Solving Burnup Equations in Serpent:

Matrix Exponential Method CRAM

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Outline

- Burnup equations and matrix exponential solution
- Characteristics of burnup matrices
- Established matrix exponential methods
- Chebyshev Rational Approximation Method (CRAM)
- Implementation in Serpent
- Numerical results

Burnup equations

- Form a system of ordinary differential equations:

$$\frac{dn_i}{dt} = -(\lambda_i + \sigma_i)n_i + \sum_{j \neq i} (\gamma_i \, \sigma_{\mathrm{f}}^j \phi + \lambda^{j \to i} + \sigma^{j \to i} \phi) n_j \tag{1}$$

- Matrix form

$$\boldsymbol{n}' = \boldsymbol{A}\boldsymbol{n} \; , \quad \boldsymbol{n}(0) = \boldsymbol{n}_0 \; , \tag{2}$$

- Matrix exponential solution

$$\boldsymbol{n} = e^{\boldsymbol{A}t} \boldsymbol{n}_0 \tag{3}$$

Matrix exponential

- Definition

$$e^{\boldsymbol{A}t} = \sum_{k=0}^{\infty} \frac{1}{k!} (\boldsymbol{A}t)^k \tag{4}$$

- Diagonalizable matrices

$$e^{\boldsymbol{A}t} = \boldsymbol{V} e^{\boldsymbol{\Lambda}t} \boldsymbol{V}^{-1}\,, \quad \boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{-1} \tag{5}$$

- 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

- Non-diagonalizable
- 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

$$t \sim 10^{1} \ldots 10^{6} \text{ s}$$

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

Established matrix exponential methods

- Truncated Taylor series based approximation
- Scaling and squaring

$$e^{\boldsymbol{A}} = (e^{\boldsymbol{A}/m})^m \,, \quad m = 2^k \tag{6}$$

- ORIGEN based on truncated Taylor series with scaling and squaring
  - Short-lived nuclides treated separately!
- Padé approximation
  - rational approximation near the origin
  - MATLAB matrix exponential function `expm` based on Padé approximation with scaling and squaring

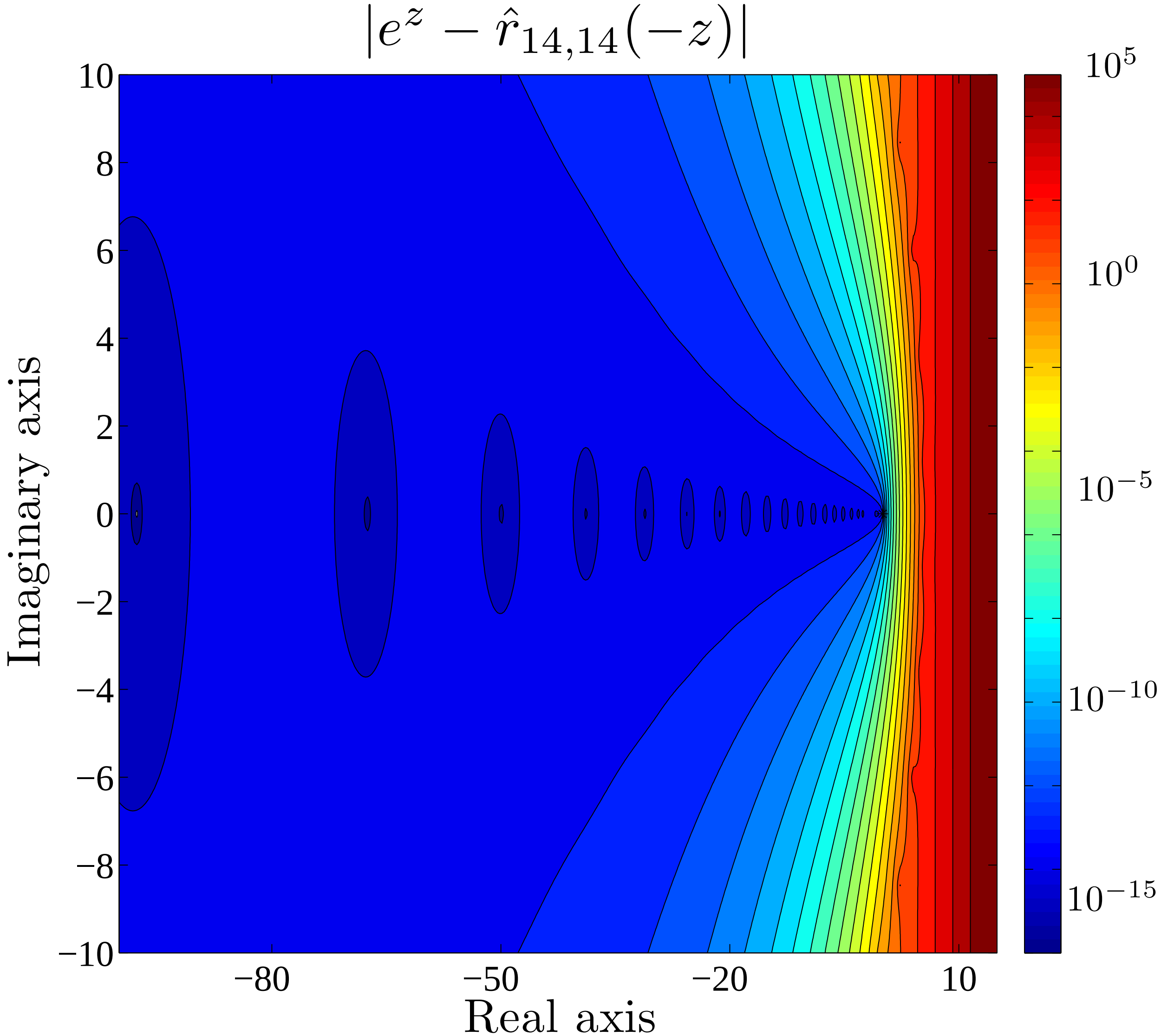
Chebyshev Rational Approximation Method (CRAM)

