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Importance of nuclear data for activation calculations of fusion systems and key differences from fission.

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Workshop on Applied Nuclear Data Activities (WANDA 2024)
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Outline

- Quick introduction to inventory solver mathematics
- Nuclear data as a graph
  - Transitive closure
  - Cycles – testing solvers
  - Show that CRAM, the matrix exponential, and BDF are on the transitive closure
- CRAM FISPACT (and further developments)
  - Some key FNS decay heat benchmark results

Inventory simulations

$$\frac{d}{dt}N_i = -N_i\lambda_i - N_i\sum_s \int_0^\infty \sigma_{is}(E)\phi(E)dE + \sum_{k\neq i} N_k \left(\lambda_{ki} + \int_0^\infty \sigma_{ki}(E)\phi(E)dE\right)$$

N is a list of the number of nuclides, ϕ is the projectile spectrum, σ is the cross sections and λ is the decay constant

$$\dot{\mathbf{N}}(t) = A\mathbf{N}(t)$$

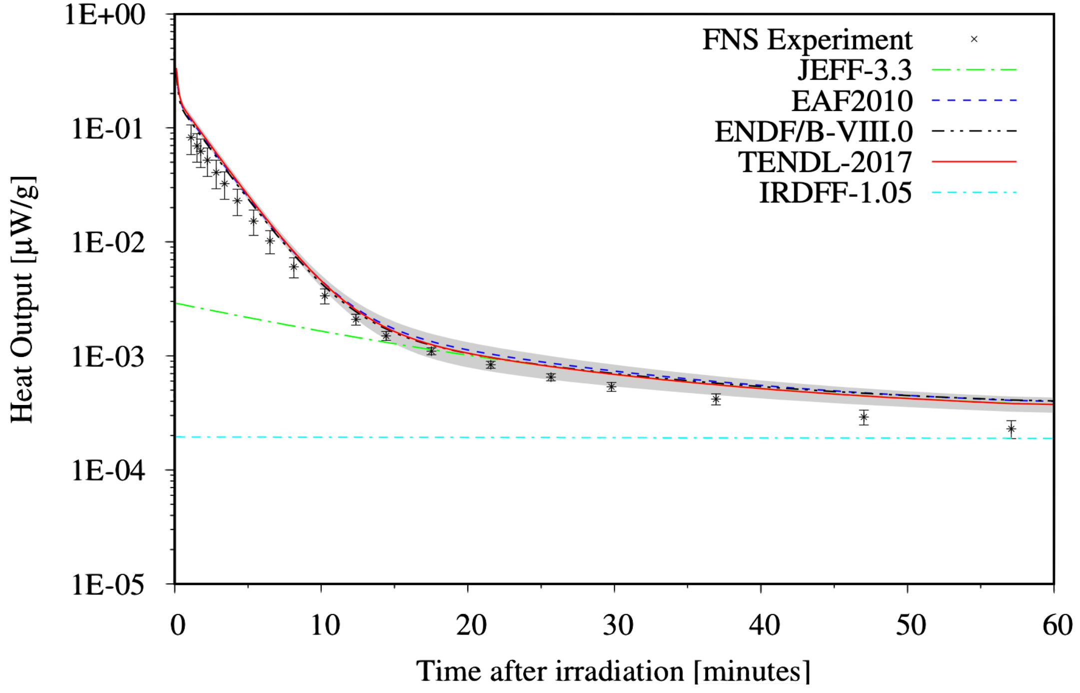
Solution:

$$N(t) = e^{At}N(t=0)$$

Where:

$$e^{At} = I + At + \frac{1}{2!}(At)^2 + \frac{1}{3!}(At)^3 + \ldots$$

Tungsten example



How do we approximate e^{At}

Chebyshev rational approximation method (CRAM)

$$\epsilon_{k,k} = \sup_{x\in\mathbb{R}_-} |\hat{r}_{kk}(x) - e^x| = \inf_{r_{kk}\in\pi_{kk}} \left\{ \sup_{x\in\mathbb{R}_-} |r_{kk}(x) - e^x| \right\}$$

Where: $r_{kk} = \dfrac{p_k(x)}{q_k(x)}$

Assumes that all the eigenvalues of A are (near to)/(along) the negative axis.

Error bounded by $\dfrac{\varepsilon_{k,k}(t)}{n_j(t)} = \epsilon_{k,k}\dfrac{n_i(0)}{n_j(t)}$

$$r_{kk}(At) = \alpha_0 + \sum_{j=1}^{k} \frac{\alpha_i}{At - \theta_j I}$$

M Pusa thesis: *Numerical methods for nuclear fuel burnup calculations*

Numerical integration

Derivatives are approximated by Taylor series

$$N(t+\Delta t) = N(t) + N'(t)\Delta t + \frac{N''(t)\Delta t^2}{2!} + .. + O(\Delta t^n)$$

Error bounded by $O(\Delta t^n)$

FISPACT-II
Backwards difference formula (BDF)

$$\sum_k a_k N_{n+k} = h\beta N_{n+s}$$

Nuclear Data as a graph: decay ⊕ activation

Adjacency matrix

Algebraic representation of the graph G(A).

$$A_{ji} = \begin{cases} 1 & \text{if } A_{ij}^{\text{coeff}} > 0 \text{ and } i \neq j \\ 0 & \text{else.} \end{cases}$$

