Business from technology

Higher-order Chebyshev Rational Approximation Method (CRAM) and application to Burnup Calculations

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Outline

- Burnup equations and matrix exponential solution
- Characteristics of burnup matrices
- Chebyshev Rational Approximation Method (CRAM)
- Computation of CRAM approximations
- Accuracy considerations
- Example results

Burnup equations

- Form a system of ordinary differential equations:

$$\boldsymbol{n}' = \boldsymbol{A}\boldsymbol{n} \; , \quad \boldsymbol{n}(0) = \boldsymbol{n}_0 \; , \tag{1}$$

- Matrix exponential solution

$$\boldsymbol{n} = e^{\boldsymbol{A}t}\boldsymbol{n}_0 \tag{2}$$

- There are various numerical algorithms but many of them are computationally expensive and of dubious numerical quality [1]

[1] C. MOLER and C. VAN LOAN, *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later, SIAM Rev.*, **45** (2003).

Burnup matrix

- Contains both positive (off-diagonal) and negative (diagonal) elements
- Extreme cases encountered:
  - Size $\sim 1700 \times 1700$
  - Norm
$$\|\boldsymbol{A}\| \sim 10^{21}$$
  - Eigenvalues
$$|\lambda| \in [0, 10^{21}]$$
  - Timestep
$$t \sim 10^1 \ldots 10^7 \text{ s}$$

$\Rightarrow$ Matrix exponential usually not computed for a full system!

  - In ORIGEN short-lived nuclides are removed from the burnup matrix before computing the matrix exponential solution

Rational approximation of matrix exponential

- Eigenvalue decomposition (General case: Jordan form)
  - $\boldsymbol{A} = \boldsymbol{T}\boldsymbol{\Lambda}\boldsymbol{T}^{-1}$

$$\Rightarrow \; e^{\boldsymbol{A}t} = \boldsymbol{T}\, e^{\boldsymbol{\Lambda}\,t}\boldsymbol{T}^{-1} \quad \text{and} \quad r(\boldsymbol{A}t) = \boldsymbol{T}\, r(\boldsymbol{\Lambda}t)\, \boldsymbol{T}^{-1}$$

- Approximate $e^{\boldsymbol{A}t}$ by $r(\boldsymbol{A}t)$, where $r(z)$ approximates e^z at the *eigenvalue*s of $\boldsymbol{A}$

- Example: Matlab's matrix exponential function `expm` based on Padé approximation
  - Approximation accurate near the origin

  $\Rightarrow$ Not applicable to burnup matrices when short-lived nuclides are included

Burnup matrix eigenvalues

- Burnup matrix eigenvalues are bounded near the negative real axis [2]
- Burnup matrices are connected with the class of singular M-matrices [3]
- Wedge condition for the spectrum around the negative real axis [3]

$$\Lambda(\boldsymbol{A}) \subset W_n = \left\{ z = re^{i\theta} \,\middle|\, r > 0\,, |\theta| \geq \frac{\pi}{2} + \frac{\pi}{n} \right\} \tag{3}$$

⇒ To compute the matrix exponential, rational approximation accurate near the negative real axis should be chosen.

[2] M. PUSA and J. LEPPÄNEN, *Computing the Matrix Exponential in Burnup Calculations, Nucl. Sci. Eng.*, **164**, 2, 140–150 (2010)

[3] M. PUSA *Numerical Methods for Nuclear Fuel Burnup Calculations* D.Sc. Thesis, Aalto University (2013). (VTT Science 32)

Chebyshev Rational Approximation Method (CRAM)

