

Implementation of a CRAM solver in MENDEL Depletion Code System

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Abstract - Accuracy on the evaluation of isotopic concentrations are an important issue for the nuclear fuel cycle studies, from nuclear facility in operation to long term disposal. Indeed, most of the physical quantities of interest (masses, activities, decay heats...) depend of concentrations.

All fuel cycle code systems are available to estimate the concentrations. ORIGEN, FISPACT, DARWIN/PEPIN2 are part of them. MENDEL is a new generation depletion code developed at CEA, devoted to the calculation of physical quantities related to fuel cycle studies. It already offers iso-capacity with DARWIN/PEPIN2. The first Bateman solver implemented in MENDEL was a 4th order Runge-Kutta solver, algorithm already used in DARWIN/PEPIN2.

The purpose of this paper is to present the recent implementation of a Chebyshev Rational Approximation Method (CRAM algorithm) in MENDEL. After a general description of both Runge-Kutta and CRAM algorithm, focus will be made on MENDEL's CRAM solver first results. They will be compared with MENDEL already existing solvers, and the lacks and advantages of all methods will be discussed.

I. INTRODUCTION

Isotopic concentrations are the most important quantities of interest for fuel cycle studies. Other interest outputs are directly computed from concentrations: masses, activities, decay heats, particle spectra...

As it is the fundamental physical quantity, one needs to compute accurately the isotopic concentrations, solving Bateman equation [1]. This accuracy is of utmost importance for nuclear power plant safety, both in normal operation and accidental situation, as well as for all fuel cycle processes, from fuel fabrication to retreatment, in order to know with a good accuracy all isotopic concentrations.

MENDEL [2, 3] is the new generation depletion code system developed at CEA, with new software architecture, dedicated to the calculation of physical quantities related to fuel cycle studies. MENDEL already offers iso-capacity with the French current industrial fuel cycle code system DARWIN/PEPIN2 [4].

MENDEL can be used as a stand alone code system to compute interest outputs for nuclear reactor fuel cycle studies: isotopic concentrations, masses, activities, decay heats, particle spectra, radiotoxicity parameters... MENDEL also provides its depletion solvers to both Monte Carlo TRIPOLI-4® [5] and deterministic APOLLO3® [6] transport code systems.

In this paper we focus entirely on the use of the stand alone fuel cycle code system.

Comparisons to other code systems will not be done in this work, as it has already been shown that MENDEL and DARWIN/PEPIN2 give the same results when used with the same input data [3].

MENDEL depletion solver was based originally on a 4th order Runge-Kutta scheme, both with a separate treatment for the calculation of saturated isotopes. In order to compute in

the same way all isotopic concentrations, an algorithm based on Chebyshev Rational Approximation Method [7] (CRAM algorithm) 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.

II. BATEMAN EQUATION SOLVERS IN MENDEL

Let's consider a material submitted to a neutron flux $\phi(t)$. The depletion (evolution in time) of the nuclei concentrations $N_i(t)$ is described by Bateman [1] equation:

$$\frac{dN_i}{dt}(t) = -(\lambda_i + \tau_{i,i})N_i(t) + \sum_{j \neq i} (b_{j,i}\lambda_j + \tau_{j,i}^r)N_j(t) + \sum_k \gamma_{k,i}\tau_k^f N_k(t) \quad (1)$$

with:

λ_i the radioactive decay constant of nuclide i ,

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

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

$\tau_{j,i}^r$ = $\int_E \sigma_j^r(E)\phi(E,t)dE$ the neutronic reaction rate from nuclide j to nuclide i with reaction r , except fission,

τ_k^f = $\int_E \sigma_k^f(E)\phi(E,t)dE$ the fission reaction rate of fissile nuclide k ,

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

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

$$\begin{cases} \frac{dN(t)}{dt} = A(t)N(t) \\ N(t_0) \end{cases} \quad (2)$$

where t_0 is the initial time and $N(t_0)$ the initial isotopic vector.

