A Krylov Subspace Method with Newton Divided Difference Applied to Depletion Calculation in ORIGEN 2.2

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1. Introduction

In conventional burnup calculation, simplified burnup chains are generally employed for computational efficiency. Although the simplified burnup chain calculation has provided sufficiently accurate results in neutronic analysis, it is still desirable to use a detailed burnup chain calculation in the extended use of the burnup calculation (e.g., source term analysis). Recently, a Krylov subspace method with Padé approximation, which showed better performance in the detailed burnup chain calculation, was suggested [1].

In this paper, the Newton divided difference (NDD) scheme is newly adopted in a Krylov subspace method as an alternative to the Padé approximation and implemented in the ORIGEN 2.2 code [2]. It is tested on a sample problem and compared with the method currently used in the ORIGEN 2.2 code.

2. Krylov Subspace Method with NDD

2.1 Krylov Subspace Method for matrix exponential

The nuclides concentration after Δt can be expressed as follows:

$$\vec{N}(t+\Delta t) = \exp[\mathbf{A}\Delta t]\vec{N}(t), \quad (1)$$

where

$\vec{N}(t)$: nuclides concentration at time t,

$\mathbf{A}$: original burnup matrix.

By the definition of Taylor series expansion, matrix exponential in Eq. (1) is expressed as follows:

$$\exp[\mathrm{A}\Delta\mathrm{t}] = \sum_{\mathrm{m}=0}^{\infty} (\mathrm{A}\Delta\mathrm{t})^{\mathrm{m}} / \mathrm{m}!, \quad (2)$$

with additional definition $(\mathbf{A}\Delta t)^0/0!=\mathbf{I}$.

In practical implementation, a truncated form of the Taylor series is used as follows:

$$\vec{N}(t+\Delta t) = c_0\vec{N}(t) + c_1(\mathbf{A}\Delta t)\vec{N}(t) + c_2(\mathbf{A}\Delta t)^2\vec{N}(t) + \cdots + c_{m-1}(\mathbf{A}\Delta t)^{m-1}\vec{N}(t), \quad (3)$$

where $c_k=1/k!$.

If each term in Eq. (3) is considered as a vector, a Krylov subspace can be defined as follows:

$$\mathbf{K}_{\mathbf{m}}(\mathbf{A}\Delta t, \vec{N}(t)) = Span\{\vec{N}(t), (\mathbf{A}\Delta t)\vec{N}(t), (\mathbf{A}\Delta t)^2\vec{N}(t), \cdots, (\mathbf{A}\Delta t)^{m-1}\vec{N}(t)\}. \quad (4)$$

An orthogonal basis of a Krylov subspace is made by the Arnoldi procedure, after which the following relationship is obtained:

$$\mathbf{H}_{\mathbf{m}} = \mathbf{V}_{\mathbf{m}}{}^{\mathbf{T}}\mathbf{A}\mathbf{V}_{\mathbf{m}}, \quad (5)$$

where

m: dimension of a Krylov subspace,

$\mathbf{V}_{\mathbf{m}} = [\vec{v}_1, \vec{v}_2, \vec{v}_3, \ldots, \vec{v}_m] \in \mathbf{R}^{n\times m}$,

$\mathbf{H}_{\mathbf{m}} \in \mathbf{R}^{\mathbf{m}\times\mathbf{m}}$: a Hessenberg (upper triangular with an extra sub-diagonal) matrix.

With minimizing the least squares residual, the following equation is obtained:

$$\vec{N}(t+\Delta t) \approx \vec{N}_{approx}(t+\Delta t) = \beta\mathbf{V}_{m+1}\exp(\mathbf{H}_{m+1}\Delta t)\vec{e}_1, \quad (6)$$

where

$$\mathbf{H}_{m+1} = \begin{pmatrix} \mathbf{H}_{\mathbf{m}} & 0 \\ \mathbf{0}\ \ \mathrm{h}_{\mathrm{m+1,m}} & 0 \end{pmatrix}, \quad \vec{e}_1 = [1,0,\ldots,0] \in \mathbf{R}^m.$$

Then, we can calculate nuclides concentration with a smaller and denser matrix $\mathbf{H}_{\mathbf{m+1}}$.

2.2 Matrix Exponential with NDD

According to the spectral decomposition property of the matrix function theory [3], we have,

$$\exp(\mathbf{H}_{m+1}\Delta t) = \sum_{i=0}^{m} a_i(\mathbf{H}_{m+1}\Delta t)^i, \quad (7)$$

where the coefficients a_i's are obtained as follows:

$$p(\lambda_i) = \exp(\lambda_i), \quad \mathrm{i}=0,1,\ldots,\mathrm{m}. \quad (8)$$

where λ_i's are the eigenvalues of $\mathbf{H}_{\mathrm{m+1}}\Delta\mathrm{t}$, and

$$p(\lambda) = \sum_{i=0}^{m} a_i\lambda^i. \quad (9)$$

Then, the set of Chebyshev nodes [4] is applied as:

$$\tilde{\lambda}_i = \frac{1}{2}(\lambda_0+\lambda_m) + \frac{1}{2}(\lambda_m-\lambda_0)\cos\left[\left(\frac{2i+1}{2m+2}\right)\pi\right], \quad (0\le \mathrm{i} \le \mathrm{m}), \quad (10)$$

where λ_0 is the smallest eigenvalue of $\mathbf{H}_{\mathrm{m+1}}\Delta\mathrm{t}$ and λ_m is the largest eigenvalue of $\mathbf{H}_{\mathrm{m+1}}\Delta\mathrm{t}$.