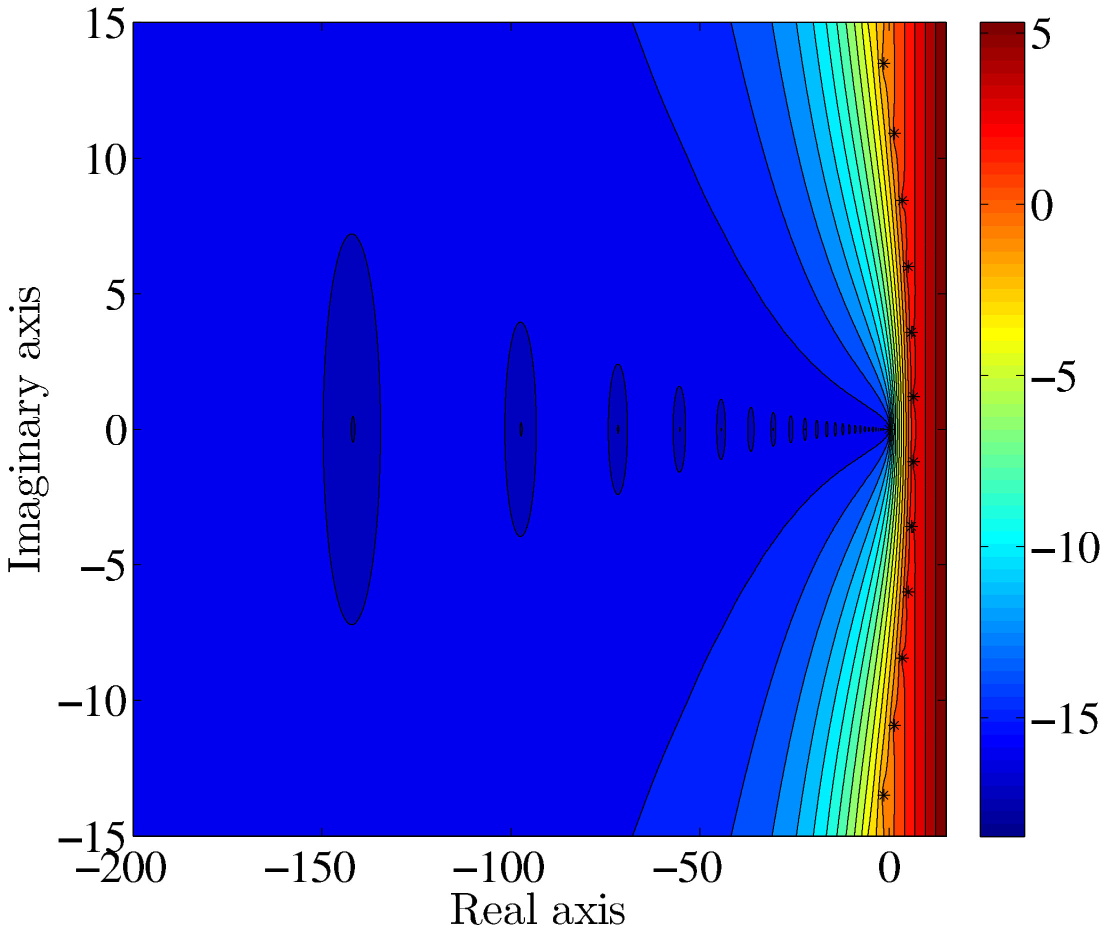
- CRAM approximation of order k is defined as the unique rational function $\hat{r}_{k,k}$ such that

$$\hat{\varepsilon}_{k,k} = \sup_{-\infty < x \leq 0} |\hat{r}_{k,k}(x) - e^x| = \inf_{r_{k,k} \in \pi_{k,k}} \left\{ \sup_{-\infty < x \leq 0} |r_{k,k}(x) - e^x| \right\} . \quad (4)$$

- It can be characterized as the *best rational approximation on the negative real axis*

Accuracy of the CRAM approximation of order 16 in the complex plane

$$\log_{10}|e^z - \hat{r}_{16,16}(z)|$$



Computation of CRAM approximations

- Determining best rational approximations is difficult
  - Requires tailored algorithms and high-precision arithmetics.
  - Polynomial coefficients for approximation orders $1, \ldots, 30$ computed previously and published with 20 digits of accuracy:

    A. J. CARPENTER, A. RUTTAN, and R. S. VARGA, *Extended Numerical Computations on the '1/9' Conjecture in Rational Approximation Theory, Rational Approximation and Interpolation* in *Lecture Notes in Mathematics*, Vol. 1105, 383–411, P. R. Graves-Morris, E. B. Saff, and R. S. Varga, Eds., Springer-Verlag (1984).