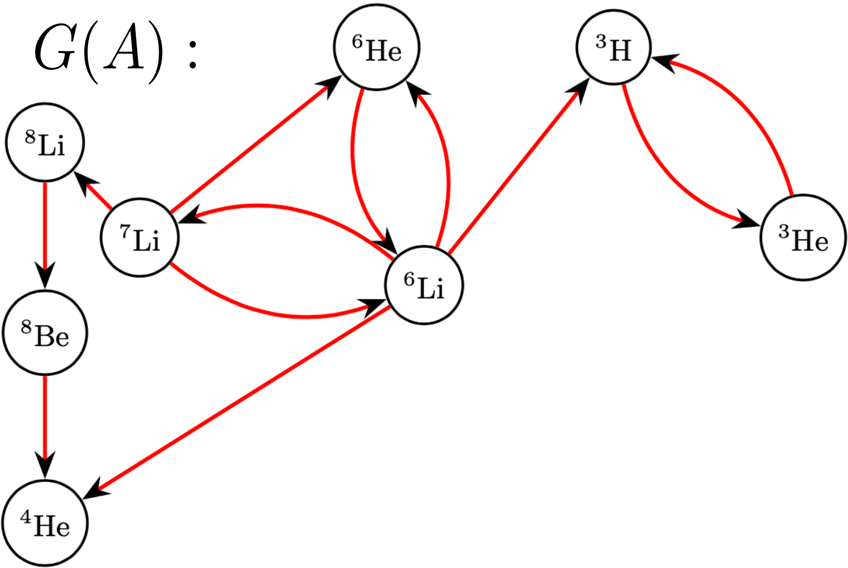
$$A_{\text{zai}} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

Nuclide graph

$$G(A) = (V, E), \text{ where}$$

$$V = \{\text{nuclides}_i | i = 1..n\} \text{ and}$$

$$E = \{(i, j) \in V \times V : a_{ij} \neq 0\}.$$



Neutron irradiation of natural Lithium, this data is built from the collapse of Tendl19 with an FNS flux.

Transmutation paths

Transitive closure:

$$A_m^+ = A + A^2 + A^3 \ldots + A^m \in \mathbb{R}^n \times \mathbb{R}^n$$

A matrix detailing if there is a directed path, of up to length m, from nuclide i to nuclide j.

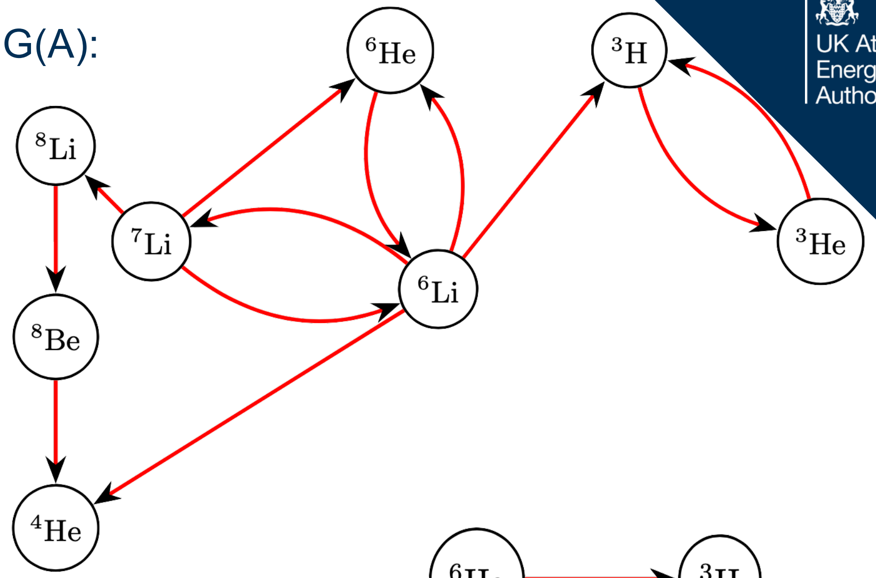
- A^+_m is a function of irradiation

Exponential matrix:

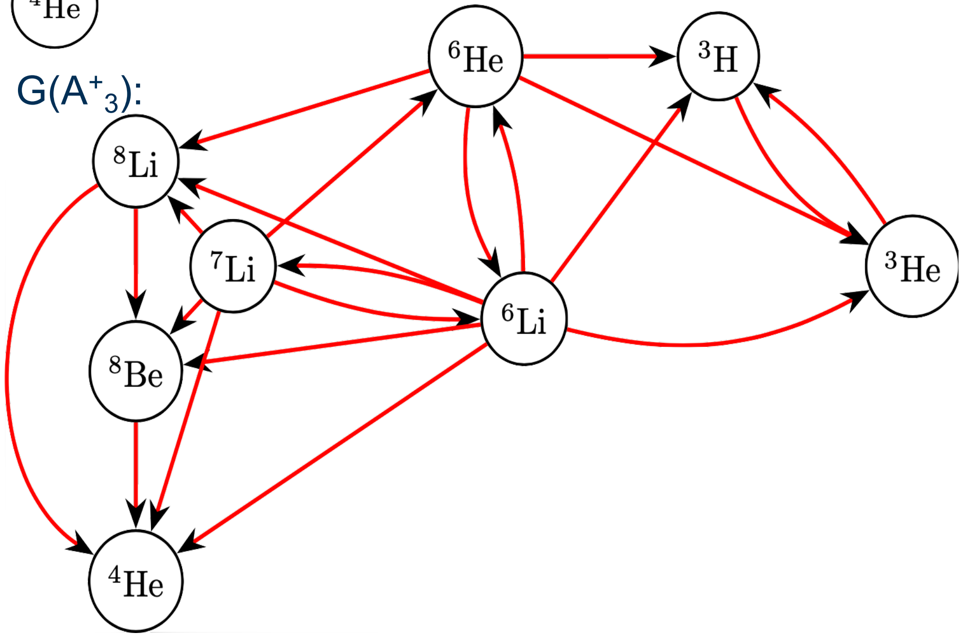
The graph of the exponential matrix is the transitive closure of A

$$e^{At} = I + At + \frac{1}{2!}(At)^2 + \frac{1}{3!}(At)^3 + \ldots$$

G(A):



G(A^+_3):

