A Two-Block Decomposition Method for Efficient and Accurate Depletion Calculations

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1. Introduction

A new method of decomposing nuclide concentration vector into two blocks is introduced in this paper. It is tested on a sample problem that includes very short-lived nuclides and compared with the ORIGEN 2.2 [1] and Krylov subspace methods [2, 3].

2. Two-Block Decomposition of Nuclide Concentration Vector

2.1 Two-Block Decomposition of System of Bateman Equations

The system of Bateman equations is written as :

$$\dot{\vec{X}} = A\vec{X}, \quad \vec{X}(0) = \vec{X}_0, \tag{1}$$

where

$\vec{X} \in R^n$: nuclide concentration vector,

$A \in R^{n\times n}$: burnup matrix.

Depending on the magnitude of the "effective" decay constant of nuclide *i*,

$$\lambda_i^{eff} = \lambda_i + \sum_{r=f,c} \sigma_r \phi, \tag{2}$$

the nuclide concentration vector $\vec{X}$ is decomposed into two blocks, short-lived nuclide block and long-lived nuclide block. Then, Eq. (1) is decomposed as :

$$\dot{\vec{X}}_S = A_S \vec{X}_S + A_{SL} \vec{X}_L, \tag{3a}$$

$$\dot{\vec{X}}_L = A_L \vec{X}_L + A_{LS} \vec{X}_S. \tag{3b}$$

The two blocks are calculated separately but with coupling, as in the following.

2.2 Short-Lived Nuclide Block Calculation by Bateman Solutions and Importance Concept

Due to very large norm of A_S, Eq. (3a) is solved by using the general Bateman solution [4] for each nuclide in the short-lived nuclide block.

To reduce computational burden in Bateman solution calculations, we introduce an "importance" concept for selecting important nuclides that produce a particular short-lived nuclide.

Consider the reaction chain involving production of short-lived nuclide *s* shown in Fig. 1.

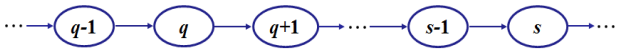

Fig. 1: Example of Reaction Chain

The importance of parent *q* for production of short-lived nuclide *s* from time *t* to *t*+Δ*t*, $\mathrm{IMP}_{s,q}(t,t+\Delta t)$, is defined as :

$$\mathrm{IMP}_{s,q}(t,t+\Delta t) \equiv \frac{\dfrac{a_{s,s-1}}{\lambda_{s-1}^{eff}} \displaystyle\int_t^{t+\Delta t} \lambda_{s-1}^{eff} x_{s-1,q}(\tau)\,d\tau}{\displaystyle\int_t^{t+\Delta t} \lambda_s^{eff} \sum_{i=q+1}^{s} x_{s,i}(\tau)\,d\tau + \sum_{i=q+1}^{s} x_{s,i}(t+\Delta t)}, \tag{4}$$

where

$$x_{s,q}(\tau) = \frac{1}{\lambda_s^{eff}} \prod_{\substack{j=1\\ j\neq s}}^{n} \left(\frac{a_{i,j}}{\lambda_j^{eff}}\right) \sum_{i=1}^{n} \lambda_i^{eff} \prod_{\substack{j=1\\ j\neq i}}^{n} \left(\frac{\lambda_j^{eff}}{\lambda_j^{eff} - \lambda_i^{eff}}\right)^{m_j} \cdot \exp\left(-\lambda_i^{eff}(\tau - t)\right) \Lambda_{i,\mu_i}, \tag{5}$$

$$\Lambda_{i,\mu_i} = \sum_{m=0}^{\mu_i} \frac{\left(\lambda_i^{eff}(\tau - t)\right)^{\mu_i}}{\lambda_s^{eff}} \cdot \sum_{l=0}^{\mu_i} \sum_{h_1=0}^{\mu_i} \cdots \sum_{h_n=0}^{\mu_i} \prod_{\substack{j=1\\ j\neq s}}^{n} \binom{h_k + \mu_k}{\mu_k} \cdot \left(\frac{\lambda_i^{eff}}{\lambda_i^{eff} - \lambda_k^{eff}}\right) \delta\left(\mu_i - m, l + \sum_{\substack{k=1\\ k\neq i}}^{n} h_k\right), \tag{6}$$