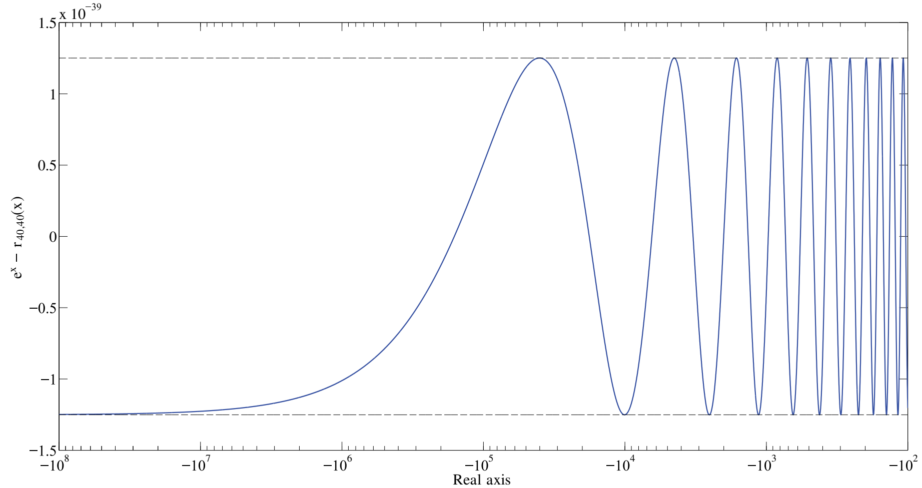
- To compute $\hat{r}_{k,k}(\boldsymbol{A}t)$, where $\hat{r}_{k,k}(z) = \hat{p}_k(z)/\hat{q}_k(z)$, the zeros of $\hat{q}_k(z)$ need to be known with a high accuracy

- Coefficients by Carpenter et al. enable computation of the poles for approximations up to order 16.

  $\Rightarrow$ Highest-order of CRAM considered previously for computing the matrix exponential

Determining best approximations

- Error functions corresponding to best approximations equi-oscillate



- Remez algorithm

1. Assume $\{t_i\}_{i=1}^{2k+2} \subset [-1,1]$ and find real polynomials p_k and q_k and a parameter $\varepsilon > 0$ such that

$$e^{\phi(t_i)} - \frac{p(\phi(t_i))}{q(\phi(t_i))} + (-1)^i \varepsilon = 0 \,, \quad i = 1, \ldots, 2k+2 \,, \tag{5}$$

where $q_{k+1} = 1$.