In MENDEL stand-alone code system, fission reaction rates and neutronic reaction rates are computed using:

- microscopic multigroup cross sections coming either from GENDF files, either from transport code systems APOLLO2 [8], APOLLO3®, ERANOS [9] or TRIPOLI-4®,
- multigroup neutron flux coming from ERANOS, TRIPOLI-4®, APOLLO2 or APOLLO3® codes.

Both cross sections and neutronic fluxes are given to MENDEL in the form of hierarchic files.

1. Runge-Kutta method

4th order Runge-Kutta [10] 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. This functionality of a non constant depletion matrix during the user time step is available in APOLLO3® and TRIPOLI-4®, leading to a predictor corrector scheme for better approximation of the depletion. It is valid only for some families of Bateman equation solvers not strictly based on exponential of matrices, like Runge-Kutta.

In MENDEL stand-alone use, neutronic flux has been computed at different times in neutron transport code (being APOLLO2 [11], APOLLO3® or TRIPOLI-4®). In APOLLO3® and TRIPOLI-4® case, MENDEL solver has already been used to deplete nuclear fuel.

Runge-Kutta 4th order algorithm description

MENDEL and DARWIN/PEPIN2 both use the standard 4th order Runge-Kutta scheme for solving the system of differential equations (1).

Time step between two flux updates is divided in several time steps to ensure both accuracy and numerical stability. Numerical stability is proved using a Courant-Friedrich-Lewy (CFL) condition [12] which defines automatically the sub-division in time.

There is no adaptation of the sub-step length between two flux updates depending on the variation of the linear or parabolic variation of the depletion matrix. It is computed taken into consideration the less favorable value of the depletion matrix. This hypothesis ensure the stability and accuracy of the resolution. Adaptation of the sub-steps length is done at each new flux update, a new sub-step value been defined whith the new values of depletion matrices.

It is equivalent to what is done in APOLLO2 and, with another algorithm, in CRONOS2 [13] (Taylor expansion of the exponential of matrix instead of Runge-Kutta).

The Runge-Kutta 4th order used in MENDEL is the classical one. Let's assume that Δt is the time step asked for the user, starting from time t_0 . For a given Runge-Kutta time step $\delta t = \frac{\Delta t}{N}$, and concentration at time $t + \delta t$ reads:

$$N(t + \delta t) = N(t) + \frac{k_1 + 2k_2 + 2k_3 + k_4}{6} \quad (3)$$

where

$$\begin{cases} k_1 = A(t)N(t) \\ k_2 = A\left(t + \frac{\delta t}{2}\right)\left(N(t) + \frac{\delta t}{2}k_1\right) \\ k_3 = A\left(t + \frac{\delta t}{2}\right)\left(N(t) + \frac{\delta t}{2}k_2\right) \\ k_4 = A(t + \delta t)(N(t) + \delta tk_3) \end{cases} \quad (4)$$

Runge-Kutta limitation and saturated isotopes

If we take into consideration all 2631 nuclei of the MENDEL standard full depletion chain, it leads to very small time steps, and the time consumption of such a method would be too important. Indeed, Runge-Kutta time step depends of the depletion matrix eigenvalues, which are not so different from the diagonal elements. Due to the very large range of radioactive decay periods, the depletion matrix is badly conditioned, leading to those very small time steps.

In order to solve this problem, we split nuclides between saturated and non-saturated isotopes. Non-saturated isotopes are computed using the Runge-Kutta 4th order scheme with an adequate sub-division of time step, much bigger than the one needed for the full matrix. Saturated isotopes are computed using a specific algorithm.

This compromise enables to run the Bateman equation solver in a reasonable time for the any depletion chain, saturated isotopes approximation being rather good.

In MENDEL, users can freely chose two criteria:

- Using more or less saturated isotopes by adjusting the saturation criteria. More saturated isotopes will lead to a faster execution time, but also to more approximation for isotopes going from the non saturated algorithm (Runge-Kutta) to the saturated isotopes algorithm.
- Accuracy criteria on final concentrations for non-saturated isotopes.

