1 INTRODUCTION

Over the last few years, ORIGEN has undergone an active modernization including the addition of an application programming interface (API) for both C++ and Fortran with modern object-oriented design and various solver enhancements. ORIGEN has the capability to generate source terms for accident analyses; characterize used fuel (including activity, decay heat, radiation emission rates, and radiotoxicity); activate structural materials; and perform fuel cycle analysis studies [1–4] using current nuclear data sources. As an integral part of SCALE 6.1 [3], ORIGEN has been subject to hundreds of validation cases using measured data from destructive isotopic assays of spent fuel, decay heat of spent fuel, gamma spectra resulting from burst fission, and neutron spectra resulting from spontaneous fission and (α,n) reactions. This wide range of applications is possible because the guiding principle has been to explicitly simulate all decay and neutron reaction pathways using the best available data and rigorously validate the result versus experiment.

This paper highlights new API capabilities for high-performance, coupled transport/depletion, currently available in beta release, and being used in the CASL core simulator, MPACT [5]. This extends the 2013 work of Skutnik, et. al. [6], which described the

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API for stand-alone depletion calculations, which was a refactoring of work by Yesilyurt, et. al. [7] to be integrated in the SCALE code system.

1.1 Overview

The fundamental purpose of ORIGEN and the new API is to solve the following system of ordinary differential equations (ODEs) describing the depletion/decay phenomena:

\[
\frac{d\tilde{n}_m}{dt} = (A_{\phi m}\Phi_m + A_\lambda)\tilde{n}_m(t) + \tilde{S}_m(t),
\]

where

- \(m\) is a material index,
- \(\tilde{n}_m\) is the nuclide number density vector for material \(m\) (atoms/barn-cm),
- \(A_{\phi m}\) is the transition matrix for the reaction transitions (barns or cm\(^2\)),
- \(\Phi_m\) is the scalar flux magnitude (1/cm\(^2\)s),
- \(A_\lambda\) is the transition matrix for decay transitions (1/s),
- \(\tilde{S}_m\) is an external source.

Using SCALE/ORIGEN as a stand-alone code typically implies a single material. Here, the focus is on using the ORIGEN API for transport/depletion coupling with traditional quasi-static time approximation. This requires solving

- the steady-state, transport Eigen-problem at each time point (with appropriate problem-dependent self-shielding of cross sections) and
- the above depletion equation over each time step.

Additionally, in typical transport/depletion coupling, the total power \(P(t)\) produced by the system is given, and the external source \(\tilde{S}_m(t)\) is zero. The remaining sections will explain the components of Eq. (1), what is provided internally in the API, and what must be provided by the API user.

1.2 Transition Representation

A visualization of the full transition matrix, \(A = A_{\phi} + A_\lambda\), for ~1200 fission products is shown in Figure 1, with a zoomed-in view of Xe-135 shown in Figure 2. Solid-colored lines are used for reaction transitions and dashed green lines for decay transitions. Note the decay of short-lived fission products indicated by nuclides in the lower right with decay transitions to the upper left.

The decay portion, \(A_\lambda\), of the transition matrix is given by row as

\[
a_{\lambda,ii'} = \begin{cases} 
\gamma_{d,i\rightarrow i'}\lambda_{d,i'} & \text{for } i \neq i' \\
-\sum_d \lambda_{d,i} & \text{for } i = i'
\end{cases}
\]

with \(d\) indicating a decay mode, the top term (off-diagonal) representing gains of nuclide \(i\) due to decay mode \(d\), and the bottom term (diagonal) representing the loss of nuclide \(i\) due to all decay modes. Note that the decay portion is independent of material \(m\).
Figure 1. The transition matrix for fission products.

Figure 2. The transition matrix zoomed in around Xe-135.
The reaction part is treated in essentially the same way, with the off-diagonal entries in the matrix \( A_{\phi m} \) defining the creation of nuclide \( i \) from reaction transitions of all other nuclides \( i' \). The structure of each row of \( A_{\phi m} \) is

\[
a_{\phi m, i'} = \begin{cases} 
Y_{xm, i' \rightarrow i} \sigma_{xm, i} & \text{for } i \neq i' \\
- \sum_x \sigma_{xm, i} & \text{for } i = i'
\end{cases}
\]

where the top term (off-diagonal) represents gains of nuclide \( i \) due to reaction type \( x \), and the bottom term (diagonal) represents the loss of nuclide \( i \) due to all reaction mechanisms. It is convenient to represent the gain term in terms of “yield,” \( Y_{xm, i' \rightarrow i} \), and reaction cross section, \( \sigma_{xm, i} \).