2. Assume $r_{k,k} \in \pi_{k,k}$ and $\varepsilon > 0$ and find the $2k+2$ local extreme points of the function

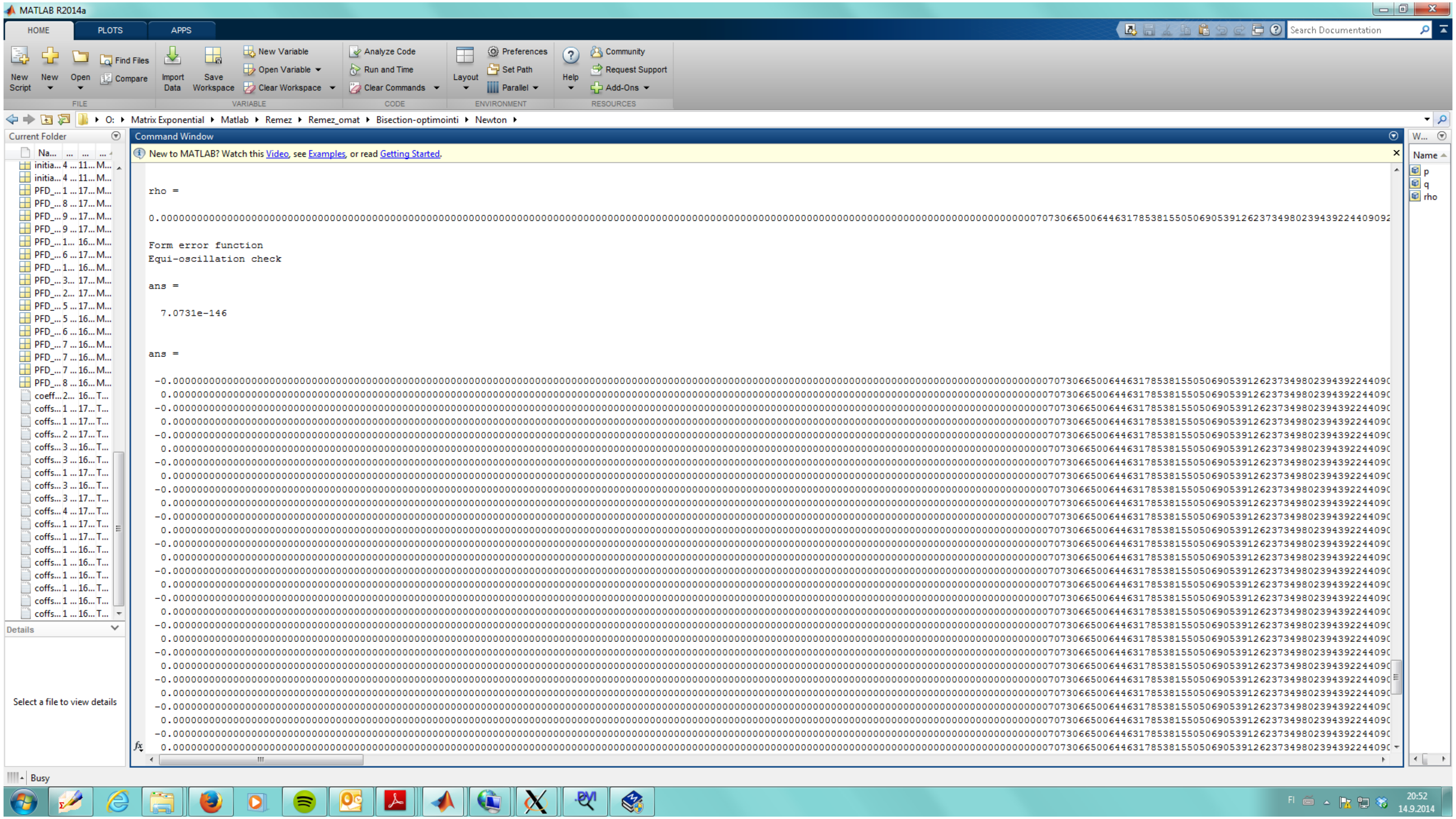
$$E(t) = e^{\phi(t)} - r_{k,k}(\phi(t)) \tag{6}$$

in the interval $[-1,1]$.

Implementation of Remez algorithm

- Remez algorithm was implemented using Matlab's Symbolic Toolbox with high-precision arithmetics (`vpa`)
- CRAM coefficients were computed for approximation orders $2, 4, \ldots, 50$.
  - Computation of approximation of order 50 (1000 digits, tolerance 10^{-200}) took 1 hour 10 minutes CPU time in Matlab.
  - In 1984, *one Newton update* took 15 hours CPU time (230 digits, tolerance 10^{-200}) for approximation order 30!

Implementation of Remez algorithm



Accuracy of CRAM

- CRAM of order 16 can provide very accurate and efficient solution to burnup equations without the need to exclude any nuclides [2, 4]
- Accuracy of CRAM or order k is compromised if a nuclide concentration diminishes significantly during the time step [5].
  - Cut-off $\approx 10^{-k} n_i(0)$
- Approximation order of CRAM should be selected according to [6]

$$k > \max_i \left(\log_{10} \left\{ \frac{n_i(0)}{\max\{e^{A_{ii}t} n_i(0), 10^{-s}\}} \right\} + d \right) , \tag{7}$$

where

- Nuclide concentrations smaller than 10^{-s} can be treated as zero
- Result is wanted with d digits of accuracy

[2] M. PUSA and J. LEPPÄNEN, *Computing the Matrix Exponential in Burnup Calculations, Nucl. Sci. Eng.*, **164**, 2, 140–150 (2010)