The saturation criteria used by MENDEL users is an integer linked to the decision of taking isotopes saturated or non saturated. The bigger the criteria, the more non saturated isotopes, and the better the accuracy for those isotopes. Saturated isotopes are always isotopes with very short radioactive decay periods and consequently low densities.

Default saturation criteria in MENDEL is fixed to 100. It is the lowest value observed in this paper.

Accuracy criteria applies only for non saturated isotopes.

2. CRAM method

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

Let's assume the depletion matrix can be considered constant between two neutron flux updates. In this time step, this assumption leads to equation (2) reads:

$$\left\{ \frac{dN(t)}{dt} = AN(t) \right. \quad (5)$$

In this approximation, an analytic solution appears to solve Bateman equation, leading to the computation of a matrix exponential:

$$N(t) = \exp(A*(t - t_0)) N(t_0) \quad (6)$$

With this assumption, it is possible to use any matrix exponential method [10]. Historically in CEA neutronics code systems, Taylor expansion has been used, in particular in CRONOS2, CEA core code system. Among the different available methods, CRAM algorithm enables to compute all nuclides without segregating the saturated ones and is nowadays more and more used.

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 reference [7].

CRAM algorithm description

CRAM is based on a rational fraction approximation using complex coefficients:

$$\exp(A\Delta t) = \alpha_0 \prod_{l=1}^{k/2} \left(I + 2\Re(\alpha_l (A\Delta t - \theta_l I)^{-1}) \right) \quad (7)$$

with:

- α_l and θ_l are the coefficients of the Chebyshev rational approximation,
- I is the identity matrix,
- k is the order of the rational approximation,
- \Re is the real part function.

Coefficients α_l and θ_l are all complex values with non zero imaginary part. Only α_0 is real. In our work, we took directly the values given in reference [7].

It is necessary, for solving Bateman equation by CRAM method, to inverse $k/2$ linear systems.

We use the MENDEL sparse matrix structure (for the fuel depletion standard chain with 2631 nuclei, non null coefficient in matrix A are much less than 1%). We solve the inversion by a LU factorization, which leads to apparition on new non null positions in the matrix. For better efficiency, we used the symbolic factorization, already well described in [14].

This method consists of a first run to know which coefficient will be null for sure, and the LU factorization is done without taking them into account. As we need to make $k/2$ factorization, this method is more efficient when k increases.

This method is particularly efficient for sparse matrices, like the MENDEL 2631 nuclei depletion matrix for which the positions of all non-zero coefficients are shown in Figure 1.

In general, all depletion matrices are sparse, and it is particularly true for high numbers of nuclei.

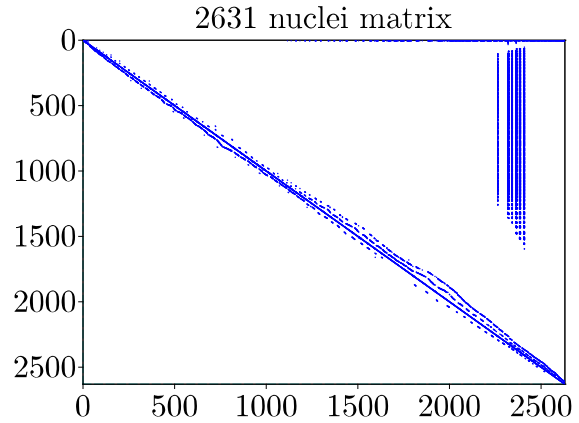


Fig. 1. Position of non zero coefficients in the MENDEL 2631 nuclei depletion matrix

Existence of the LU factorization

The LU factorization is done on the $A\Delta t - \theta_l I$ matrix, where θ_l are complex coefficients. One first problem is to prove the existence of the LU factorization, which is equivalent to the fact that all principle sub-matrices are invertible.

Let's assume $(A_k \Delta t - \theta_l I_k)$ the k^{th} one.

