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Q. Wang and D. L. Henderson

Department of Nuclear Engineering and Engineering Physics
University of Wisconsin-Madison
1500 Engineering Drive
Madison, WI 53706

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Abstract

As a part of the RACC code improvement and upgrade project, a number of matrix exponential calculational methods were analyzed with respect to the evaluation of the nuclear transmutation and decay matrix equation system. The objective was to determine which method implemented in RACC-Pulse provides the most reasonable computational performance for pulsed/intermittent activation calculations for nuclear fusion devices. The combination of the Taylor series expansion method for pre-shutdown calculation and linear chain method for the post-shutdown calculation resulted in the best performance of the new RACC-Pulse code.

1. Introduction

The neutron transmutation and decay processes in a fusion device can be described by a system of coupled first order ordinary differential equations which can be written in a general matrix form:

$$\frac{d\overline{N}}{dt} = \mathbf{A}\,\overline{N}(t)\,. \tag{1}$$

The mathematical solution of the above matrix equation can be written in a simple concise form,

$$\overline{N}(t) = e^{\mathbf{A}t} \times \overline{N}(0) \tag{2}$$

where $e^{\mathbf{A}t}$ is called the matrix exponential and $\overline{N}(0)$ is the initial number density vector. The matrix $\mathbf{A}$ contains both the total destruction rates $(\lambda + \sigma_t\phi)$ of all nuclides which are the diagonal elements a_{ii} and the production rates ($\sigma_i\phi$ or λ) of all nuclides which are the off-diagonal elements (a_{ij}).

There are a number of ways to evaluate the matrix exponential $e^{\mathbf{A}t}$. Cleve Moler and Charles Van Loan described nineteen dubious ways to compute the exponential of a matrix[1]. In the RACC code all nuclides involved in the transmutation and decay processes in a material zone of a fusion device are sorted by their ZA numbers (Z is the atomic number and A is the mass number). The production rates and destruction rates of all these nuclides form a single matrix $\mathbf{A}$ for this zone. The dimensional size of matrix $\mathbf{A}$ can be greater than 100 and depends on the number of input nuclides and the nuclides occurring in the transmutation and decay scheme. However, the maximum number of the transmutation types of a nuclide in the current data library is 10, though this number could exceed 30. Since a nuclide is usually not coupled to many nuclides occurring in the transmutation decay scheme, matrix $\mathbf{A}$ is a very sparse general matrix.

During the operation period matrix $\mathbf{A}$ can be tightly coupled depending on the number of transmutation/decay chain loops. Matrix $\mathbf{A}$ is separable during the post shutdown period because there are no decay chain loops for pure decay processes.

The Taylor series expansion method, Schür decomposition method, Parlett method, and linear chain method were all analyzed for evaluation of the matrix exponential of **A** during both the operation period and the post-shutdown period.

2. Methods Utilized for the Operation Period

Because transmutation/decay chain loops occur in matrix **A** during the operation period, the only reliable and efficient method to compute $e^{\mathbf{A}t}$ during this period is the Taylor series expansion method combined with the scaling and squaring technique. After taking advantage of the sparsity of matrix **A**, this technique has proven itself to be very efficient for the calculation of $e^{\mathbf{A}t}$. The new RACC-Pulse code utilizes this technique to perform the radioactivity calculation for the operation period. As we will discuss in the next section, other methods either cannot be applied for the operation period calculation or are computationally inefficient.

2.1. Taylor Series Expansion Method

This technique uses a Taylor series expansion of matrix **A** combined with scaling and squaring to compute $e^{\mathbf{A}t}$ as follows:

$$B = (e^{\frac{t*\mathbf{A}}{2^n}})^{2^n} = (e^{\mathbf{C}})^{2^n}$$

$$e^{\mathbf{C}} = \mathbf{I} + \mathbf{C} + \frac{\mathbf{C}^2}{2!} + ... + \frac{\mathbf{C}^k}{k!} + ...$$

The truncation criteria for the Taylor series is:

$$||\mathbf{C}^k/k!|| < eps * max(abs(c_{ij}))$$

$$||\mathbf{C}^k/k!|| := \sum(abs(c_{ij}))\,.$$

During the operation period, if transmutation/decay chain loops are present, this technique is the only reliable and efficient technique and can be quite efficient after taking advantage of the sparsity of all matrices.