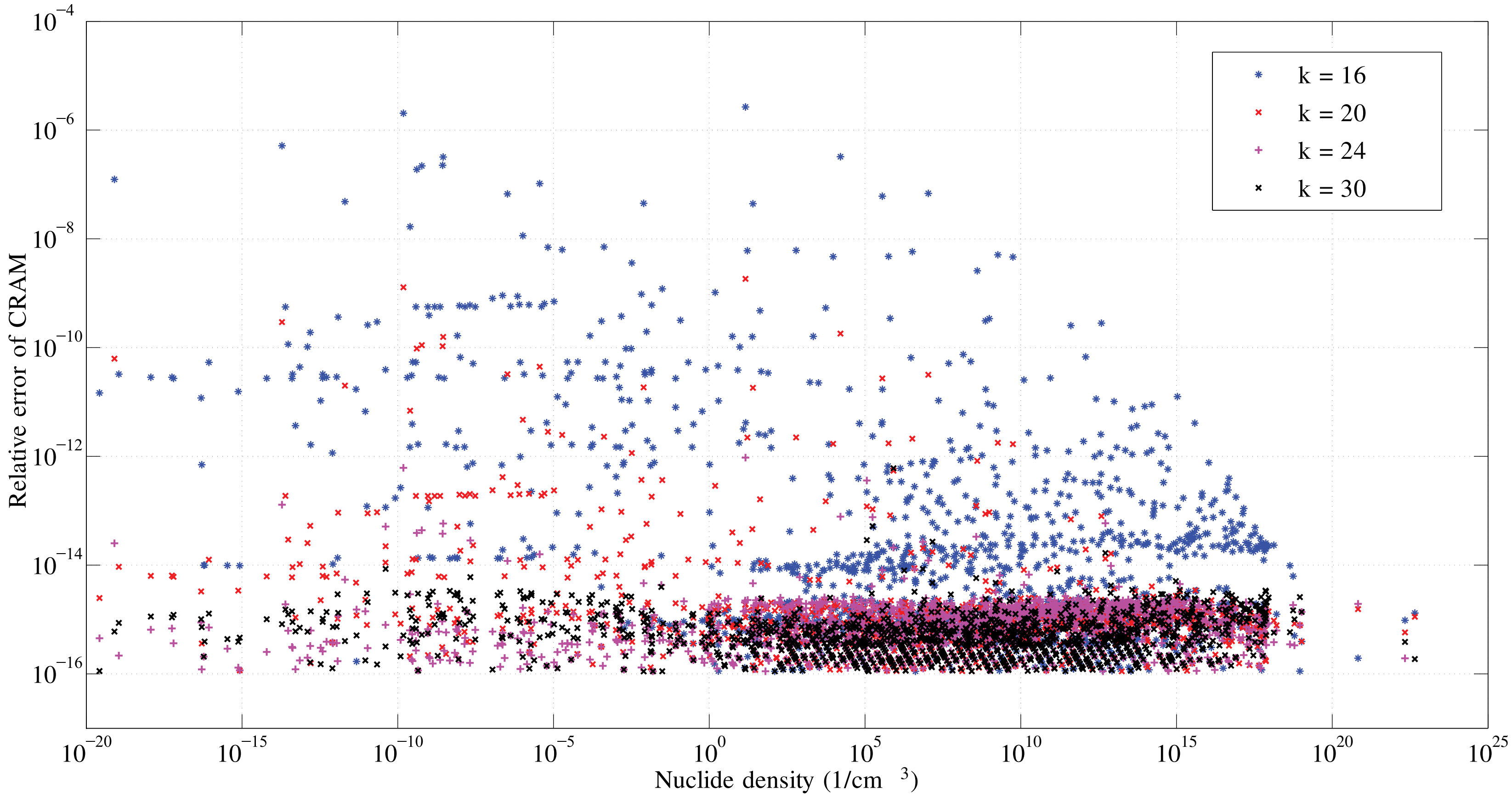
[4] A. ISOTALO and P. A. AARNIO, *Comparison of depletion algorithms, Ann. Nucl. Energy*, **38**, 2–3, 261–268 (2011).