As $\Delta t \neq 0$, if $(A_k \Delta t - \theta_l I_k)$ is not invertible, then:

$$\begin{aligned} \exists X \neq 0, (A_k \Delta t - \theta_l I_k) X = 0 &\Leftrightarrow A_k \Delta t X = \theta_l X \\ &\Leftrightarrow A_k X = \frac{\theta_l}{\Delta t} X \end{aligned} \quad (8)$$

In the general case of a depletion matrix, it is not possible to prove anything more, which is a first problem in the CRAM algorithm structure. To counter this absence of formal demonstration a test has been introduced in MENDEL pivot decomposition. For all tests done, LU decomposition was possible.

Even if formal demonstration is not possible, the probability of occurrence of the case when $\frac{\theta_l}{\Delta t}$ is an eigenvalue is very small. Indeed, by the A_k matrix structure, eigenvalues have a positive real part, but it is not possible to characterize their imaginary part. When looking at the θ_l coefficient values in [14], depending on the approximation order, between 30% and 50% of them might be attained. But the probability to be exactly on the $\left\{ \frac{\theta_l}{\Delta t}, 1 \leq l \leq \frac{k}{2} \right\}$ complex half-lines in complex plan is extremely scarce.

If one obtains an eigenvalue exactly equal to $\frac{\theta_l}{\Delta t}$ and do not succeed to create the LU decomposition, one simple solution would be to divide the time step by 2, and making two CRAM iterations.

In conclusion for the LU decomposition existence lack of proof, we have here a theoretical limitation of the CRAM algorithm in our context, but its occurrence is low enough to use the algorithm. If the LU decomposition cannot be done, time step will be reduced.

III. COMPARISONS BETWEEN BOTH METHODS

Before showing results physically interesting in the field of nuclear fuel cycle, we compare in this section Runge-Kutta and CRAM schemes for solving the Bateman equation. We will focus on the strong and weak points of both methods.

All data provided in this abstract are computed using MENDEL standard isotopic chains:

- the 2631 nuclei chain for fuel depletion in reactor, based on JEFF-3.1.1 nuclear data and describing both decay ways and neutronic reactions,
- the simplified chain for fuel depletion in reactor, with 159 nuclei, based on JEFF-3.1.1,
- the 3849 nuclei chain for decay ways, based on JEFF-3.1.1 nuclear data and describing only the decay ways.

In this study MENDEL uses neutronic data (multigroup neutron fluxes and multigroup self-shielded cross-sections) issued from APOLLO3® [6] transport code.

The communication between codes is done through hierarchical file in HDF5 format (with the named MPO for “Multiple Parameters Outputs”) generated by APOLLO3®.

When comparing MENDEL results by Runge-Kutta and CRAM solvers, we need to deal with several differences in modelisation:

- CRAM assumes a constant matrix during each time steps. This hypothesis requires a relevant choice of consecutive periods of flux updates.
- CRAM accuracy will depend of the approximation order.
- Runge-Kutta scheme separates saturated and non saturated isotopes. When comparing the isotopic concentrations of a nuclei considered as saturated or as non saturated by modifying the saturation criteria, relative differences on concentrations can be important. It concerns only isotopes of very low concentration in the medium. It means that Runge-Kutta accuracy will depend of both asked accuracy and saturation criteria.

In order to compare efficiently the methods, we will show results for several saturation criteria in Runge-Kutta method and several approximation orders in CRAM algorithm (orders 4, 8 and 16).

1. Results on accuracy and saturated isotopes with Runge-Kutta method

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.

The 16th order CRAM is chosen for a better accuracy in this section.

In order to demonstrate the convergence or the saturation criteria value of the Runge-Kutta scheme to the CRAM results, we use the OECD-NEA benchmark described in [15] on the

2631 nuclei depletion chain of MENDEL. It concerns an UOX 4.1% PWR fuel cell.

Accuracy criteria in Runge-Kutta is fixed to 10^{-4} for the determination of the sub-steps. 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). Value 10^4 corresponds to the fewest number of saturated isotopes used here. This configuration should be nearer the CRAM results.