According to the Newton divided difference (NDD) [5], p(λ) is expressed with the set of Chebyshev nodes:

$$p(\lambda) = \sum_{i=0}^{m} K[\tilde{\lambda}_0, \ldots, \tilde{\lambda}_i]\prod_{j=0}^{i-1}(\lambda - \tilde{\lambda}_j), \quad (11)$$

where

$K[\tilde{\lambda}_i] = f(\tilde{\lambda}_i)$,

$K[\tilde{\lambda}_i, \ldots, \tilde{\lambda}_{i+k}] = \dfrac{K[\tilde{\lambda}_{i+1}, \ldots, \tilde{\lambda}_{i+k}] - K[\tilde{\lambda}_i, \ldots, \tilde{\lambda}_{i+k-1}]}{\tilde{\lambda}_{i+k} - \tilde{\lambda}_i}$.

3. Numerical Results

A 4.15% enriched UO_2 PWR fuel that is depleted to 1.56MWd/t (≈3600sec) is considered as a test problem. The burnup matrix **A** is constructed with 1696 nuclides, in which half-lives of extremely short-lived nuclides (whose half-lives are shorter than 0.5sec) are set to 0.5sec. Reference calculation is performed by a simple Taylor series expansion with a small time step ($\Delta t=10^{-5}$s) and a large number of expansion terms (53 terms). The computing time of reference calculation is 9776.252sec (2.71hour).

In the conventional ORIGEN 2.2 calculation, fission-induced successive short-lived nuclides chains (e.g., fisson→^{106}Ru→^{106}Rh→^{106}Pd) are not included in the burnup matrix, but they are calculated by a Gauss-Seidel method with secular equilibrium assumption. However, all burnup chains are included in the burnup matrix in the modified ORIGEN 2.2 using the Krylov subspace method with NDD.

The conventional ORIGEN 2.2 calculations are performed with various time steps (Δt=120sec, 40sec, 36sec, 18sec). The modified ORIGEN 2.2 calculations are performed with various Krylov subspaces (m=12, 15, 20, 25). The time steps are determined by the interpolation error theorem [4]. The relative RMS errors (RMSE) are shown in Fig. 1, while the maximum errors (MAXE) are shown in Fig. 2.

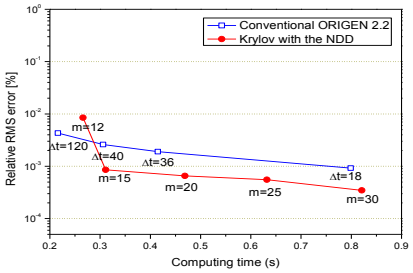

Fig. 1 Relative RMS errors vs. computing time of each method

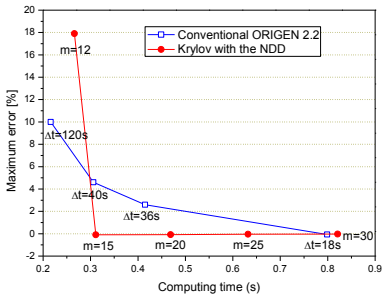

Fig. 2 Maximum errors vs. computing time of each method

Sufficient accuracy in RMS errors and maximum errors are obtained (8.5E-4% in RMSE, 7.6E-2% in MAXE) by the modified ORIGEN 2.2 with a sufficient dimension of the Krylov subspace (m≥15). Computing time of the modified ORIGEN 2.2 at m=15 is 0.311sec, while that of the conventional ORIGEN 2.2 calculation is 0.799sec for similar accuracy (9.2E-4% in RMSE, 7.3E-2% in MAXE).

The conventional ORIGEN 2.2 results (Δt=40sec, 50 terms in simple Taylor series expansion and 287 short-lived nuclides) and the modified ORIGEN 2.2 results (m=15 and Δt=25sec) are compared due to the similar computing times. The relative errors of 26 nuclides, which show discrepancies >0.01%, are shown in Fig. 3.

In the conventional ORIGEN 2.2 calculation, the 26 nuclides show considerable discrepancies (2.6E-3% in RMSE, 4.8% in MAXE), while in the modified ORIGEN 2.2 they show much reduced discrepancies (8.5E-4% in RMSE, 7.6E-2% in MAXE).

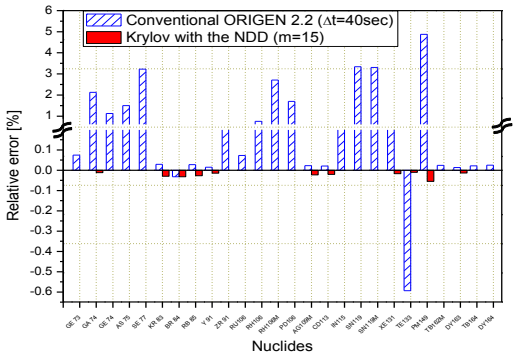

Fig. 3 Relative errors in the 26 nuclides

4. Conclusions

In this paper a Krylov subspace method with Newton divided difference was introduced. It was implemented in the ORIGEN 2.2 code. With a sufficient dimension of the Krylov subspace (m≥15), the Krylov subspace method with NDD provides improved results, i.e., ~2.5 times speedup in computing time for similar accuracy. In the case of similar computing time, the Krylov subspace method with NDD shows 100 times smaller MAXE and 10 times smaller RMSE, since all reactions in the burnup chain are considered in the Krylov subspace method with NDD.

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