[5] M. PUSA *Accuracy Considerations for Chebyshev Rational Approximation Method (CRAM) in Burnup Calculations* In proc. M&C 2013, Sun Valley, ID, May 5-9, 2013.

[6] M. PUSA *Higher-Order Chebyshev Rational Approximation Method (CRAM)* In Proc. PHYSOR 2014, Kyoto, Japan, Sept 28 – Oct. 3 (2014).

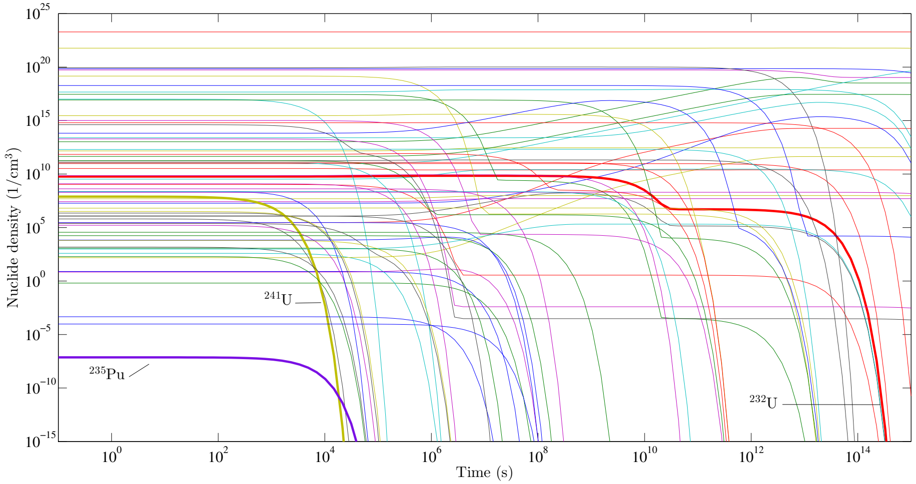
Example: burnup system with 1606 nuclides

- PWR pin-cell lattice irradiated to 0.1 MWd/kgU, $t = 12.5$ days



Example: Decay system with 1531 nuclides

- In the absence of neutron irradiation, some of the nuclide concentrations tend fast to zero