We obtain very close results between Runge-Kutta and CRAM algorithms, as shown in Figure 2. This figure gives an histogram of the number of nuclei (y-axis) for a given discrepancy between the two algorithms (x-axis).

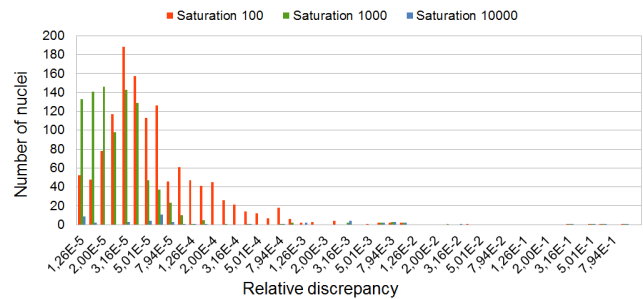


Fig. 2. Relative discrepancy between concentrations computed by CRAM and RK4 with constant reaction rates over time. Relative discrepancy is normalized to 1.

This discrepancy is computed as $\frac{|RK - CRAM|}{RK}$ where RK is the concentration computed by Runge-Kutta and $CRAM$ the concentration computed by CRAM. A discrepancy of value 1 would correspond to 100%. Discrepancies less than 10^{-5} are not represented on this graph.

For the standard value of the saturation criteria, we observe that the mode of the discrepancies distribution is around 3.10^{-5} (red histogram).

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.

The green histogram (saturation 1000) shows a slight reduction of the mode and of the number of represented isotopes (non negligible discrepancies). The blue histogram (saturation 10^4) shows no bar higher than 12 isotopes.

Nevertheless, some isotopes of larger discrepancy (around 10^{-3} to 10^{-2}) still appears on the histogram.

The reduction of the number of saturated nuclei leads to an increase of calculation time for the Runge-Kutta method, as shown in Table V. 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.

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 when the number of saturated nuclei tends to zero.

It is also for MENDEL a first validation for given nuclear data, for all nuclei, of the splitting between saturated and non saturated isotopes, by comparing with a method making a priori no difference between very short life time isotopes and others.

2. Accuracy when changing CRAM order

Another way of testing the accuracy is to compare the Runge-Kutta 4th order scheme with standard saturation criteria and the CRAM algorithm at several orders for several sub-steps. The number of sub-steps with Runge-Kutta is automatically computed by MENDEL and not written here.

Results are given in Table I for the same benchmark as previously.

	2631 nuclei chain	
	4th order	16th order
1 sub-step	8.6×10^{-5}	2.9×10^{-7}
2 sub-steps	1.7×10^{-4}	2.9×10^{-7}
10 sub-steps	8.6×10^{-4}	2.9×10^{-7}

TABLE I. Mean relative discrepancy (weighted by concentration) of nuclei concentrations in CRAM algorithm.

Those results show that from a given order (here, order 16), CRAM approximation is good enough even without making any subdivision. It is stable and accurate.

Nevertheless, when the order is not enough, like for order 4, we observe an augmentation on the discrepancy while subdividing the time step.

When using the 159 nuclei simplified depletion chain, we obtain similar results as shown in Table II.

	159 nuclei chain	
	4th order	16th order
1 sub-step	8.6×10^{-5}	7.1×10^{-7}
2 sub-steps	1.7×10^{-4}	7.1×10^{-7}
10 sub-steps	8.6×10^{-4}	7.1×10^{-7}

TABLE II. Mean relative discrepancy (weighted by concentration) of nuclei concentrations in CRAM algorithm.

Those results tend to demonstrate that the subdivision of the time step is not enough to ensure the stability of the system, and an optimum between order, accuracy and time consumption should be found.

In MENDEL, we consider the CRAM 16th order approximation as being the standard approximation order, but lower and upper CRAM orders are also available (orders 4, 8, 16 and 32).

3. Isotopic concentration positivity

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

This problem has been proved inherent to CRAM method, which do not ensure the positivity of the outputs (isotopic concentrations).

For a formal demonstration and better understanding of

this problem, we no more consider in this section the exponential of a matrix but the exponential function on real values $f(x) = \exp(x)$.