$a_{i,j}$: production reaction rate of nuclide *i* from nuclide *j*,

m_i : number of effective decay constants λ_j^{eff}'s making $\dfrac{1}{\lambda_j^{eff} - \lambda_i^{eff}}$ infinite,

$\mu_i = m_i - 1, \ \tau \in [t, t+\Delta t]$,

$\delta(i, j)$: Kronecker delta function.

The nuclide *q* is selected as an important nuclide for production of short-lived nuclide *s* if $\mathrm{IMP}_{s,q}(t,t+\Delta t)$ is larger than criterion (IMP) set by the user.

With only important parents for the short-lived nuclide *s*, general Bateman solution is written as:

$$x_s(\tau) = \sum_{j=1}^{n_{IMP}} \frac{x_{j0}}{\lambda_s^{eff}} \prod_{\substack{j=1\\ j\neq s}}^{n_{IMP}} \left(\frac{a_{i,j}}{\lambda_j^{eff}}\right) \sum_{i=1}^{n_{IMP}} \lambda_i^{eff} \prod_{\substack{j=1\\ j\neq i}}^{n_{IMP}} \left(\frac{\lambda_j^{eff}}{\lambda_j^{eff} - \lambda_i^{eff}}\right)^{m_j} \cdot \exp\left(-\lambda_i^{eff}(\tau - t)\right) \Lambda_{i,\mu_i}, \tag{7}$$

where

$x_s(\tau) \in \vec{X}_S(\tau)$,

n_{IMP}: number of important nuclides determined by importance calculation, ($n_{IMP} \le n$).

2.3 Long-Lived Nuclide Block Calculation with Time-Dependent Short-Lived Nuclide Concentrations

The solution of long-lived nuclide block, Eq. (3b) is expressed as :

$$\vec{X}_L(t+\Delta t) = \exp\left(A_L \Delta t\right) \cdot \left(\vec{X}_L(t) + \sum_{i=1}^{G_n} w_i \exp(-A_L \tau_i) A_{LS} \vec{X}_S(\tau_i) \right), \quad (8)$$

where

G_n: number of Gaussian quadrature set,

w_i: weights for Gaussian quadrature, $\sum_{i=1}^{G_n} w_i = \Delta t$,

τ_i: abscissas for Gaussian quadrature, $\tau_i \in [t, t+\Delta t]$.

In contrast to A_S in Eq. (3a), the norm of A_L is small enough to calculate matrix exponentials efficiently in Eq. (8).

3. Numerical Results

In order to get a realistic initial condition, 3.19w/o enriched PWR fuel is burned for 100 days by the ORIGEN code [1] with Δt=20 days. Then the 100 days burned PWR fuel is irradiated by constant neutron flux 1.98E+14#/cm^3-sec for 20 days. The burnup matrix consists of 976 nuclides. Reference calculation is performed by simple Taylor series expansion with the ORIGEN code using a small time steps (Δt=2.0E-07 days) and a large number of expansion terms (70 terms). Computing time of the reference calculation is 1.668E+05 sec (~1.30 days) on Intel i5 2.67-GHz CPU.

The magnitude of the effective decay constant used for decomposition is $\lambda_i^{eff} \times \Delta t = |\ln(0.001)| \sim 6.9$ (as used in ORIGEN 2.2 for its own treatment of short-lived nuclides). The decomposition method calculations are performed for various IMPs with a fixed number of G_n (G_n=20) and Δt (Δt=20 days and 1 day).