The use of a “yield” \( Y \) in all types of transitions is convenient for modeling not only fission (where it is a necessity) but also for modeling isomeric branching and byproduct production. For an isomeric branching example, consider a case where the \((n, \gamma)\) reaction cross section of U-234 is 1 barn, producing both U-235 (99%) and U-235m (1%). ORIGEN would have \( \sigma_{(n,\gamma),U5m} = 1 \text{ barn} \), \( Y_{(n,\gamma),U5m \rightarrow U4} = 1\% \), and \( Y_{(n,\gamma),U5m \rightarrow U4} = 99\% \), indicating that 1% of reactions go to the first metastable state of U-235 and 99% go directly to the ground state.

Neutrons, protons, deuterons, tritons, helions (He-3), and alphas emitted in reaction/decay transitions are tracked by ORIGEN explicitly as if they were actual nuclides. In this case, the yield is used as the multiplicity of the product \([i.e., an \ (n, \alpha) \ reaction \ results \ in a \ gain \ term \ for the \ alpha \ byproduct \ of \ Y_{(n,\alpha),\alpha \rightarrow} = 1, \ and \ an \ (n, 2\alpha) \ results \ in \ Y_{(n,2\alpha),2\alpha \rightarrow} = 2, \ with "*" used to indicate validity for any parent nuclide]. In the case of fission and isomeric reaction transitions, the yield term is dependent on the neutron spectrum. For byproducts, the yield is a constant.

ORIGEN contains an extensive multigroup reaction cross-section library based on JEFF/3.0-A with over 12,000 cross sections for the following reactions: \((n,2n); (n,3n); (n,f); (n,na); (n,n3a); (n,2na); (n,3n a); (n,3n p); (n,2n2a); (n,nd); (n,n); (n,3He); (n,nd2a); (n,2n2a); (n,4n); (n,He); (n,p); (n,d); (n,He); (n,He); (n,2a); (n,3a); (n,2p); (n,pa); (n,2a); (n,2a2); and (n,n'). Note that in typical activation problems where self-shielding is not important, given a multigroup neutron flux spectrum, this JEFF library is sufficient to calculate the one-group cross sections and yields needed to perform transmutation calculations. In reactor physics applications in SCALE where self-shielded ENDF/B-VII.1 data is available, it is used instead of JEFF data.

Given the group-wise neutron spectrum \( \phi^g_{m} \), where \( g \) is the multigroup energy index, the one-group cross sections used by ORIGEN are calculated with standard flux weighting.

\[
\sigma_{xm, i} = \frac{\sum_g \sigma^g_{xm, i} \phi^g_{m}}{\sum_g \phi^g_{m}}
\]

For isomeric reaction branching, energy-dependent yields are calculated as

\[
Y_{xm, i' \rightarrow i} = \frac{\sum_g Y^g_{x, i' \rightarrow i} \sigma^g_{x, i} \phi^g_{m}}{\sigma_{x, i} \phi_{m}},
\]

where the multigroup yield term \( Y^g_{x, i' \rightarrow i} \) and weighting cross section \( \sigma^g_{x, i} \) are contained in the JEFF library and are independent of material. For fission yields, the average energy of fission is
calculated and linear interpolation is performed on yields tabulated at one to three discrete energy points,
\[
Y_{fm,i\rightarrow i'} = \text{interp}(E_{fm,i'}, Y_{f,i\rightarrow i}(E_1), Y_{f,i\rightarrow i}(E_2), \ldots)
\]
where the average energy of fission in actinide \(i'\), which creates fission products \(i\), is given as
\[
E_{fm,i'} = \frac{\sum_g E_g \sigma_{f,lm}^g \phi_m^g}{\sum_g \sigma_{f,lm}^g \phi_m^g},
\]
where \(E_g\) is some average energy for group \(g\) that depends only on the group structure.