When use CRAM approximation for orders 4, 8 and 16 on function $f(x) = \exp(x)$ for $x < 0$ and we obtain the results shown in Figure 3.

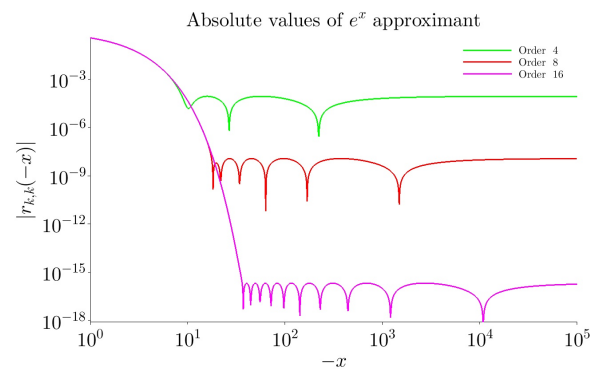


Fig. 3. Absolute discrepancy between exact value and CRAM approximation of $\exp(-x)$.

The y-axis shows the absolute value of the discrepancy between CRAM approximation and the exact value of the exponential for negative values of x (x -axis).

The first conclusion is that the accuracy greatly increases with the order of the CRAM method. Accuracy is roughly in 10^{-N} , where N is the CRAM approximation order. This has already been proved in reference [7] and is a huge positive aspect of the CRAM algorithm.

This change of order of magnitudes in the accuracy led to the necessity of a logarithmic y-axis, and the use of absolute differences.

The second information of Figure 3 is the presence of vertical lines (vertical asymptotes), corresponding to a sign change in the CRAM approximation, while the exponential itself is positive. Those sign changes correspond to small exponential values (*id est* small concentrations for isotopes).

This appearance of negative values exists for all CRAM approximation orders, and the number of changes is linear in the order.

It also means 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. The assumption taken generally when using CRAM method of making only one sub-step is therefore not so safe.

Let's assume x_N the biggest value $x > 0$ so that the CRAM approximation in x is negative. x_N is decreasing when N increases.

It means there are several ways to ensure that negative concentration occurrences do not appear :

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

Both those ways have been successfully tested in MENDEL.

In Table III, we give the number of negative concentrations occurrences in a 2631 nuclei depletion chain for one step of time in the same UOX PWR fuel cell as previously. 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.

Sub-steps have been taken constant between the time step.

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

Most authors consider that negative concentrations are small enough to put them equal to zero. As the occurrence of negative concentrations do not affect the stability of the CRAM algorithm, 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.

4. Comparison to polynomial approximation

The negative concentrations do not occur when using polynomial expansions like Taylor. It is therefore interesting to compare the accuracy of those methods.

We continue in this section to work on the function $f(x) = \exp(x)$, $x < 0$.

Figure 4 represents the polynomial approximation by Taylor expansion (orders 4, 8 and 16) and CRAM rational approximation (orders 4, 8 and 16) compared to the exact value of the exponential.

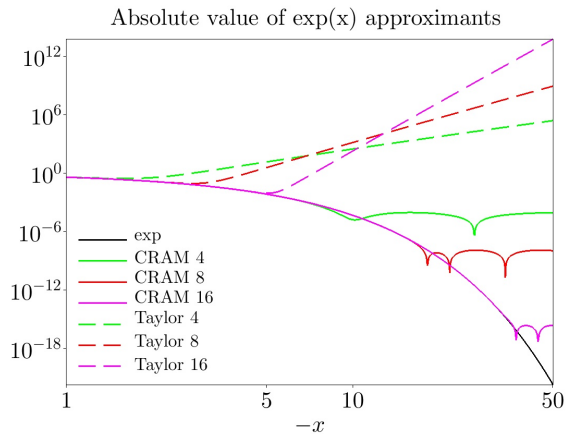


Fig. 4. Comparison between Taylor expansion and CRAM approximation.