- Burnup matrix eigenvalues confined to a region near the negative real axis!
  - Real parts of eigenvalues non-positive (stable system)
  - Fraction of the eigenvalues have small imaginary parts ($\sim 10^{-8}$ or smaller)
- CRAM approximation of order k is is defined as the unique rational function $\hat{r}_{k,k}$ such that

$$\sup_{-\infty<x\leq 0} |\hat{r}_{k,k}(-x) - e^x| = \inf_{r_{k,k}\in\pi_{k,k}} \left\{ \sup_{-\infty<x\leq 0} |r_{k,k}(-x) - e^x| \right\} . \quad (7)$$

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

Accuracy of the CRAM approximation of order 14 in the complex plane



Implementation (1)

- The rational approximation is computed using partial fraction form
  - Scalar function

$$r_{k,k}(x) = \frac{p_k(x)}{q_k(x)} = \alpha_0 + 2\,\mathrm{Re}\left(\sum_{j=1}^{k/2} \frac{\alpha_j}{x - \theta_j}\right) \tag{8}$$

  - Matrix function

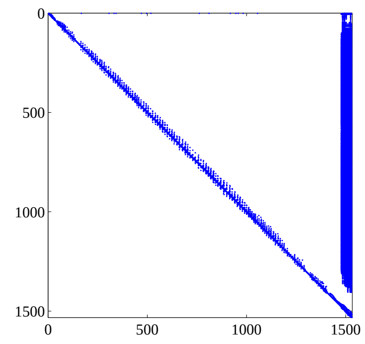
$$\boldsymbol{n} \approx r_{k,k}(\boldsymbol{A}t)\boldsymbol{n}_0 = \alpha_0 \boldsymbol{n}_0 + 2\,\mathrm{Re}\left(\sum_{j=1}^{k/2} \alpha_j (\boldsymbol{A}t - \theta_j \boldsymbol{I})^{-1} \boldsymbol{n}_0\right) . \tag{9}$$

$\Rightarrow$ Only solving a set of linear equations is required in addition to the partial fraction coefficients

$\Rightarrow$ Computation of approximation of order k takes $k/2$ matrix inversions

Implementation (2)

- Matrix sparsity pattern can be exploited in the inversion
- Matrix inversion in Serpent: symbolic LU factorization and Gaussian elimination on this factorization [3]
- Computational efficiency:
  - Example: for a system with ~ 1300 nuclides, CRAM of order 6 takes 0.06 s and CRAM of order 16 takes 0.1 s
  - The order of approximation can be adjusted to suit needs for accuracy and speed



[2] R. E. TARJAN, *Graph Theory and Gaussian Elimination,* Tech. Rep. CS-TR-75-526, Stanford University, Department of Computer Science,

Stanford, CA, USA (1975).