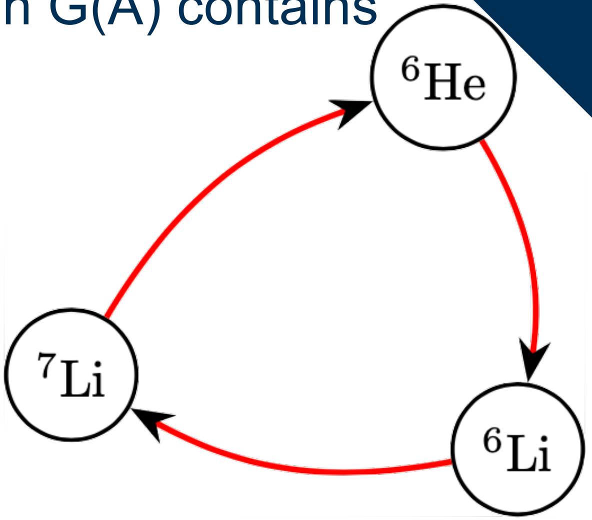


Complex eigenvalues – cycles in the data

The number of closed cycles, of length s, that the directed graph G(A) contains can be counted as:

$$l_s = \frac{1}{s}\mathrm{Tr}(A^s)$$

This is important because if $l_3 \neq 0$ G(A) must contain at least one directed triangle ∴.



$$PA^{\mathrm{coeff}}_{\mathrm{sub}}P^T = \begin{pmatrix} -a & 0 & c \\ a & -b & 0 \\ 0 & b & -c \end{pmatrix}$$

Which has one complex eigenvalue if a≈b and c<<1

$$N(t) = c_1 v_1 e^{i\omega t} + \dots$$

Deviation away from CRAM regions of approximation, $\mathbb{R}_-$

CRAM's graph

$$r_{kk}(At) = \alpha_0 + \sum_{j=1}^{k} \frac{\alpha_i}{At - \theta_j I}$$

If ∃ a path from p to q in G(A) of length l then:

$$(A)^l_{pq} \neq 0$$

Cayley-Hamilton method

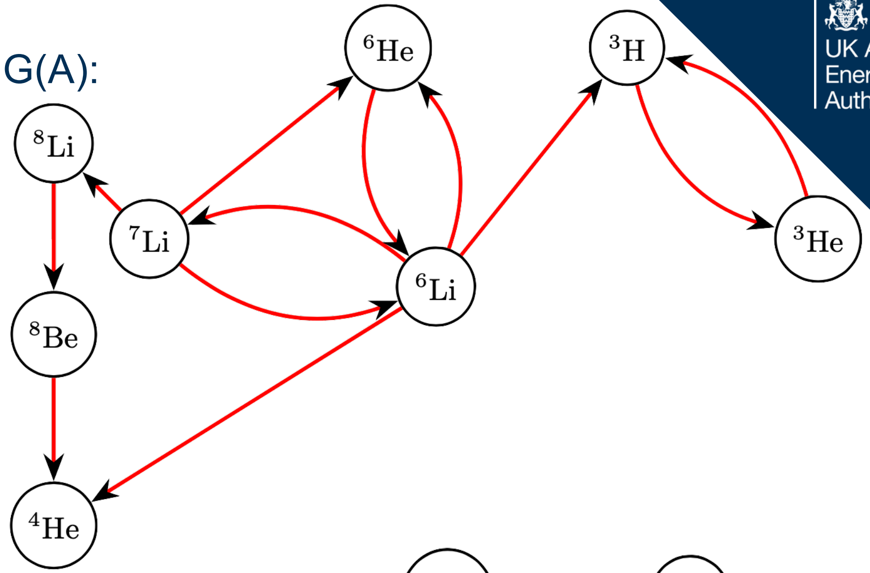
$$A^{-1} = \boxed{\frac{1}{\det(A)}} \boxed{\sum_{s=0}^{n-1} A^s} \boxed{\sum_{k1,k_2,k_{n-1}} \prod_{l=1}^{n-1} \frac{(-1)^{k_l+1}}{l^{k_l} k_l!}} \boxed{\mathrm{Tr}(A^l)^{k_l}}$$

Number

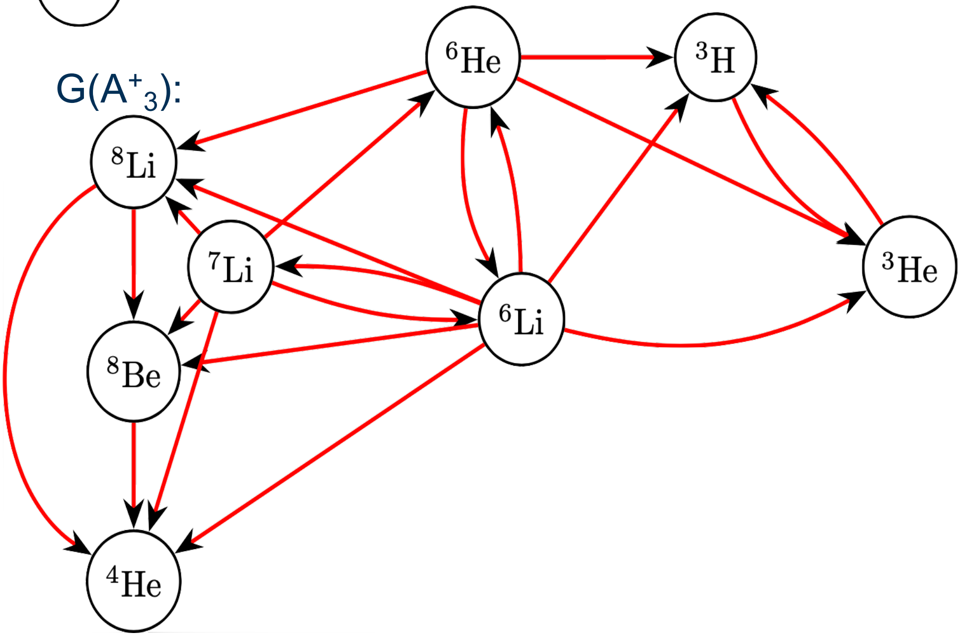
$$\therefore (A^{-1})_{pq} \neq 0$$

CRAM is on the transitive closure of A

G(A):