3. Methods Utilized for the Post-Shutdown Period

For the post-shutdown period, a number of calculations need to be performed, one for each after shutdown time period specified. During this period, decay processes are the only relevant nuclear processes occurring which means that only linear chains are present in the decay scheme. This leads to a simple structure for matrix **A** which can be separated into lower and upper triangular matrices. The advantage of the triangular structure is that very efficient methods exist for the evaluation of their matrix exponentials. In this section the Taylor series expansion method, Schür decomposition method, Parlett method, and the linear chain method are analyzed. The linear chain method is the most efficient method for performing post-shutdown calculations.

3.1. Taylor Series Expansion Method

The post-shutdown calculation requires the computation of activity for several post-shutdown periods. This means that a Taylor expansion for each individual time step is performed which has proven itself to be computationally inefficient.

3.2. Schür Decomposition Method

The Schür decomposition of a matrix is the following:

$$\mathbf{A} = \mathbf{Q}\mathbf{T}\mathbf{Q}^T$$

where **T** is an upper-triangular matrix. Once matrix **A** has been decomposed, the matrix exponential is evaluated from the expression:

$$e^{\mathbf{A}t} = \mathbf{Q}e^{\mathbf{T}t}\mathbf{Q}^T \,.$$

LAPACK routines [2] are used to perform the Schür decomposition. The evaluation of the matrix exponential of an upper-triangular matrix is performed using an algorithm developed by Parlett [3,4].

This method does a Schür decomposition of matrix **A** once for all post-shutdown periods. However, for each individual period the matrix exponential $e^{\mathbf{T}t}$ must be evaluated. This method has also been proven to be computationally inefficient.

3.3. Parlett's Method

Because the decay processes are the only nuclear processes occurring during the post shutdown period, only linear decay chains are present in the nuclide decay scheme. From a physics point of view this means that all decay chains do not interfere with each other and every decay chain can be represented by lower or upper triangular matrices; therefore matrix **A** can be separated as follows:

$$\mathbf{A} = \mathbf{U} + \mathbf{L}$$

where **L** is a lower triangular matrix and **U** is an upper triangular matrix.

The system of equations given by Eq. 1 can thus be separated into components:

$$\frac{d\overline{N_1}}{dt} = \mathbf{L}\,\overline{N_1}(t) \tag{3}$$

and

$$\frac{d\overline{N_2}}{dt} = \mathbf{U}\,\overline{N_2}(t) \tag{4}$$

where

$$\overline{N(0)} = \overline{N_1}(0) + \overline{N_2}(0)$$

and

$$\overline{N(t)} = \overline{N_1}(t) + \overline{N_2}(t)\,.$$

The separation of both **A** and $\overline{N}(0)$ is based on the decay information represented in matrix **A**, from which every individual decay chain can be constructed. The initial densities of these radioactive nuclides can then be found, from which the beginning nuclide of the individual linear decay chains can be determined.

The solutions of equations (3) and (4) are:

$$\overline{N_1}(t) = e^{\mathbf{L}t} \times \overline{N_1}(0) = \mathbf{E}^l \times \overline{N_1}(0) \tag{5}$$

and

$$\overline{N_2}(t) = e^{\mathbf{U}t} \times \overline{N_2}(0) = \mathbf{E}^u \times \overline{N_2}(0)\,. \tag{6}$$

Because **L** and **U** are lower and upper triangular matrices, $\mathbf{E}^l$ and $\mathbf{E}^u$ are determined by using the following recurrence relations as described in [3,4]:

$$e^l_{ii} = e^{l_{ii}t} \tag{7}$$

$$e^u_{ii} = e^{u_{ii}t}\,. \tag{8}$$

For lower triangular matrix $\mathbf{E}^l$, $i > j$,

$$l_{ii} \times e^l_{ij} - e^l_{ij} \times l_{jj} = \sum_{k=0}^{i-j-1} (e^l_{i,i-k} \times l_{i-k,j} - l_{i,j+k} \times e^l_{j+k,j})\,. \tag{9}$$

For upper triangular matrix $\mathbf{E}^u$, $i < j$,

$$u_{ii} \times e^u_{ij} - e^u_{ij} \times u_{jj} = \sum_{k=0}^{j-i-1} (e^u_{i,i+k} \times u_{i+k,j} - u_{i,j-k} \times e^u_{j-k,j})\,. \tag{10}$$

In our case, matrices **A**, **L** and **U** are all very sparse. Parlett's method mentioned above does not take advantage of the sparsity of these matrices, hence, a numerical example has shown it to be computationally inefficient.