Implementation (3)

- Originally only approximation order 14 was implemented into Serpent
  - Partial fraction coefficients taken from [3]
- These coefficients were later discovered to be inaccurate
- New sets of partial fraction coefficients have been computed for approximation orders 6, 8, 10, 12, 14 and 16 [4]

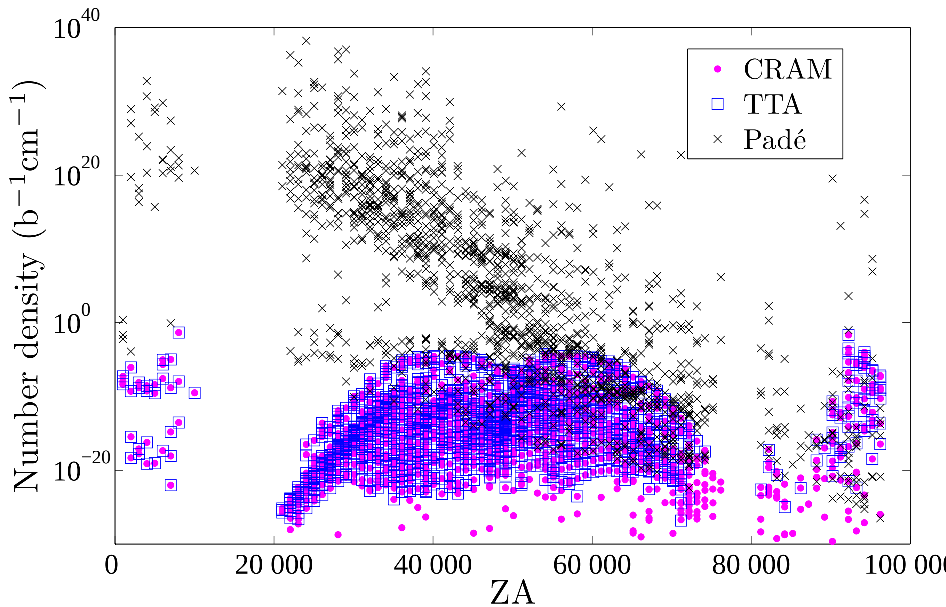
  $\Rightarrow$ These approximation orders are implemented in Super-Serpent

[3] E. Gallopoulos, and Y. Saad *Efficient Solution of Parabolic Equations by Krylov Approximation Methods, SIAM J. Sci. Stat. Comput.*, **13**, 5, 1236–1264 (1992).

[4] M. PUSA, *Rational Approximations to the Matrix Exponential in Burnup Calculations, Nucl. Sci. Eng.*, **169**, 2, 155–167 (2011)

Numerical Results (1)

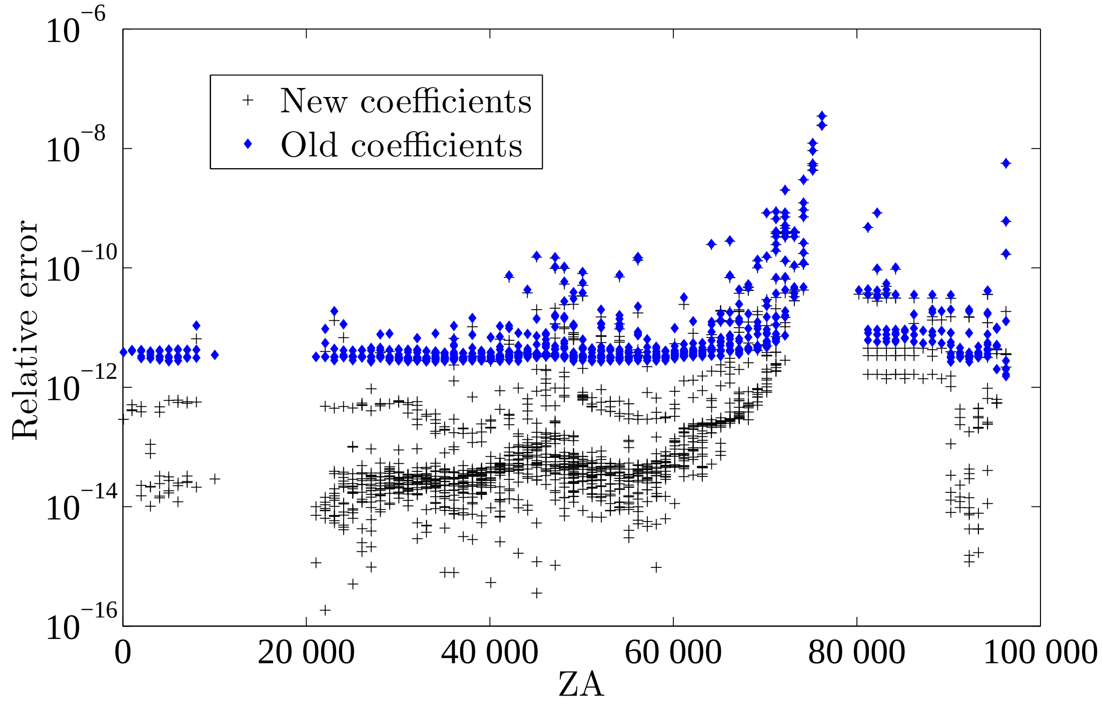
- PWR pin cell lattice irradiated to 25 MWd/kgU burnup [5]
- $\boldsymbol{A} \in \mathbb{R}^{1532\times 1532}$, $\|\boldsymbol{A}\| \sim 10^{21}$, $t \sim 10^{6}$ s