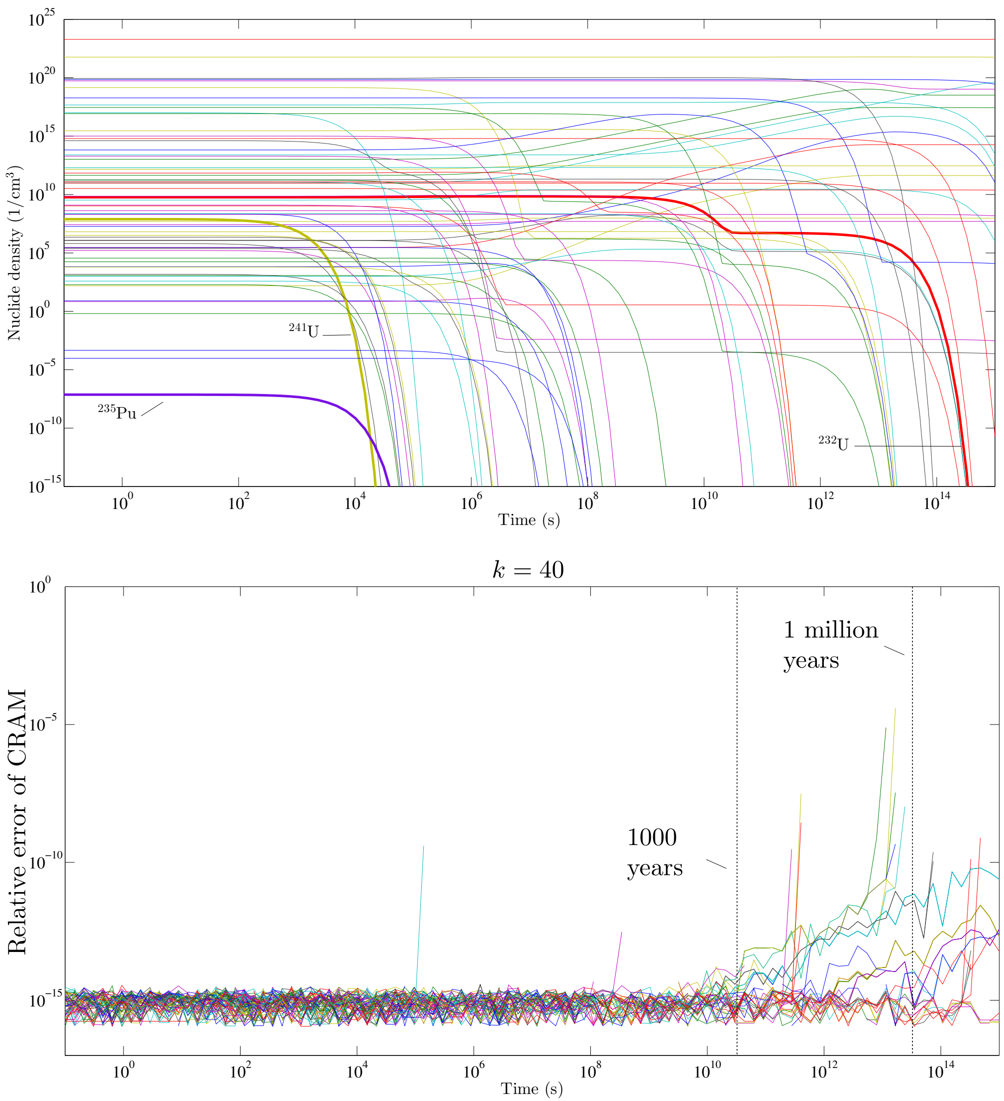


- Define cut-off $10^{-15} 1/\text{cm}^3$ (single nuclide in a cubic km)

$\Rightarrow$ Accuracy considerations:

  – For $t < 10^4$ s, low approximation orders can be used
  – To reach 5 digits of accuracy, approximation order $k = 36$ is required for $t = 10^5$ s and $k = 40$ for $t = 10^{15}$ s$= 32$ million years
  – For $k = 44$, time-step can be extended to infinity without compromising the accuracy of the solution!

Example: Decay system with 1531 nuclides



Summary

- The computation of matrix exponential has been considered challenging in the context of burnup equations
- Burnup matrix eigenvalues were discovered to lie around the negative real axis and CRAM can be characterized as the best rational approximation there
- Computation of CRAM approximations is difficult

  $\Rightarrow$ Approximations up to order 16 considered previously
- Coefficients computed recently for approximation orders $2, 4, \ldots, 50$ based on Remez algorithm.
- CRAM of order 16 can provide very accurate solution to burnup equations without excluding any nuclides
- Higher-orders of CRAM enable accurate simulation of decay systems for time steps of the order of millions of years.

Further reading

- M. PUSA and J. LEPPÄNEN, *Computing the Matrix Exponential in Burnup Calculations, Nucl. Sci. Eng.*, **164**, 2, 140–150 (2010)
- M. PUSA, *Rational approximations to the matrix exponential in burnup calculations, Nucl. Sci. Eng.*, **169**, 2, 155–167 (2011)
- M. PUSA, *Correction to partial fraction decomposition coefficients for Chebyshev rational approximation on the negative real axis*, `arXiv:1206.2880v1 [math.NA]` (2012).
- M. PUSA *Accuracy Considerations for Chebyshev Rational Approximation Method (CRAM) in Burnup Calculations* In proc. M&C 2013, Sun Valley, ID, May 5-9, 2013.
- M. PUSA and J. LEPPÄNEN, *Solving linear systems with sparse Gaussian elimination in the Chebyshev rational approximation method (CRAM)*, Nucl. Sci. Eng., **175** (2013) 250-258.
- M. PUSA, *Numerical methods for nuclear fuel burnup calculations*, D.Sc. Thesis, Aalto University, VTT Science 32 (2013). `http://montecarlo.vtt.fi/download/S32.pdf` (2013).
- M. PUSA *Higher-Order Chebyshev Rational Approximation Method (CRAM)* In Proc. PHYSOR 2014, Kyoto, Japan, Sept 28 – Oct. 3 (2014).