1.3 Time Approximation

In transport/depletion coupling, the \(A_{\phi m}(t)\) matrix is expensive to calculate, requiring global self-shielding and transport operations, whereas \(\Phi_m(t)\) only requires the evaluation of a simple formula relating the relative material flux and power level in the system. For this reason, the coupled transport/depletion calculation is assumed to be broken down into steps and substeps. During each step \(j\), the matrix is fixed at some “average” value, \(\bar{A}_{\phi m,j}\), but the flux is represented as \(\tilde{\Phi}_{m,j}\phi_{j+s/N}\), where the normalization factor \(\Phi_{m,j+s/N}\) is recalculated on each substep with \(N\) as the total number of substeps. The following depletion equation is then solved \(N\) times (once over each substep \(s\)),
\[
\frac{d\tilde{n}_m}{dt} = (\bar{A}_{\phi m,j}\tilde{\Phi}_{m,j} \phi_{j+s/N} + A_{\chi})\tilde{n}_m(t),
\]
over substep \(t_{j+(s-1)/N} \leq t \leq t_{j+s/N},\)
with initial condition \(\tilde{n}_m(t_{j+(s-1)/N}) = \tilde{n}_m(t_{j+(s-1)/N}),\) for \(s=1, 2, \ldots, N\)
where
- \(\tilde{\Phi}_{m,j}\) is the step-average material total flux \((1/cm^2s)\),
- \(\phi_{j+s/N}\) is the substep system power normalization (-),
- \(\bar{A}_{\phi m,j}\) is the step-average reaction transition matrix \((barn)\).

The substep system power normalization term is given as
\[
\Phi_{j+s/N} = \frac{\tilde{P}_j}{\sum m \sum_i \kappa_{L,i} \sigma_{Lm,j,i} \tilde{\Phi}_{m,j} V_m n_{m,j+s-1/N,i}}
\]
where
- \(\tilde{P}_j\) is the given total system power \((Watts)\);
- \(m\) is the material index;
- \(i\) is the nuclide index;
- \(\kappa_{L,i}\) is the energy release per loss \((\text{capture+fission})\) of nuclide \(i\) \((\text{Joules})\);
- \(\sigma_{Lm,j,i}\) is the loss cross section over step \(j\) of nuclide \(i\) \((\text{barn})\);
- \(\tilde{\Phi}_{m,j}\) is the relative \((\text{total})\) flux in material \(m\) over step \(j\) \((n/cm^2s)\);
- \(V_m\) is the volume of material \(m\) \((cm^3)\);
- \(n_{m,j+s-1/N,i}\) is the beginning-of-substep \(s\) number density of nuclide \(i\) \((\text{atom/barn-cm})\).
The loss cross section (also called the total capture or removal cross section) is defined as

\[ \sigma_{L,i} = \sum_x \sigma_{x,i} \]  

(10)

It represents the sum of all reactions that destroy nuclide \( i \) [i.e., not only normal absorption mechanisms such as \((n,g)\); \((n,\alpha)\); and \((n,f)\), but including \((n,2n)\); multi-byproduct reactions like \((n,np)\); and even inelastic scattering \((n,n')\) if it creates a meta-stable isomeric state]. The energy release per loss of nuclide \( i \), \( \kappa_{L,i} \), is defined by the relation

\[ \kappa_{L,i} \sigma_{L,i} = \kappa_{f,i} \sigma_{f,i} + \kappa_{c,i} (\sigma_{L,i} - \sigma_{f,i}) \]  

(11)

where the energy release per fission \( \kappa_{f,i} \) and “capture” \( \kappa_{c,i} \) are fixed for each nuclide.

1.4 Data Delivered by API Caller

The ORIGEN API for coupled transport/depletion is currently a simple two-level hierarchy, shown below in Figure 3.