G(A$^+_3$):



Numerical integration

Euler integration (explicit integrator)

(*this is an example and not globally a good approach*).

$$N_{t+1} = (A\Delta t + I)N_t$$

$$N(t=0) = ({}^{7}\mathrm{Li} = x, {}^{6}\mathrm{Li} = y, 0, 0,)^{\mathrm{T}}$$

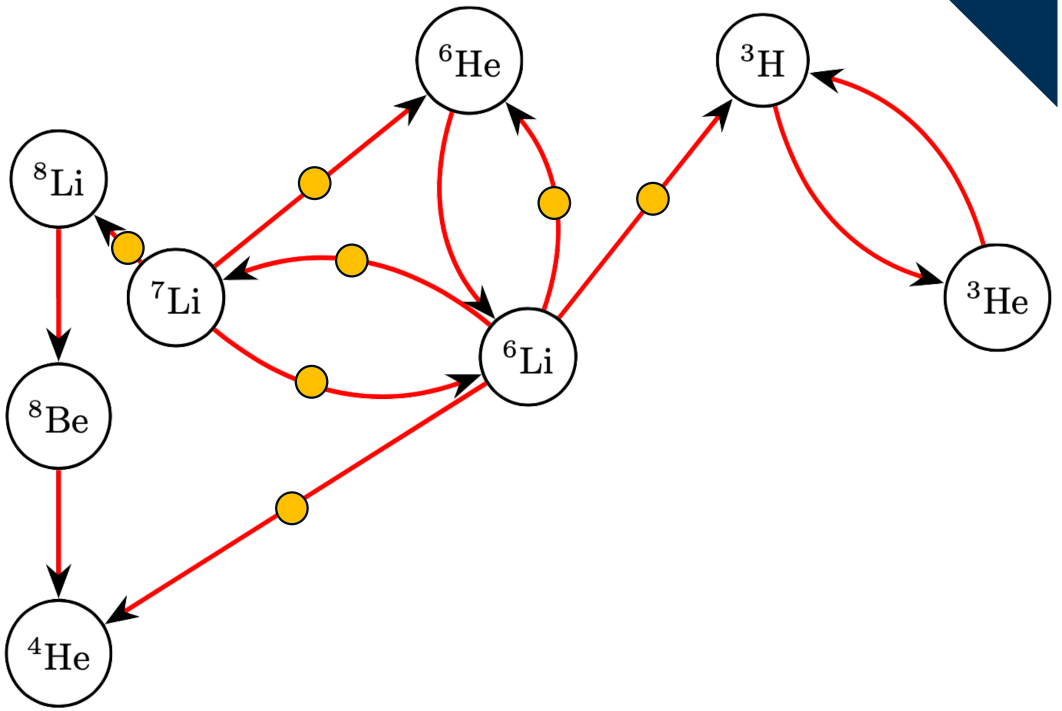
- Switches on the ● edges
- Next set of edges get switched on the next iteration

Backwards difference formula (implicit integrator):

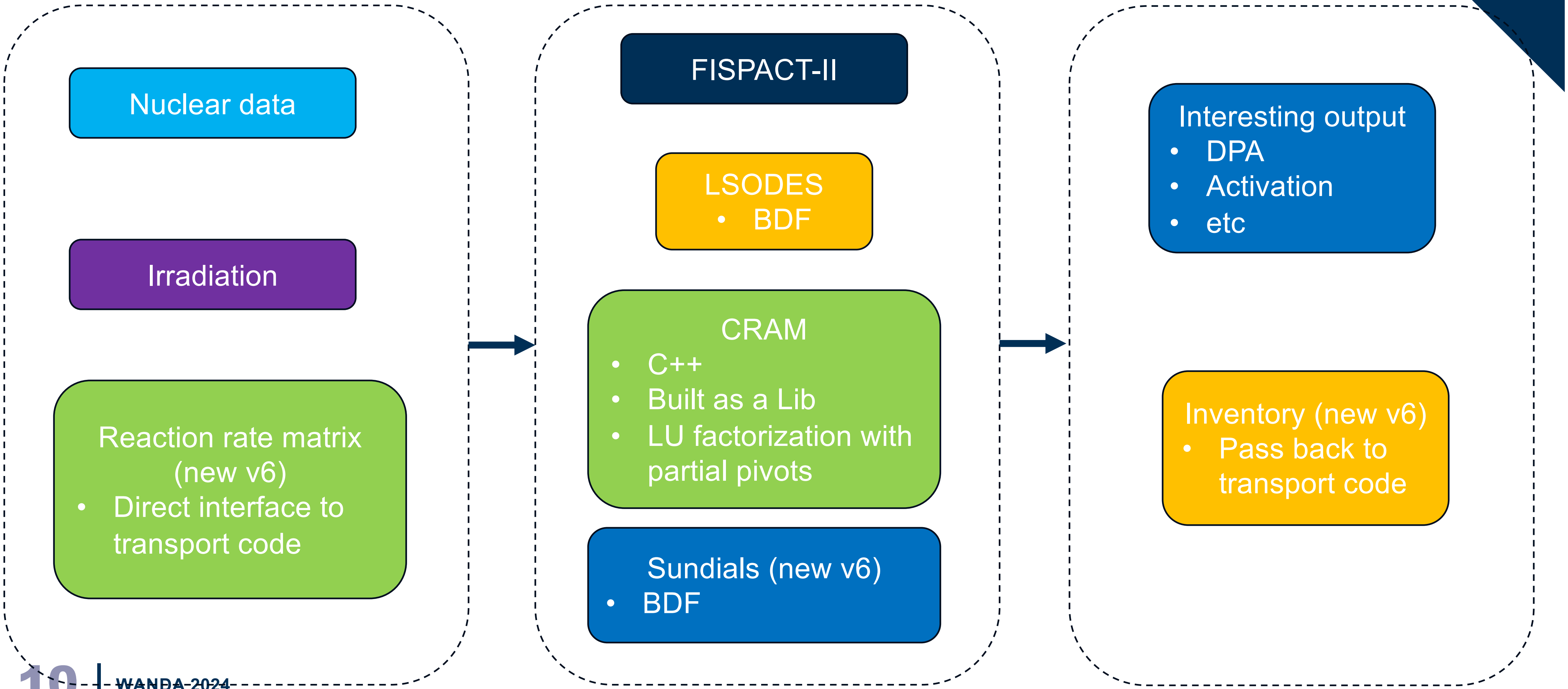
$$N_{s+n} = (\Delta t A - a_s I)^{-1} \sum_{k}^{s-1} a_k N_{n+k}, \text{ where } s > k$$