The method is compared with the ORIGEN code and Krylov subspace method with Chebyshev Rational Approximation (Krylov+CRA) [2]. Krylov subspace method with Padé approximation [3] diverges for all Krylov subspaces, since the norm of A is too large (~2.92136E+11). The results are summarized in Fig. 3 and Fig. 4.

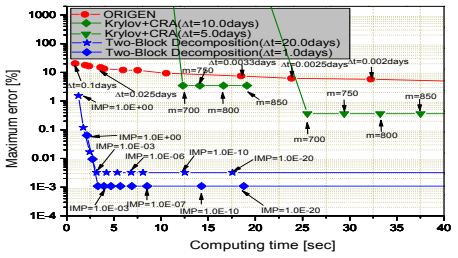

Fig. 3. Maximum errors vs computing time

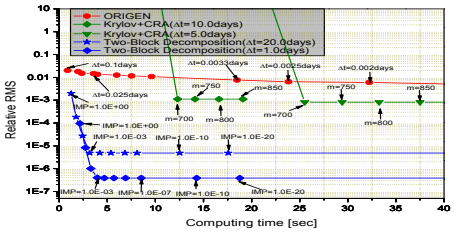

Fig. 4. Relative RMS errors vs computing time

The ORIGEN code calculations are performed for various time steps. The Krylov+CRA calculations are performed for various Krylov subspaces.

Sufficient accuracies in relative RMS errors (RMSE) and maximum errors (MAXE) are obtained by the two-block decomposition method (1.09E-03% in MAXE, 3.89E-07 in RMSE) with sufficient IMP (IMP≤1.0E-03). Computing time of the method for IMP=1.0E-03 and Δt=1 day is 3.75 sec, while that of Krylov+CRA at m=700 and Δt=5 days is 25.52 sec for similar accuracy (2.09% in MAXE, 2.21E-04 in RMSE).

The two-block decomposition method results (Δt=1 day, IMP=1.0E-03, 599 short-lived nuclides) and the ORIGEN results (Δt=0.025 days, 53 terms in simple Taylor series expansion, 495 short-lived nuclides) are compared for the similar computing times. The relative errors of 10 nuclides for which ORIGEN results show discrepancies >3.6% are shown in Table 1.

Table 1 : Relative errors of 10 nuclides

Nuclide	Relative error (%)		Nuclide	Relative error (%)	
	ORIGEN	Two-block		ORIGEN	Two-block
Pd-109	9.46	4.32E-06	Ag-113	6.17	9.18E-07
Pd-109m	-13.46	-1.18E-06	Cd-113	5.23	-4.41E-07
Ag-109m	9.55	-6.49E-05	Pr-148	-4.60	-1.47E-06
Ag-111	4.63	-1.36E-05	Pm-153	-4.52	-2.50E-06
Ag-111m	3.87	-4.42E-05	Pm-154	-3.61	-2.52E-06

In the ORIGEN results, the 10 nuclides show considerable discrepancies (13.46% in MAXE, 8.67E-03 in RMSE), while the two-block decomposition method shows much reduced discrepancies (1.09E-03% in MAXE, 3.89E-07 in RMSE).

4. Conclusions

In this paper, two-block decomposition of the nuclide concentration vector is introduced for efficient and accurate depletion calculations and its performance was compared to those of existing methods.

With a wide range of importance values, the two-block decomposition method shows remarkably improved results, e.g., ~10 times speedup in computing time for similar accuracy compared to the Krylov subspace method. For similar computing time, the two-block decomposition method shows 1000 times smaller MAXE and RMSE compared to the ORIGEN code.

References

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[3] A. Yamamoto et al., "Numerical Solution of Stiff Burnup Equation with Short Half Lived Nuclides by the Krylov Subspace Method", *J. Nucl. Sci. Technol.*, **44**, 147, 2007.

[4] J. Cetnar, "General Solution of Bateman Equations for Nuclear Transmutations," *Ann. Nucl. Energy*, **33**, 640, 2006.