![Figure 3. Basic coupled/transport depletion Solver API structure.](image)

The “Solver Kernel” is given by Eq. (8). It requires a transition matrix \( \tilde{A}_{\phi_{m,j}} \), step-average material flux \( \tilde{\phi}_{m,j} \), and power level \( \tilde{P}_j \), as well as beginning-of-step isotopics \( \tilde{n}_{m,j} \) to produce end-of-step isotopics \( \tilde{n}_{m,j+1} \). The “MultiZoneDepleter” class wraps the solver kernel and management of depletable materials in the system and drives the solver execution and recalculation of the normalization factor in Eq. (9) over a step. Note that the API currently assumes the coupling with transport (e.g., predictor-corrector) to occur at the caller level.

Routines are provided in the API to create or update transition matrices \( \tilde{A}_{\phi_{m,j}} \) given user-specified multigroup flux \( \phi_{m}^\theta \) and one-group cross sections \( \sigma_{xm,i} \). The “TransitionMatrixUpdater” class manages the update procedure, as shown in Figure 4. A base reaction matrix, \( A_{\phi} \), is used by the class to define the nuclides and transitions considered in the update. The multigroup flux, \( \phi_{m}^\theta \), is used in Eqs. (4), (5), (6), and (7). Any user-provided cross sections \( \sigma_{xm,i} \) are used in Eq. (3) preferentially over those calculated in Eq. (4).
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2 RESULTS

The ORIGEN API is currently being used by the following codes:
- SCALE/ORIGAMI, a simplified assembly isotopes depletion code;
- SCALE/Polaris, a new lattice physics code; and
- the CASL core simulator MPACT.

This section first presents run-time and parallel scaling studies for stand-alone depletion (i.e., without transport coupling components) and then for the coupled system, including MPACT results with an experimental reduced-size burnup chain. The purpose here is to demonstrate the runtime performance of the ORIGEN API and that it is viable in a high-performance computing environment. Results of stand-alone depletion/decay calculations with ORIGEN are essentially unchanged from those described in references [1-4]. Coupled transport/depletion results are presented in the MPACT paper [5] and detailed stand-alone ORIGEN results in the companion paper [8].

2.1 Stand-alone Depletion Tests

A simple test case was used to analyze performance of the ORIGEN API for multi-zone depletion, shown in Table I, consisting of an irradiation history designed to mimic a single reactor cycle, but with a supplied flux level, i.e. without using Eq. (9) to calculate the flux level based on the power. The last column shows the average time in milliseconds to run the solver kernel to solve Eq. (8) with a single substep. Runtime scales proportionally with the number of substeps. In this case where flux, $\Phi_p$, is provided to the solver kernel, substeps are only required to converge the solution, e.g. for long time steps. In typical reactor calculations where system power is provided, substeps also serve the purpose of redistributing power, and in this case, the number of substeps is small in typical problems (~4). Note that the final two decay steps are an order of magnitude faster than the irradiation steps. This is due to the fact that the transition matrix without reaction transitions is about an order of magnitude smaller.
To assess the parallel performance, a strong scaling study was performed where 24,576 materials were depleted by up to 256 parallel processes. Two depletion modes were compared:

1. “deplete by flux,” where the flux magnitude is provided and the flux renormalization to system power is avoided (as shown in Table I) and

2. “deplete by power,” where the system power is provided to produce a flux magnitude of approximately 1e14.

As expected, the “depletion by flux” case exhibited near 100% parallel efficiency (not shown). The “depletion by power” case in Table II shows approximately 95% efficiency with 96 materials per process and a total of 24,576 materials. Due to the testing machines used, tests beyond 256 processes have not been performed. Because the single material solve time is relatively small, MPI communication does become a bottleneck as the number of materials per core approaches one. However, fewer than a hundred materials per core is rare in large-scale problems. For example, transport/depletion of a single 3D assembly with 49 axial levels, 264 fuel pins, and 1 depletable material per pin would contain ~13000 materials.