Performed on the transitive closure of G(A)

CRAM is also ‘implicit’



FISPACT-II + CRAM (+development)



Nuclear data

Irradiation

Reaction rate matrix (new v6)
- Direct interface to transport code

FISPACT-II

LSODES
- BDF

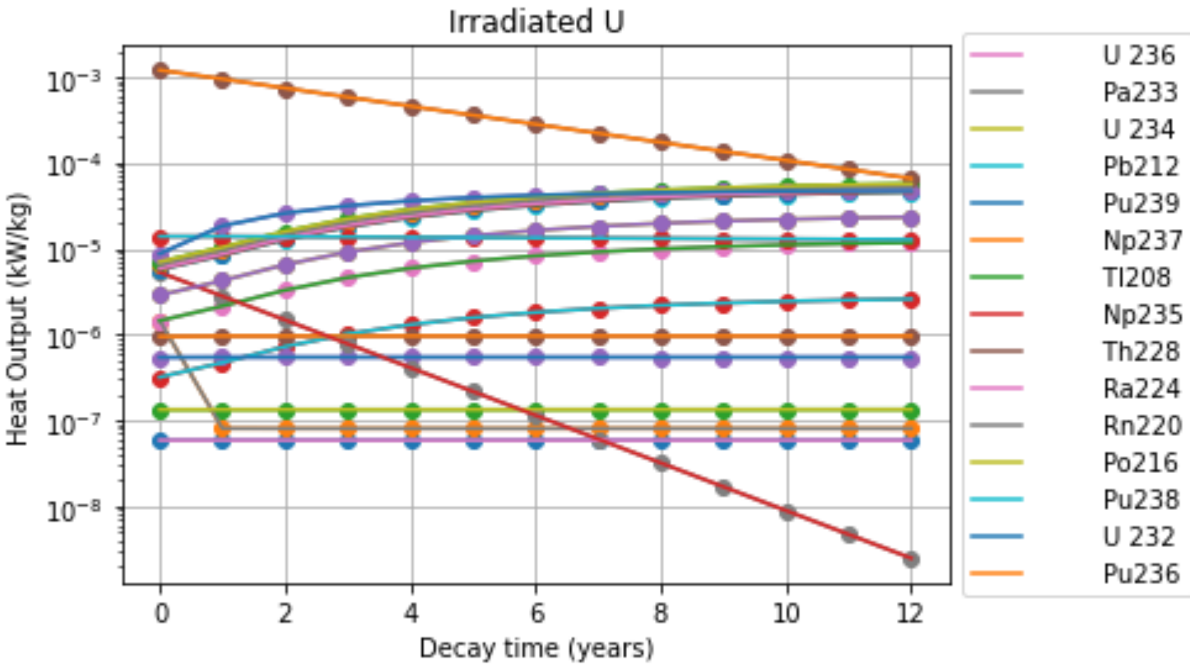
CRAM
- C++
- Built as a Lib
- LU factorization with partial pivots

Sundials (new v6)
- BDF

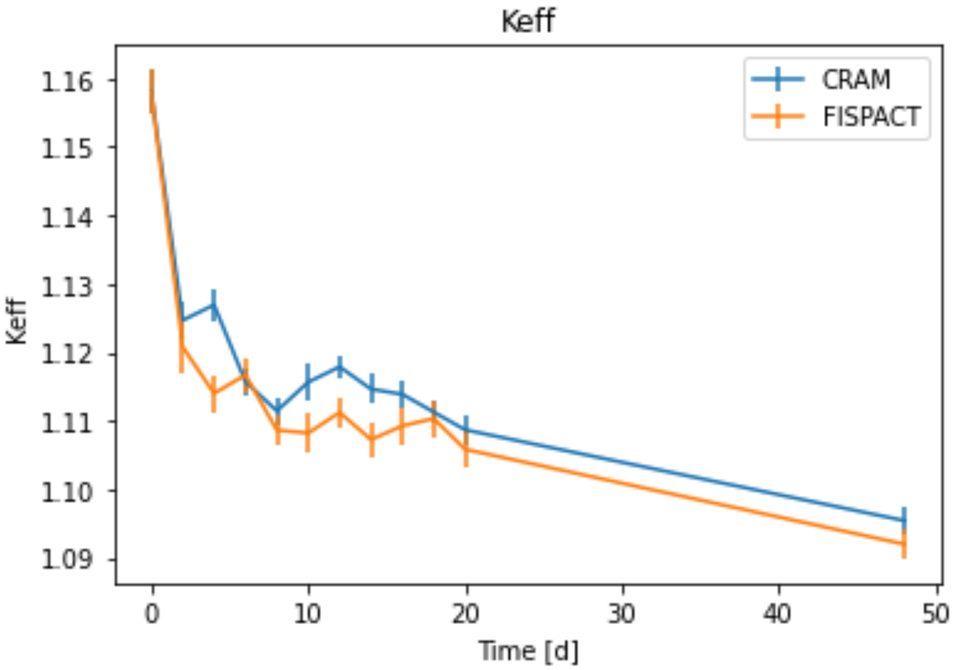
Interesting output
- DPA
- Activation
- etc