This figure shows a much better accuracy for CRAM

method, following the exponential decay much longer than the polynomials. CRAM order 4 seems this way more precise than Taylor order 16.

The use of rational function in CRAM also enables to create an approximation which do not tend to $+\infty$ when x (*id est* the norm of $A\Delta t$) tends to $+\infty$, which is a negative point of Taylor expansion.

It explains in particular that the necessity of the subdivision of the time step in Runge-Kutta and Taylor methods do not necessarily applies for CRAM algorithm.

5. Decay Heat

We have previously shown in sections 1. and 2. that, despite the risk of negative occurrences, most of the isotopic concentrations are computed correctly both by CRAM and Runge-Kutta. Using the same OCDE benchmark, we will verify in this section that the isotopes for which the discrepancies exist do not impact integrated parameters, like the decay heat.

The decay heat corresponds to the residual power of nuclear waste due to radioactive decay and reads:

$$PR(t) = \sum_{i=0}^M N_i(t)\lambda_i E_i \quad (9)$$

with:

- λ_i the radioactive decay constant,
- E_i the radioactive decay energy due to any decay way: $E_i = E_i^\alpha + E_i^\beta + E_i^\gamma$.

In MENDEL, concentrations are computed at the end of irradiation with CRAM or Runge-Kutta solvers, then an analytical solver is used to compute the concentrations at any cooling time.

We compute the relative discrepancy of decay heat between the use of both solvers during the irradiation phase. Cooling phase is done with the analytical solver in both case. Results are given for several cooling times in Figures 5 and 6.

For Runge-Kutta, saturation is fixed to default value (100). For CRAM, the 16th order approximation is chosen.

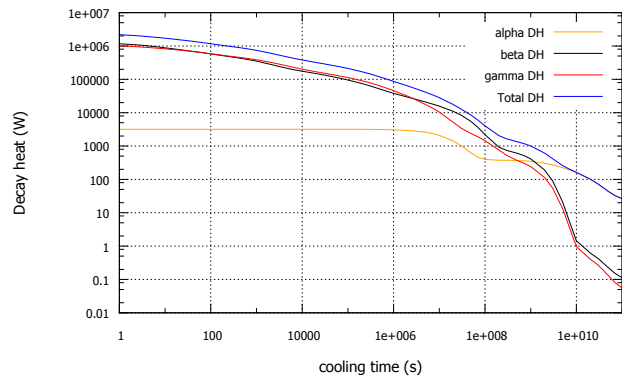


Fig. 5. Total decay heat and its components (W).

Figure 5 represents the evolution in cooling time of the total decay heat (blue line) and its components from 1 second

to 3000 years. Isotopic concentrations during the irradiation phase have been computed using the CRAM algorithm.

Figure 6 represents the relative discrepancy, in percent, between decay heat computed from concentrations issued of Runge-Kutta solver and concentrations issued from CRAM solver.

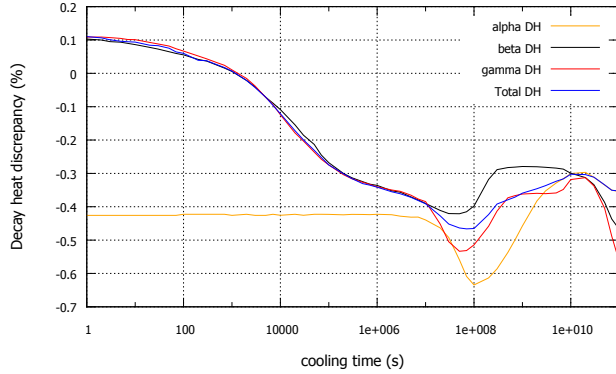


Fig. 6. Discrepancy on total decay heat and its components (discrepancies in %) between CRAM 16th order and Runge-Kutta default settings.

Discrepancy on decay heat is directly issued from discrepancies on isotopic concentrations.

Discrepancy is low enough, as experimental data on decay heat do not attain this precision.

