New Capabilities for the Chebyshev Rational Approximation method (CRAM)

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Chebyshev Rational Approximation Method (CRAM)*

• Fast, accurate depletion algorithm for large systems
  – Overall accuracy almost independent of step lengths

• Limitations
  – Cannot handle source term (model external feed)
  – Some concerns about decay reliability (nuclides whose concentration decreases greatly)

• In this presentation:
  – Solutions to these limitations
  – A method for extracting additional results

Source Term and External Feed

• External feed
  – Continuous flow of material to the modeled composition from outside the modeled composition
    • Molten salt reactors
    • Reprocessing facilities

• Source term models external feed

\[
\frac{d\mathbf{x}(t)}{dt} = A\mathbf{x}(t) + \mathbf{s}(t)
\]

– Also needed in adjoint calculations for time-integral responses (e.g., total absorption by a nuclide over time)
External Feed*

• CRAM only evaluates matrix exponential, $e^{At} x(0)$ which is the solution of a homogeneous system

• Solution: homogenize the system

$$\frac{d\mathbf{x}(t)}{dt} = A\mathbf{x}(t) + \mathbf{s}(t) \quad \Rightarrow \quad \frac{d\tilde{\mathbf{x}}(t)}{dt} = \tilde{A}\tilde{\mathbf{x}}(t)$$

  – Constant or exponentially decreasing source term does not affect overall accuracy
  – Polynomial source term reduces maximum accuracy by roughly one digit per order of the highest order polynomial

Substeps*

- Accuracy of CRAM improves rapidly over steps with equal step length and microscopic reaction rates
  - Divide steps into equidistant substeps
  - Improvement is not driven by (sub)step lengths!

- Substeps multiply the number of CRAM solutions required

- Reuse LU-decompositions on substeps:
  - 2/4/8 substeps increase cost by 25/50/100%
  - We call these internal substeps

Extracting Integral Results*

- Add imaginary “tally nuclides” that are produced in proportion to the concentrations of the physical nuclides without the parent being removed

- The final concentration of such nuclide is

\[ d_j(T) = \int_0^T \sum w_{j,i} x_i(t) \, dt \]

- Number of fissions tally: \( w_i = \sigma_{i,f} \phi \)
  - Fuel performance codes

- Energy release tally: \( w_i = \sum K_{i,r} \sigma_{i,r} \phi + \lambda_i K_{i,d} \)
  - Local burnups, coupling diagnostics

Energy Release in Burnup Calculations

• Constant power (input) × step length (input) → burnup

• In depletion: power → average flux → composition
  – Not exact
  – Burnup of the compositions differs from assumed

• Tally nuclide for energy release gives the burnup of the compositions
  – A measure of normalization accuracy
  – Were step lengths short enough?
Results: Depletion of Fresh Fuel
Results: Depletion of Used Fuel

Initial, no substeps

Initial, 4 substeps

Feed, no substeps

Feed, 4 substeps
Results: Decay of Spent Fuel

Initial, no substeps

Initial, 4 substeps

Feed, no substeps

Feed, 4 substeps
Results: Order 6 Polynomial Feed Rate for $^{235}\text{U}$
Results with Lots of Substeps

Depletion of fresh fuel, 64 substeps

Depletion of used fuel, 4 substeps

Depletion of fresh fuel as feed, 64 substeps

Deca of used fuel, 32 substeps
Running Times

• Timings with new CRAM solver of ORIGEN
  – Uses the SuperLU library
  – Library data includes 1946 nuclides and 35,013 transitions
  – Basic depletion solution took 23ms on Intel Xeon E5-1607 and 41ms on AMD Optron 6212

• Source term for all nuclides
  – Depletion: ~10% + 2.5% per highest source term order
  – Decay: ~10% + 10% per highest source term order

• 2/4/8 substeps increase the total running time by roughly 25/50/100%
Running Times

• Tally nuclides:
  – Number of fissions: <1%
  – Energy released in depletion calculations: +8–10%
  – Energy released in decay calculations: +20–30%
  – Average concentrations of all nuclides
    • Decay calculations: +110–130%
    • Depletion calculations: +80–90%

• Other tallies can be constructed from average concentrations
  – Running time effect is never more than 80-130%.
Results: Burnup calculation

Cumulative normalization error and the error in the change to HM inventory with different coupling schemes when depleting a 2D PWR assembly segment with Gd rods.

The former is obtained by adding a single tally nuclide while determining the latter requires having an accurate reference solution.
Results: Burnup Calculation

Absolute errors in the Gd-155 and U-235 atomic densities with different coupling schemes when depleting a 2D PWR assembly segment with Gd rods.

Normalization is not the only error source so a small normalization error does not guarantee results to be all around accurate.
Summary

• New capabilities for CRAM
  – Source term
  – Improved accuracy
  – Evaluating integral results
  – Source term and tally nuclides are applicable with some other depletion algorithms in addition to CRAM

• This work was carried out with ORIGEN in SCALE
  – ORIGEN now has a CRAM solver
    • LU decompositions by the SuperLU–library
  – Presented features are not yet available in Serpent
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