Inventory (new v6)
- Pass back to transport code

FISPACT CRAM/BDF



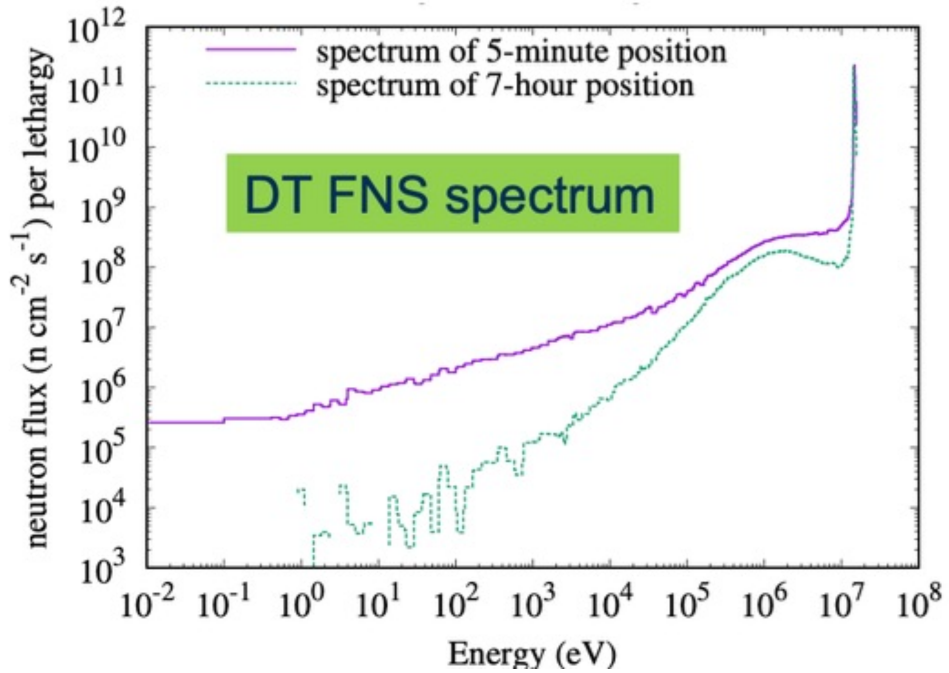
Comparison of irradiated U, lines are BDF dots are CRAM

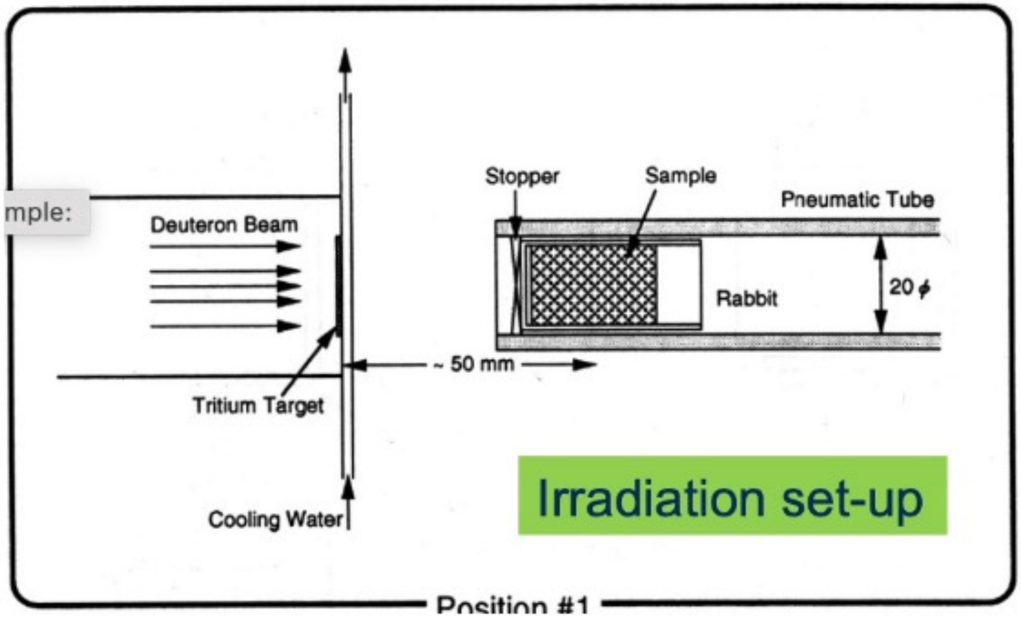


FISPACT-II performing burnup in OpenMC for a pin-cell (low statistics, preliminary)

