# Implementation of a CRAM solver in MENDEL Depletion Code System

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## INTRODUCTION

MENDEL [1, 2] is the new generation depletion code system in CEA. It offers iso-capacity with the French current industrial fuel cycle code system DARWIN/PEPIN2 [3].

It can be used as a fuel cycle study stand alone code system to compute reactor cycle interest outputs: isotopic concentrations, masses, activities, decay heat, particle spectra... MENDEL also provides its depletion solvers to both Monte Carlo TRIPOLI-4® [4] and deterministic APOLLO3® [5] transport code systems.

As it is the fundamental physical quantity, one needs to compute accurately the isotopic densities, solving Bateman equation [6]. MENDEL depletion solver was based originally on a 4th order Runge-Kutta scheme or a Euler scheme, both with a separate treatment for the calculation of saturated isotopes. Euler method, less efficient, will not be treated in this paper. In order to compute in the same way all isotopic densities, an algorithm based on Chebyshev Rational Approximation Method [7] (CRAM) was recently added to the MENDEL solvers.

The purpose of this paper is to present the first results of MENDEL's CRAM solver. They will be compared with MENDEL Runge-Kutta solver, and the lacks and advantages of both methods will be discussed.

## BATEMAN EQUATION SOLVERS

If we consider a material submitted to a neutron flux $\phi(t)$, the evolution in time of the nuclei densities $N_i(t)$ is described by Bateman [6] equation:

$$\frac{dN_i}{dt}(t) = -\left(\lambda_i + \tau_{i,i}\right) N_i(t) + \sum_{j \neq i} \left(b_{j,i}\lambda_j + \tau^r_{j,i}\right) N_j(t) + \sum_k \gamma_{k,i}\tau^f_k N_k(t) \quad (1)$$

with:

$\lambda_i$ the radioactive decay constant of nuclide $i$,

$\tau_{i,i} = \int_E \sigma^d_i(E)\phi(E,t)dE$ the global disappearance reaction rate by neutronic reactions,

$b_{j,i}$ the radioactive decay branching ratio from father nuclide $j$ to daughter $i$,

$\tau^r_{j,i} = \int_E \sigma^r_j\phi(E,t)dE$ the neutronic reaction rate from nuclide $j$ to nuclide $i$ with reaction $r$,

$\gamma_{k,i}$ the independent fission product yields from fissile nuclide $k$ to fission product nuclide $i$,

$\tau^f_k$ the fission reaction rate of fissile nuclide $k$.

Bateman equation (1) can be written in matrix form:

$$\begin{cases} \frac{dN}{dt}(t) &= A(t)N(t) \\ N(0) &= N_0 \end{cases} \quad (2)$$

### Runge-Kutta method

4th order Runge-Kutta [8] method is the historical way to compute Bateman equation in both DARWIN/PEPIN2 and MENDEL code systems. This method offers the advantage of taking into account the non-constant form of matrix $A(t)$.

In MENDEL, matrix $A(t)$ can be considered constant, linear or quadratic in time.

Time step between two flux updates is divised in several time steps to ensure both numerical stability (using a CFL condition) and accuracy. This sub-division is done automatically by the code. If we take into consideration all 2631 nuclei of the MENDEL standard full depletion chain for under irradiation depletion, it leads to very small time steps, and the time consumption of such a method would be too important. In order to solve this problem, we split nuclides between saturated and non-saturated isotopes. Non-saturated isotopes are computing using the Runge-Kutta 4th order scheme with an adequate sub-division of time step. Saturated isotopes are computed using a specific algorithm.

The aim of the implementation of a CRAM solver in MENDEL is to compute all nuclei with the same algorithm.

### CRAM method

When the depletion matrix is considered constant between two neutron flux calculations, $A(t) = A$ and equation (2) reads:

$$N(t) = \exp\left(A*(t - t_0)\right) N(t_0) \quad (3)$$

With this assumption, it is possible to use matrix exponential methods. Among them, CRAM algorithm enables to compute all nuclides without segregating the saturated ones. As a first step in using such a method, we implemented in MENDEL the CRAM method using the Incomplete Partial Fractions method (IPF), as detailed in [7].

CRAM is based on a rational fraction approximation:

$$\exp\left(A\Delta t\right) = \alpha_0 \prod_{l=1}^{k/2} \left(I + 2\Re\left(\alpha_l \left(A\Delta t - \theta_l I\right)^{-1}\right)\right) \quad (4)$$

Both Runge-Kutta and CRAM methods will be described more precisely in the full paper.

## COMPARISONS BETWEEN BOTH METHODS

Full paper will establish a precise comparison between Runge-Kutta and CRAM schemes for solving the Bateman equation .

All data provided in this abstract are computed using a 2631 nuclei depletion chain based on JEFF-3.1.1 nuclear data. MENDEL uses neutronic data (multigroup neutron fluxes and multigroup self-shielded cross-sections) issued from APOLLO3® [5] transport code. The communication between codes is done through a HDF5 format file (with the named MPO for "Multiple Parameters Outputs").

### Results on accuracy

For stability and positivity issues, we compare here CRAM order-16 and Runge-Kutta order-4 methods. CRAM decomposition is done once per user time step (once between two flux updates) while Runge-Kutta automatically sub-divise this time step.

When using the OCDE-NEA benchmark described in [9], we obtain very close results between Runge-Kutta and CRAM algorithms, as shown in Figure 1. The discrepancy shows more or less the Runge-Kutta scheme error, which is around $10^{-4}$, when CRAM accuracy is roughly $10^{-n}$, where $n$ is the CRAM method order.