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

Numerical Results (2)

- Relative error of CRAM approximation of order 14 for the same test case [4]



[4] M. PUSA, *Rational Approximations to the Matrix Exponential in Burnup Calculations, Nucl. Sci. Eng.*, **169**, 2, 155–167 (2011)

Numerical Results (3)

- Convergence results for the same test case [4]

Approximation order	Mean error	Maximum error	Mean relative error	Maximum relative error
2	3.3901×10^{-7}	3.3110×10^{-4}	8.3015×10^{-2}	1.9561×10^{0}
4	4.0252×10^{-9}	3.8736×10^{-6}	5.6140×10^{-3}	6.3820×10^{-1}
6	4.7339×10^{-11}	4.5163×10^{-8}	2.2452×10^{-4}	3.8184×10^{-2}
8	5.5808×10^{-13}	5.2486×10^{-10}	7.1664×10^{-6}	1.5762×10^{-3}
10	6.5685×10^{-15}	6.0944×10^{-12}	1.9529×10^{-7}	5.1640×10^{-5}
12	7.6474×10^{-17}	6.9690×10^{-14}	4.7280×10^{-9}	1.4323×10^{-6}
14	9.5452×10^{-19}	9.5339×10^{-16}	1.0384×10^{-10}	3.4990×10^{-8}
16	2.0748×10^{-19}	1.6377×10^{-16}	2.1196×10^{-12}	7.7286×10^{-10}

[4] M. PUSA, *Rational Approximations to the Matrix Exponential in Burnup Calculations*, *Nucl. Sci. Eng.*, **169**, 2, 155–167 (2011)

General observations

- Generally the accuracy of CRAM depends relatively little on burnup matrix size or norm
- Typically CRAM yields better relative accuracy for depleted fuel cases compared to fresh fuel cases
- Particular nuclide chains may result in reduced relative accuracy for some nuclides with low approximation orders
- For CRAM approximation order 16 the maximum relative error has been at most of order 10^{-6} in all test cases

Summary

- The computation of matrix exponential has been considered challenging in the context of burnup equations
- Established matrix exponential methods are based on approximation near origin
- Burnup matrix eigenvalues were discovered to lie around the negative real axis and CRAM can be characterized as the best rational approximation there
- Results suggest that CRAM is capable of providing a robust and accurate solution with a very short computation time
- Serpent was the first reactor physics code using this method

Further Reading

- Introduction to the topic and comparison between CRAM and established matrix exponential methods:
  - M. PUSA and J. LEPPÄNEN, *Computing the Matrix Exponential in Burnup Calculations, Nucl. Sci. Eng.*, **164**, 2, 140–150 (2010)
- More detailed analysis on the accuracy and convergence of CRAM:
  - M. PUSA, *Rational Approximations to the Matrix Exponential in Burnup Calculations, Nucl. Sci. Eng.*, **169**, 2, 155–167 (2011)
- Comparison between CRAM, ORIGEN and TTA-based methods:
  - A. Isotalo and P. A. Aarnio, *Comparison of depletion algorithms, Ann. Nucl. Energy*, **38**, 2–3, 261–268 (2011).