FNS decay-heat

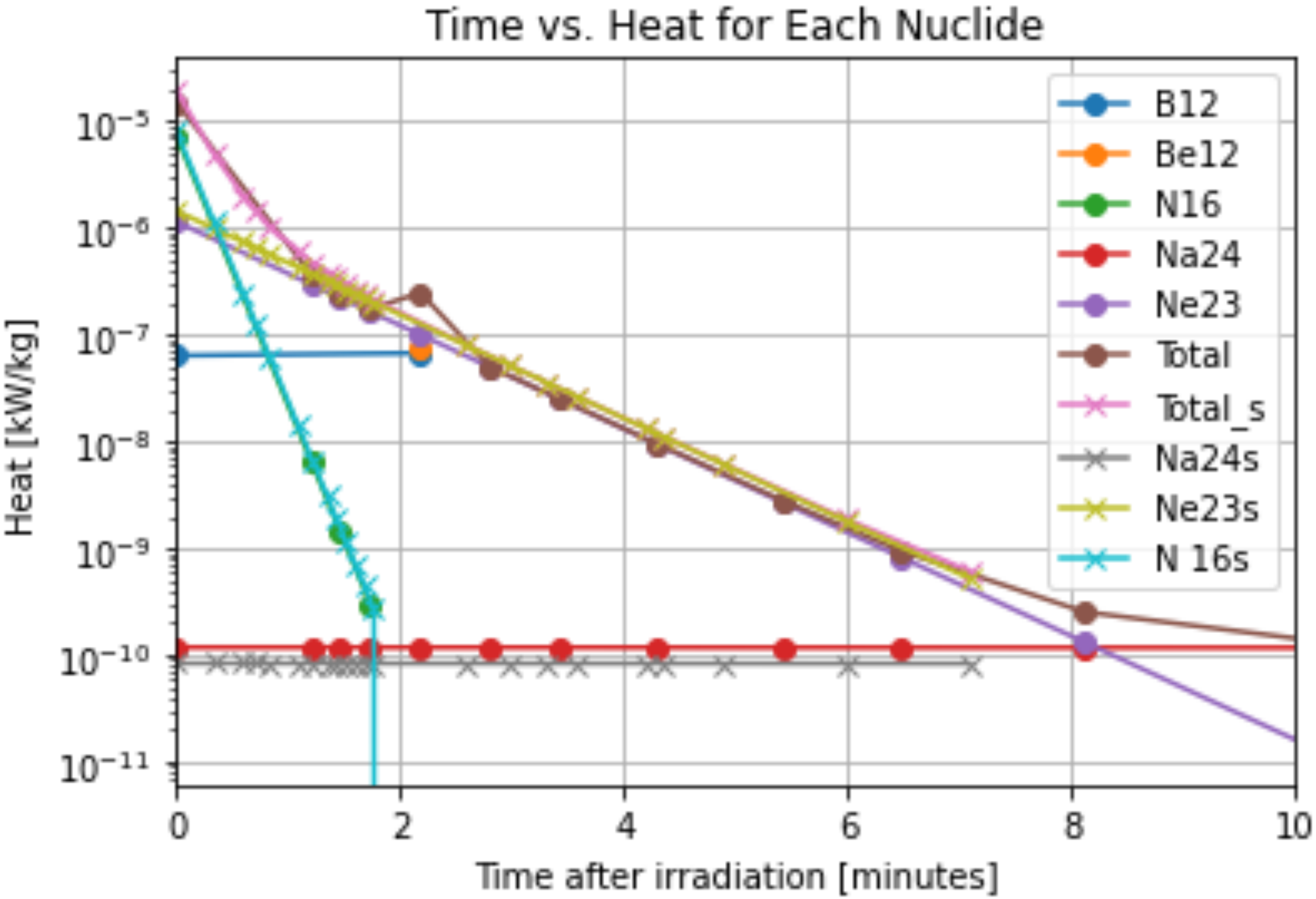
- The Japan Atomic Energy Agency (JAEA) used their Fusion Neutron Source (FNS) to irradiate several materials
- 2 mA deuteron bean onto a tritium target producing a fusion neutron flux (14MeV peak) ~10^10 n/cm2/s





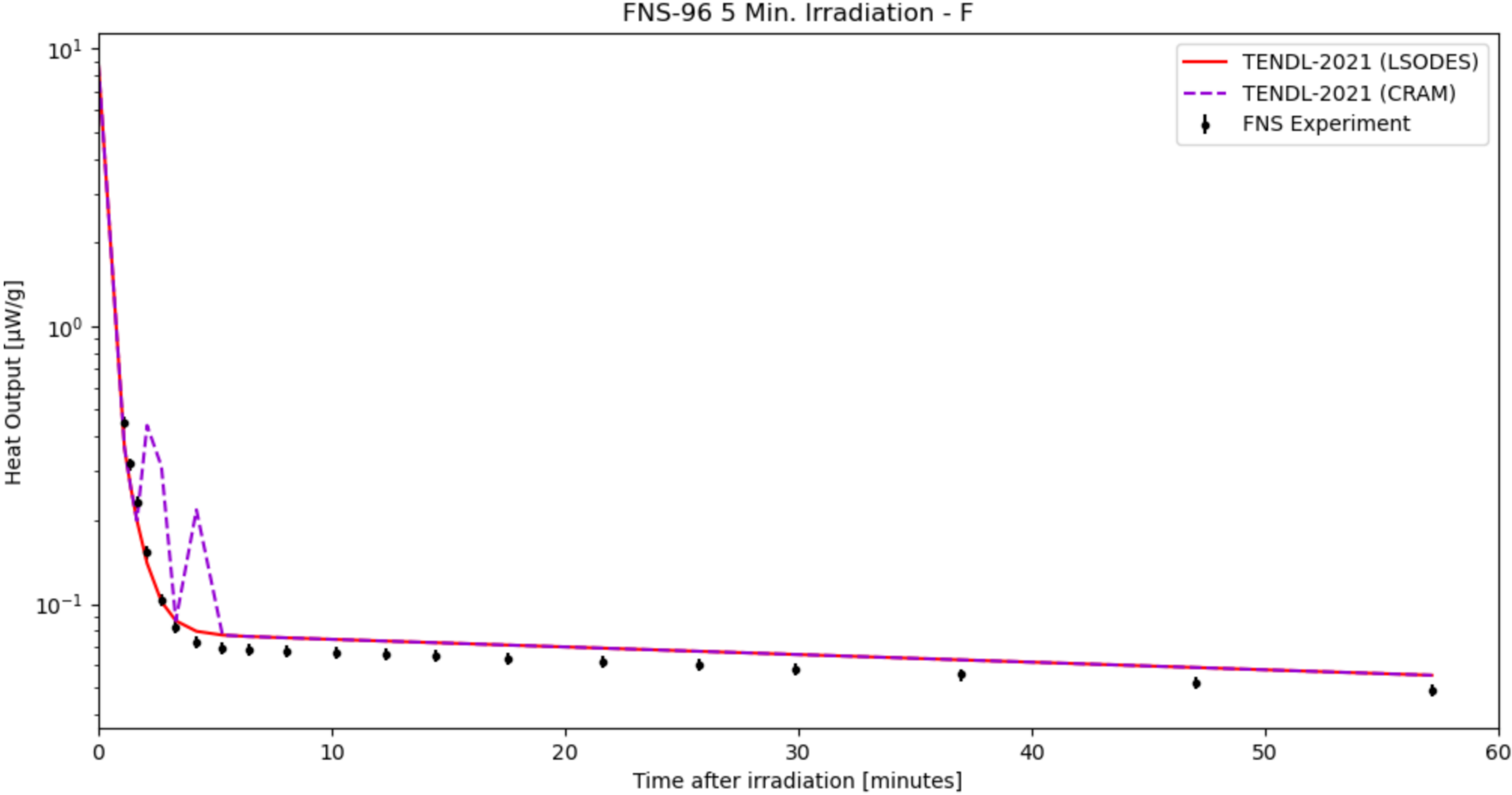
- M.R. Gilbert and J.C. Sublet (2018) used the FNS heat results to validate FISPACT-II for 73 materials

