Removal of Round off Errors in the Matrix Exponential Method for Solving the Heavy Nuclide Chain

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1. Introduction

Many nodal codes for core simulation adopt the micro-depletion procedure for the depletion analysis. Unlike the macro-depletion procedure, the micro-depletion procedure uses micro-cross sections and number densities of important nuclides to generate the macro cross section of a spatial calculational node. Therefore, it needs to solve the chain equations of the nuclides of interest to obtain their number densities.

There are several methods such as the matrix exponential method (MEM) [1] and the chain linearization method (CLM)[2] for solving the nuclide chain equations. The former solves chain equations exactly even when the cycles that come from the alpha decay exist in the chain while the latter solves the chain approximately when the cycles exist in the chain. The former has another advantage over the latter. Many nodal codes for depletion analysis, such as MASTER [2], solve only the hard coded nuclide chains with the CLM. Therefore, if we want to extend the chain by adding some more nuclides to the chain, we have to modify the source code. In contrast, we can extend the chain just by modifying the input in the MEM because it is easy to implement the MEM solver for solving an arbitrary nuclide chain. In spite of these advantages of the MEM, many nodal codes adopt the chain linearization because the former has a large round off error when the flux level is very high or short lived or strong absorber nuclides exist in the chain.

In this paper, we propose a new technique to remove the round off errors in the MEM and we compared the performance of the two methods.

2. Methods and Results

2.1 Matrix Exponential Method

The ordinary differential equation for a given nuclide chain can be expressed in matrix form as follow:

$$d\mathbf{N}/dt = \mathbf{A}\mathbf{N}, \quad (1)$$

where $\mathbf{N}$: number density vector,
$\mathbf{A}$: coefficient matrix.

It is trivial to show that the solution of Eq. (1) is

$$\mathbf{N}(t) = \exp(\mathbf{A}t)\mathbf{N}(0). \quad (2)$$

Taylor's series expansion is used to evaluate the exponential term in Eq. (2) as follow :

$$\exp(\mathbf{A}t) = \sum_{m=0}^{\infty} (\mathbf{A}t)^m / m!. \quad (3)$$

Inserting Eq. (3) into Eq. (2), we obtain the following :

$$\mathbf{N}(t) = \sum_{m=0}^{\infty} \mathbf{N}^{(m)} \approx \sum_{m=0}^{M} \mathbf{N}^{(m)}, \quad (4)$$

where $\mathbf{N}^{(m)} = (t/m)\mathbf{A}\mathbf{N}^{(m-1)}$, $\mathbf{N}^{(0)} = \mathbf{N}(0)$.

The summation procedure in Eq. (4) stops when $\mathbf{N}^{(M+1)}$ is so small that the following terms can be ignored.

2.2 Round off Errors in the Matrix Exponential Method

The jth diagonal term of the matrix A is $-(\lambda^j + \sigma_a^j \phi)$. If the jth nuclide is a short lived or strong absorber nuclide or the flux level is very high, the absolute value of the diagonal term becomes large and it causes a very large round off error.

Let's consider a 1x1 case of A for simplicity. The value of $\exp(-20.0)$ can be evaluated by the following Taylor's expansion:

$$\exp(-20.0) = \sum_{m=0}^{\infty} (-20.0)^m / m!. \quad (5)$$

The expansion in Eq. (5) converges mathematically and the value is approximately 2.06115×10^{-9}. However, we get 5.62188×10^{-9} due to the round off error if we evaluate it using a double precision variable which has about 16 digit effective precision. The large round off error comes from the fact that the largest term in absolute value in the summation is approximately -4.30998×10^{7}. It means that we subtract a huge number from another huge number to get a tiny number, which is the cause of the loss of the precision. We need at least 19 digits to get more than a 3 digit precision. In contrast, when we evaluate $\exp(20.0)$ we loose no precision because all the terms in the summation are positive.

Noting that only the diagonal elements of the matrix A are negative, we can remove the round off error in evaluating Eq. (4) using the following identity:

$$\exp(\mathbf{A}t) = \exp\left[(\mathbf{A} - \lambda\mathbf{I} + \lambda\mathbf{I})t\right], \quad = \exp(\lambda t)\exp(\mathbf{A}'t) \quad \text{where } \mathbf{A}' = \mathbf{A} - \lambda\mathbf{I} \tag{6}$$

If we use the largest diagonal element of matrix A in absolute value as λ, we can make all the elements of $\mathbf{A}'$ nonnegative and we can remove the loss of precision. However, we choose λ properly to make the most negative diagonal element of the matrix $\mathbf{A}'$ be -13.815 in the actual implementation so that no significant loss of precision can arise.

2.3 Application and Result

Figure 1 shows the heavy nuclide chain which is commonly used in nodal codes for depletion analysis and Table 1 shows the typical one-group cross sections and decay constants of the nuclides in the chain [2].