### Table II. Strong scaling for depletion by power

<table>
<thead>
<tr>
<th># MPI Processes</th>
<th># Materials per Process</th>
<th>Runtime (s)</th>
<th>Scaling (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>24576</td>
<td>13516</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td>12288</td>
<td>6690</td>
<td>99</td>
</tr>
<tr>
<td>4</td>
<td>6144</td>
<td>3311</td>
<td>98</td>
</tr>
<tr>
<td>8</td>
<td>3072</td>
<td>1656</td>
<td>98</td>
</tr>
<tr>
<td>16</td>
<td>1536</td>
<td>811</td>
<td>96</td>
</tr>
<tr>
<td>32</td>
<td>768</td>
<td>410</td>
<td>97</td>
</tr>
<tr>
<td>64</td>
<td>384</td>
<td>203</td>
<td>96</td>
</tr>
<tr>
<td>128</td>
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<td>101</td>
<td>96</td>
</tr>
<tr>
<td>256</td>
<td>96</td>
<td>50</td>
<td>95</td>
</tr>
</tbody>
</table>

### 2.2 Coupled Depletion/Transport Tests

A coupled depletion/transport test on a standard UO₂ pin cell was performed with the CASL core simulator MPACT [5] to assess the API timing. For CASL LWR depletion problems, a simplified burnup chain has been developed, and the runtime benefit is assessed, compared to the general purpose ORIGEN burnup chain. The general purpose ORIGEN burnup chain contains ~2200 nuclides, ~4000 decay transitions, and ~50,000 reaction transitions. The solve time is on the order of 200 milliseconds for the full set of isotopes, which is expensive (competing with transport solve time) with full-core pin-by-pin depletion.
A target of ~100 milliseconds was established for a single ORIGEN depletion calculation and in order to meet this target, a simplified burnup chain for LWRs was developed containing ~300 nuclides and ~8000 total transitions. The various ORIGEN API component solve times are shown in Figure 5 for the general ORIGEN burnup chain with 2200 nuclides and an experimental CASL burnup chain with 255 nuclides. Note that times are representative of the time required per depletion material in the system. The multigroup library in this case was 47 groups.

The “flux update” time is the time it takes to collapse up to ~12,000 47-group cross sections from the JEFF library [Eqs. (4) and (5)] and interpolate fission yields [Eqs. (6) and (7)]. The “user xs update” is the time it takes to collapse and update the self-shielded MPACT fission; absorption; (n,2n); and (n,3n) cross sections from MPACT's ENDF/B-VII.0-based multi-group library. There are ~300 nuclides in the MPACT transport library, so this is equivalent to about 1200 47-group cross sections. The “transition matrix update” is the time it takes to write the data into the transition matrix format, basically the structure defined in Eq. (3). The solver time is the time for the pure solver kernel in Eq. (8).

For these timing studies, the total time was about 30 milliseconds for a single substep. Thus for typical MPACT calculations with 4 substeps the target of ~100 milliseconds would be achieved.

With the general chain, the solver kernel time dominates at over 200 milliseconds. With the simplified chain, the most significant change is the solver time being reduced by over a factor of 20. A factor of approximately 10 is expected due to the decrease in the number of transitions by a factor of 10, as runtime generally scales with number of transitions. The extra factor of two is not yet understood.

### 3 CONCLUSIONS

An API to perform completely in-memory depletion/decay calculations with ORIGEN has been developed and tested for high-performance parallel depletion. This API will be available in SCALE 6.2. At the highest level, the API manages a set of materials to be depleted in parallel with appropriate flux level normalization via a specified system power, as is common in reactor
depletion problems. The efficiency of the parallel depletion was found acceptable using a strong scaling study in which 24,576 materials were depleted with up to 256 parallel processes (96 materials per process); the efficiency was greater than 95% in all cases.

Other aspects of the API include solver kernels and algorithms to update transition matrices with material-dependent reaction rate information. With the general ORIGEN burnup chain with 2200 nuclides and 54,000 transitions, a single time step requires ~40 milliseconds to update the transition matrix and ~250 milliseconds (per substep) to solve the system and update isotopics. With the simplified burnup chain developed in CASL with 300 nuclides and 8000 transitions, the runtime is ~20 milliseconds for the update and ~10 milliseconds (per substep) for the solve.

Future work includes extending the API to the various emission calculations of ORIGEN, including neutron, gamma, alpha, and beta. The gamma emission capability, in particular, may be useful for high-fidelity gamma transport and deposition modeling. The modernized ORIGEN framework allows new solvers to be easily added. Recently, a Chebyshev Rational Approximation Method (CRAM) was added; it is described in a companion paper [8]. Future work may also include adding additional solver types.

4 ACKNOWLEDGMENTS

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5 REFERENCES
