Efficient and Accurate Calculation of Burnup Problems with Short-Lived Nuclides by a Krylov Subspace Method with the Newton Divided Difference

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1. Introduction

Nowadays lattice physics codes tend to utilize a detailed burnup chain including short-lived nuclides in order to perform more accurate burnup calculations. But, since production codes, for example, ORIGEN2, take account of nuclides which have relatively long half-life, it is inappropriate for such detailed burnup chain calculation. To enhance that drawback, many matrix exponential calculation methods have been developed. Recently, a Krylov subspace method with the PADE approximation was used [1].

In this paper, a Krylov subspace method based on spectral decomposition property of the matrix function theory with the Newton divided difference (NDD) is introduced. It is tested with a sample problem and compared with simple Taylor expansion method.

2. Methods and Results

2.1 Krylov Subspace Method

The nuclide number density after Δt can be expressed as follows:

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

where,

$\vec{N}(t)$: nuclide number density at time t,

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

By Taylor series expansion, matrix exponential can be expressed as follows:

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

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

Due to implementation problem, a truncated form of the Taylor series is used in production codes. It can be expressed as follows:

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

where, $c_k=1/k!$.

If better combination of c_k is provided, then above equation can give better results. This is possible by the Krylov subspace method since it amplifies the eigenvector of **A** corresponding to the absolute largest eigenvalue which is closely related with short-lived nuclides in burnup chain. In order to find better combination of c_k, Krylov subspace has to be made, which is defined as follows:

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

Krylov subspace can be made by Arnoldi procedure which is followed below [2]:

i) Set $\beta = \| \vec{N}(t) \|_2$, where β is length of vector $\vec{N}(t)$.
ii) Set $\vec{v}_1 = \vec{N}(t)/\beta$.
iii) Repeat iv)-ix) from j=1 to m.
iv) Set $\vec{p} = A\vec{v}_j$.
v) Repeat vi)-vii) from i=1 to j.
vi) Set $h_{ij} = \vec{v}_i^T \vec{p}$.
vii) Set $\vec{p} = \vec{p} - h_{ij}\vec{v}_i$.
viii) Set $h_{j+1,j} = \| \vec{p} \|_2$.
ix) Set $\vec{v}_{j+1} = \vec{p}/h_{j+1,j}$.

After the procedure, the following relationship called Partial Hessenberg reduction can be derived as follows:

$$\mathbf{AV_m} = \mathbf{V_m H_m} + h_{m+1,m}\vec{v}_{m+1}\vec{e}_m^T, \tag{5}$$

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

With eq (5) and some modification of the Hessenberg matrix $\mathbf{H}_m$ for better accuracy, we can calculate nuclide density by using the following equation [2]:

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

where,

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

2.2 Matrix Exponential with the Newton Divided Differences

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

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

where, the coefficients, a_i in eq (7) can be obtained from the following polynomial interpolation:

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

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

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

According to the Newton divided difference (NDD), $p(\lambda)$ can be set as follows [4]:

$$p(\lambda)=\sum_{i=0}^{m}K[\lambda_0,\ldots,\lambda_i]\prod_{j=0}^{i-1}(\lambda-\lambda_j), \qquad (10)$$

where,

$$K[\lambda_i]=\exp(\lambda_i),$$

$$K[\lambda_i,\ldots,\lambda_{i+k}]=\frac{\exp(\lambda_i)}{k!} \quad \text{if } \lambda_i=\lambda_{i+k},$$

$$K[\lambda_i,\ldots,\lambda_{i+k}]=\frac{K[\lambda_{i+1},\ldots,\lambda_{i+k}]-K[\lambda_i,\ldots,\lambda_{i+k-1}]}{\lambda_{i+k}-\lambda_i} \quad \text{if } \lambda_i\neq\lambda_{i+k}.$$

2.3 Test Problems

In order to validate the method, we tested it with a sample problem which is simplified thermal neutron fission of 4.1wt% UO_2 PWR fuel with neutron flux 10^{13}neutrons/cm$^2\cdot$s. The burnup matrix **A** is constructed with 46 nuclides. Initial condition of fuel and lists of short-lived nuclides and related data are followed below:

Table I: Initial condition of UO_2 PWR fuel

Element	Number density
U-234	$7.6551\cdot10^{18}$/ cm^3
U-235	$9.5264\cdot10^{20}$/ cm^3
U-238	$2.1994\cdot10^{22}$/ cm^3
O-16	$4.508\cdot10^{22}$/ cm^3

Table II: Short-lived nuclides, their half-life and their products

Nuclides	Half-life	Products
^{105m}**Rh**	45s	^{105}Pd
^{110}**Ag**	24.5s	^{110}Pd, ^{110}Cd
^{106}**Rh**	29.9s	^{106}Pd
^{137m}**Ba**	153s	^{137}Ba

Some assumptions are used to simplify the problem. First, only U-235 and Pu-239 do fission. Second, fission rate is constant.

We selected Δt as 2298s. Burnup calculation is performed by simple Taylor expansion method, a Krylov method with the NDD. The number of expansion terms of the NDD is the same as dimension of the Krylov subspace, m. Reference calculation was performed by simple Taylor expansion method with a very large n (n=300, Δt=22.98s). It took 46.9s. Result of calculation is presented as Figure 1. We did not plot the case when the error is less than 1 %.

Percent errors of short-lived nuclides and their products which have relatively large errors are listed in the Table III

In terms of computing time, a Krylov method with the NDD takes less time (0.45s) than simple Taylor series (0.88s) when the dimension of the Krylov subspace and the number of expansion terms in Taylor series are 11

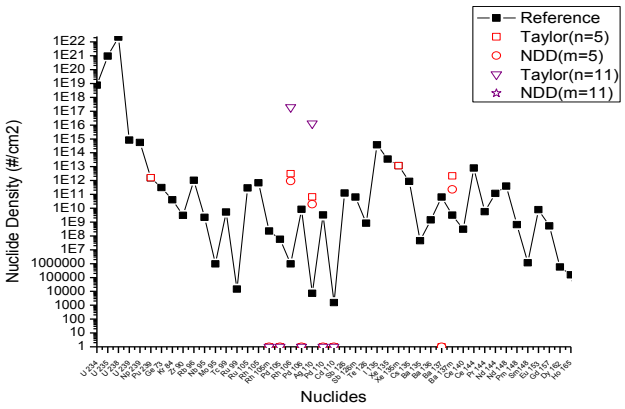

Fig. 1.Nuclides density after 1 time step (Δt=2298s)

Table III: Percent error of nuclide density vs order

Nuclides	Taylor (n=5)	Krylov method with NDD (m=5)	Taylor (n=11)	Krylov method with NDD (m=11)
^{105m}**Rh**	7.4E+05	2.0E+05	3.8E+09	0.0001
^{106}**Rh**	3.2E+08	9.6E+07	2.0E+13	0.2552
^{110}**Cd**	1.2E+07	3.8E+06	2.5E+12	0.0046
^{110}**Ag**	8.8E+08	2.6E+08	1.7E+14	0.32
^{137m}**Ba**	6.7E+04	7086	1.8E+05	5.5E-06

3. Conclusions

From the above test problem, we confirmed when a Krylov subspace method with the NDD is applied to the burnup calculation with short-lived nuclides, it showed better performance than simple Taylor series expansion method in errors of nuclide density and in computing time.

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