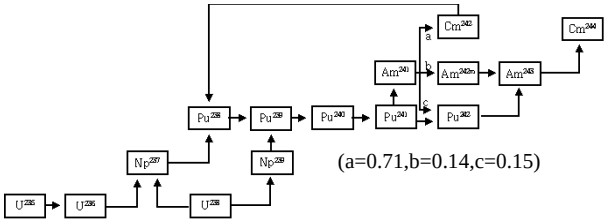

Figure 1 Typical Heavy Nuclide Chain

Table 1 Typical one-group cross sections and the decay constants of the nuclides in the chain

Nuclide	σ_a (barns)	σ_c (barns)	$\sigma_{(n,2n)}$ (barns)	λ (sec^{-1})
U235	4.32467E+01	8.17256E+00	-	-
U236	6.97011E+00	6.65920E+00	-	-
U238	9.44159E-01	8.29020E-01	5.02019E-03	-
Np237	3.24165E+01	3.18610E+01	-	-
Np239	1.65286E+01	-	-	3.441e-06
Pu238	2.98800E+01	2.75977E+01	-	-
Pu239	1.16503E+02	4.07190E+01	-	-
Pu240	1.79394E+02	1.78761E+02	-	-
Pu241	1.09738E+02	2.82835E+01	-	1.536e-09
Pu242	3.54136E+01	3.49450E+01	-	-
Am241	8.89344E+01	8.78909E+01	-	-
Am242m	5.69911E+02	9.46616E+01	-	-
Am243	5.18868E+01	5.14110E+01	-	-
Cm242	4.56404E+00	-	-	4.922e-07
Cm244	1.73249E+01	-	-	-

Table 2 shows the initial condition and the solutions of various methods. The exact solution at 1.728e+6 sec (20 days) with flux level of 2.06357e+14 #/cm.sec was obtained using MATHEMATICA. The MEM also gives the exact solution while the CLM gives an approximate solution though the error is very small.

Table 3 shows the conventional MEM and the revised MEM (RMEM) using Eq. (6). In this case, the half life of the Np239 was halved to magnify the round off error. The error of the Np239 in the conventional MEM is greater than 4000% but practically all the round off error was removed by the RMEM.

The CPU time of the RMEM is slightly shorter than that of CLM. The CPU time of the RMEM was 10.7 μ sec when 1.0e-6 was given as the convergence criteria while that of CLM was 12.7 μ sec. The compressed sparse row (CSR) data structure [4] was used to represent the matrix A in the RMEM for the efficiency of calculation.

Table 2 Initial condition and the solutions of various methods.

Nuclide	N(0) (#/barn-cm)	N(20days) (Exact)	Error of MEM (%)	Error of CLM (%)
U235	1.17975E-03	1.16170E-03	0.00	0.00
U236	6.13658E-05	6.46209E-05	0.00	0.00
U238	2.13599E-02	2.13527E-02	0.00	0.00
Np237	1.79179E-06	1.95795E-06	0.00	0.00
Np239	1.05257E-06	1.06057E-06	0.00	0.00
Pu238	1.27992E-07	1.49068E-07	0.00	0.00
Pu239	7.34848E-05	7.66660E-05	0.00	0.01
Pu240	6.84912E-06	7.48101E-06	0.00	0.00
Pu241	2.60075E-06	2.94174E-06	0.00	0.00
Pu242	1.19625E-07	1.46032E-07	0.00	0.00
Am241	2.98219E-08	3.61277E-08	0.00	0.00
Am242m	4.23231E-10	4.76517E-10	0.00	0.00
Am243	5.23399E-09	6.79026E-09	0.00	0.00
Cm242	1.78703E-09	1.26258E-09	0.00	-0.07
Cm244	2.77381E-10	3.85104E-10	0.00	0.00

Table 3 Solution of MEM with short half live of Np239

Nuclide	N(0) (#/barn-cm)	N(20days) (Exact)	Error of MEM (%)	Error of RMEM (%)
U235	1.17975E-03	1.16170E-03	0.00	0.00
U236	6.13658E-05	6.46209E-05	0.00	0.00
U238	2.13599E-02	2.13527E-02	0.00	0.00
Np237	1.79179E-06	1.95795E-06	0.00	0.00
Np239	1.05257E-06	1.52184E-07	4175.25	0.00
Pu238	1.27992E-07	1.49068E-07	0.00	0.00
Pu239	7.34848E-05	7.75434E-05	24.55	0.00
Pu240	6.84912E-06	7.49325E-06	0.10	0.00
Pu241	2.60075E-06	2.94212E-06	0.00	0.00
Pu242	1.19625E-07	1.46033E-07	0.00	0.00
Am241	2.98219E-08	3.61281E-08	0.00	0.00
Am242m	4.23231E-10	4.76517E-10	0.00	0.00
Am243	5.23399E-09	6.79026E-09	0.00	0.00
Cm242	1.78703E-09	1.26258E-09	0.00	0.00
Cm244	2.77381E-10	3.85104E-10	0.00	0.00

3. Conclusion

In this paper, a technique to remove the round off error in the MEM for solving the nuclide chain was proposed. The numerical test shows that practically all the round off errors was removed by the technique.

The revised MEM with this has several advantages over the CLM. The RMEM solves the chain exactly regardless of the existence of cycle in the chain. It is easy to implement a RMEM solver to solve the general nuclide chain. The CPU time of the RMEM is shorter than CLM though the difference is small.

REFERENCES

[1] S. J. Ball and R. K. Adams, "MATEXP, a General Purpose Digital Computer Program for Solving Ordinary Differential Equations by the Matrix Exponetial Method," ORNL/TM-1933 (August 1967)

[2] C. H. Lee et al., "Verification of Extended Nuclide Chain of MASTER with CASMO-3 and HELIOS," KAERI/TR-947/98,January 1998.

[3] Stephen Wolfrom, "The MATHEMATICA Book 4th Edition," Cambridge University Press, 1999.

[4] Yousef Saad, "Iterative Methods for Sparse Linear Systems," 2000.