Nevertheless, when trying to converge the results by reducing the number of saturated isotopes inn Runge-Kutta, we observed no improvement. Indeed, results on decay heat in this particular case between a saturation put the the default value (100) and to a greater value (10000) gives nearly no difference, as shown in Figure 7. Only numerical noise can be observed.

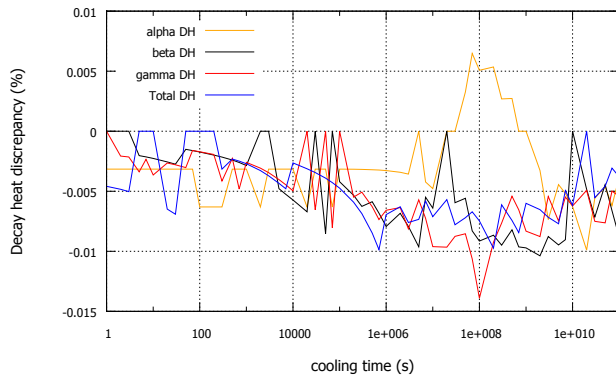


Fig. 7. Discrepancy on total decay heat and its components (discrepancies in %) between two Runge-Kutta schemes different by their saturation criteria.

Table IV shows the relative discrepancy between the two methods for the 5 more important contributors at cooling time 0s and 300years.

Values on the output ASCII files of MENDEL for decay heat are given with 6 digits.

Cooling time	Isotopes name	discr. on density (%)	Total DH contribution (%)
0 sec	U239	4.36×10^{-3}	2.6432
	NP239	4.82×10^{-1}	2.5362
	CS138	1.69×10^{-1}	1.7521
	I134	1.72×10^{-1}	1.7434
	CS140	1.89×10^{-1}	1.4746
300 years	AM241	4.70×10^{-2}	72.1326
	PU240	6.03×10^{-1}	11.1083
	PU238	5.22×10^{-1}	8.5916
	PU239	1.89×10^{-2}	6.5745
	AM243	6.59×10^{-1}	0.6405

TABLE IV. Relative discrepancy of main contributors total decay heat

It appears a clear adequateness between dominating isotopes discrepancy and decay heat discrepancy. Saturated isotopes, which have no important effect of decay heat, are not to reduced in number with the Runge-Kutta scheme as no better results will occur.

We observe a good accuracy for the total decay heat main contributors, for very short time as well as for longer times.

Those results assures the fact that CRAM and Runge-Kutta can both be used for computing fuel depletion in reactors, with result discrepancies far below the decay heat measurements uncertainty bars (generally 1% or more).

IV. TIME CONSUMPTION

Using the benchmark described in [15], we obtain, for both methods, the time consumption shown in Table V (for Runge-Kutta) and in Table VI (for CRAM).

saturation criteria	Runge-Kutta		
	100	1000	10000
total time	16.30 s	25.88 s	138.60 s
RK time	0.57 s	6.82 s	85.71 s
sat time	0.54 s	4.82 s	39.22 s

TABLE V. Time consumption in CPU time for Runge-Kutta solver for different saturation criteria. The total time corresponds to the execution time of the whole benchmark, the solver time at the time spent in Bateman equation solving by Runge-Kutta (RK time) or the solver for saturated isotopes (sat time).

solver order	CRAM			
	4	8	16	32
total time	11.18 s	12.14 s	13.96 s	17.05 s
solver time	1.87 s	2.72 s	4.41 s	7.73 s

TABLE VI. Time consumption in CPU time for CRAM solvers at different orders. The total time corresponds to the execution time of the whole benchmark, the solver time at the time spent in Bateman equation solving by CRAM.

Execution of the OCDE benchmark was done on a Intel®

Xeon® CPU E5-2620 processor at 2.10 Ghz on Linux system.

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

In Runge-Kutta scheme, the solver for saturated isotopes is not yet completely optimized.

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.

V. CONCLUSIONS

CRAM solver is now available in MENDEL.

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. And if we want to obtain a better accuracy with Runge-Kutta by reducing the number of saturated isotopes, CRAM is very competitive in time.

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

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