We used several options to predict the number of saturated nuclei considered in the Runge-Kutta scheme. Value **saturation 100** corresponds to the standard industrial assumptions used in MENDEL (default value). We observe that the mode of the discrepancies distribution is around $3.10^{-3}$% ($3.10^{-5}$ on the graph, as normalization is done to 1). When reducing the number of saturated isotopes, by computing more of them with the Runge-Kutta method, we observe a huge improvement of the adequateness between CRAM and Runge-Kutta (**saturation 10000**, in blue bars).

The reduction of the number of saturated nuclei leads to an increase of calculation time for the Runge-Kutta method, as shown in Table II. Indeed, by adding new nuclei, the infinite norm of the non-saturated nuclei depletion matrix $A$ will increase. This norm is inversely proportional to the Runge-Kutta scheme elementary time step. By increasing the number of elementary steps, time consumption will increase.

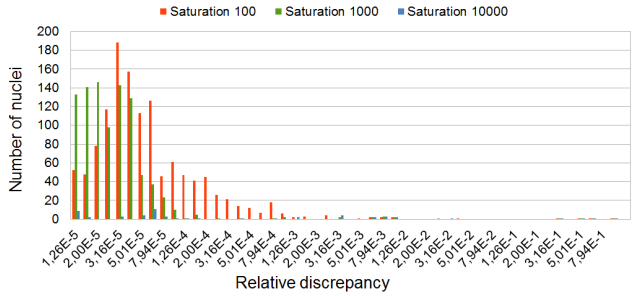


Fig. 1. Relative discrepancy between concentrations computed by CRAM and RK4 with constant reaction rates over time. Relative discrepancy is normalized to 1.

Those results prove the global efficiency of CRAM method to compute all nuclei concentrations, as well as the apparent convergence between CRAM results and Runge-Kutta results were number of saturated nuclei tends to zero.

### Isotopic density positivity

Nevertheless, with no subdivision of the time steps, concentrations at the end of CRAM algorithms can become negative for some nuclei.

This problem, as been proved inherent to CRAM method, which do not ensure the positivity of the outputs. When observing the CRAM approximation on the real exponential function for orders 4, 8 and 16, we obtain the results shown in Figure 2.

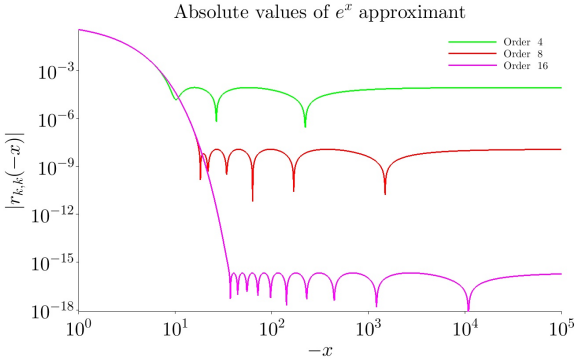


Fig. 2. Relative discrepancy between concentrations computed by CRAM and RK4 with constant reaction rates.

Each vertical asymptote corresponds to a sign change in the CRAM approximation, while the exponential itself is positive. Those sign changes correspond to small exponential values.

It means in particular that, for any order of the CRAM approximation, if $x$ is negatively big enough, the approximation of its exponential value $\exp(x)$ by CRAM might become negative.

In this example, $x$ is equivalent to the $A\Delta t$ in Bateman equation. There are two ways to ensure that negative concentration occurrences do not appear :

- reduce the time step to assure that the negative elements of matrix $A\Delta t$ are small enough,
- increase the order of CRAM approximation.

Both those ways have been successfully tested.

In Table I, we give the number of negative concentrations occurrences in a 2631 nuclei depletion chain for one step of time in an UOX PWR fuel cell. This example is quite relevant for the global trend, but readers need to beware that the 16th order CRAM method do not automatically ensure the concentration positivity.

Most authors consider that negative concentrations are small enough to put them equal to zero. We decided for the moment to let the negative occurrences in MENDEL at intermediate time steps and put them equal to zero only at the end of calculation. Work for an automatic and robust choice for the number of time steps and order of CRAM approximation to ensure the positivity of all concentrations is still undergoing.

| CRAM order | 1 sub-step | 2 sub-steps | 10 sub-steps |
|---|---|---|---|
| order 4 | 114 | 40 | 0 |
| order 8 | 10 | 0 | 0 |
| order 16 | 0 | 0 | 0 |

TABLE I. Number of negative concentrations in one call to Bateman solver, for a 2631 nuclei depletion chain example.

### Time consumption

Using the benchmark described in [9], we obtain, for both methods, the time consumption shown in Table II.

| solver | CRAM16 | RK4 (sat $10^2$) | RK4 (sat $10^4$) |
|---|---|---|---|
| total time | 10.39 s | 12.26 s | 161.52 s |
| solver time | 6.41 s | 8.41 s | 156.54 s |
| nb of sat. | 0 | 1624 to 1928 | 950 to 1394 |

TABLE II. Time consumption in CPU time. The number of saturated nuclei in Runge-Kutta scheme varies from one depletion step to another.

CRAM solver is not to be considered completely optimized in its current implementation in MENDEL.

Those computational times were considered taking only one CRAM time step between two flux updates.

If we take into account the positivity remarks, CRAM time consumption might greatly increase.

## CONCLUSIONS

CRAM proves to be very efficient to compute all nuclei without taking apart saturated ones. For nuclei considered as saturated by the Runge-Kutta scheme when time consumption is equivalent, accuracy is much better.

Nevertheless, some numerical problems are still not completely solved, as the choice of the optimal sub-step and/or approximation order to ensure the concentration positivity in amount of the calculation. Work on this aspect is still undergoing to obtain a good predictor way of chosing order and sub-steps.

In conclusion, MENDEL will continue to use CRAM-like solvers, and improve their efficiency.

## ACKNOWLEDGMENTS

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