3.4. Linear Chain Method

During the post-shutdown period, matrix **A** is separable from the decay chain construction point of view, hence, the linear chain method, based on the Bateman solution, is a reasonable choice.

All decay chains occurring during the post-shutdown period can be constructed from matrix **A** and the nuclear densities of all radioactive nuclides at shutdown. Once the decay chains have been constructed, the linear chains are evaluated utilizing the Bateman equation solution scheme implemented in the DKR-ICF [5] code.

In constructing linear chains from decay matrix **A**, we need to first determine the starting nuclides of all the decay chains from the nuclear densities of all radioactive nuclides at shutdown, which can be obtained from the solution of the pre-shutdown calculation.

Every radioactive nuclide with nonzero nuclear density at shutdown is a beginning nuclide of a specific decay chain. Starting from these nuclides and by searching the decay matrix **A**, all decay chains can be constructed. In constructing all decay chains an array based balance binary tree data structure is utilized [6]. Because of the sparsity of matrix **A** this technique introduces some memory overhead. However, it is an efficient technique because of the tree structure.

This method is the best method of all methods we have evaluated so far and has been implemented in the RACC-Pulse code for the after shutdown radioactivity calculations.

4. Results and Conclusions

The sample problem of RACC-Pulse, which is described in detail in Appendix B of the RACC-Pulse manual [7], is used to benchmark the above methods. The sample problem is the water cooled 316SS nonbreeding blanket/shield design of the ITER fusion facility considered during the ITER blanket option trade-off study. The calculation is performed for a nominal fusion power of 3.0 GW and an average wall loading of 2.0 MW/m^2. There are a total of 15 zones and approximately 350 nuclides (stable + radioactive) involved in the calculation. A 1 period 3 level pulsing scheme is used for this problem.

The total radioactivity results (Ci) for the above methods and the performance parameters of these methods are shown in Table 1.

Table 1. Comparison Results

After Shutdown Time	Taylor Expansion	Schür Decomposition	Parlett	Linear Chain
0.000000s	0.2451e+07	0.2437e+07	0.2451e+07	0.2451e+07
1.00e+02s	0.2324e+07	0.2315e+07	0.2324e+07	0.2324e+07
1.00e+03s	0.2002e+07	0.1995e+07	0.2002e+07	0.2002e+07
1.00e+04s	0.1580e+07	0.1577e+07	0.1580e+07	0.1580e+07
1.00e+05s	0.1120e+07	0.1119e+07	0.1120e+07	0.1120e+07
1.00e+06s	0.9767e+06	0.9761e+06	0.9767e+06	0.9767e+06
1.00e+07s	0.6669e+06	0.6665e+06	0.6669e+06	0.6669e+06
1.00e+08s	0.2787e+06	0.2787e+06	0.2788e+06	0.2788e+06
1.00e+09s	0.4310e+04	0.4309e+04	0.4310e+04	0.4310e+04
1.00e+10s	0.5898e+03	0.5897e+03	0.5898e+03	0.5898e+03
CPU Time	2427.5s	8517.9s	4757.1s	1639.4s
MLDC	—	—	—	4

MLDC: Maximum Length of Decay Chain considered

As noted from the table, the radioactivity results obtained from the Taylor series expansion method, Parlett's method and linear chain method are identical. However, the result obtained from the Schür decomposition method differs from the others. From additional cases we have investigated with these methods, the Schür decomposition method suffered some significant errors for a number of them. In the linear chain method we set the maximum length of the decay chain to be 4, which is a very good choice because more than ninety percent of all decay chains have the decay chain length less than or equal to 4. From Table 1 it can be clearly seen that the linear chain method's performance is the best and is the preferred technique for the post-shutdown period.

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