FISPACT CRAM

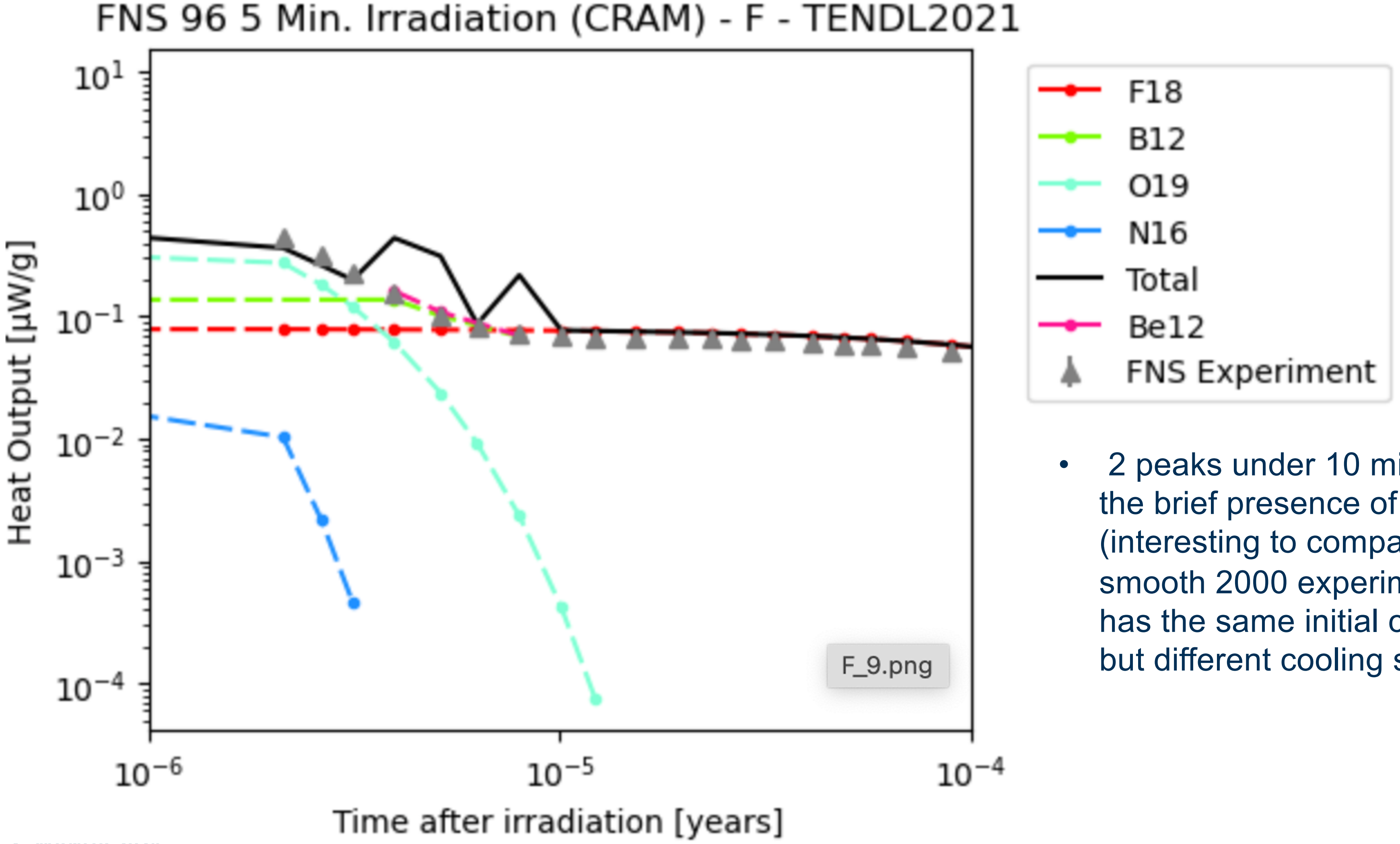


- Peak at ~2mins, due to the brief appearance of B12
- Spike can be removed by selection of time step (re-step ‘nuclide’s)
- Occurrence is likely due to fit

FISPACT CRAM/BDF Florine

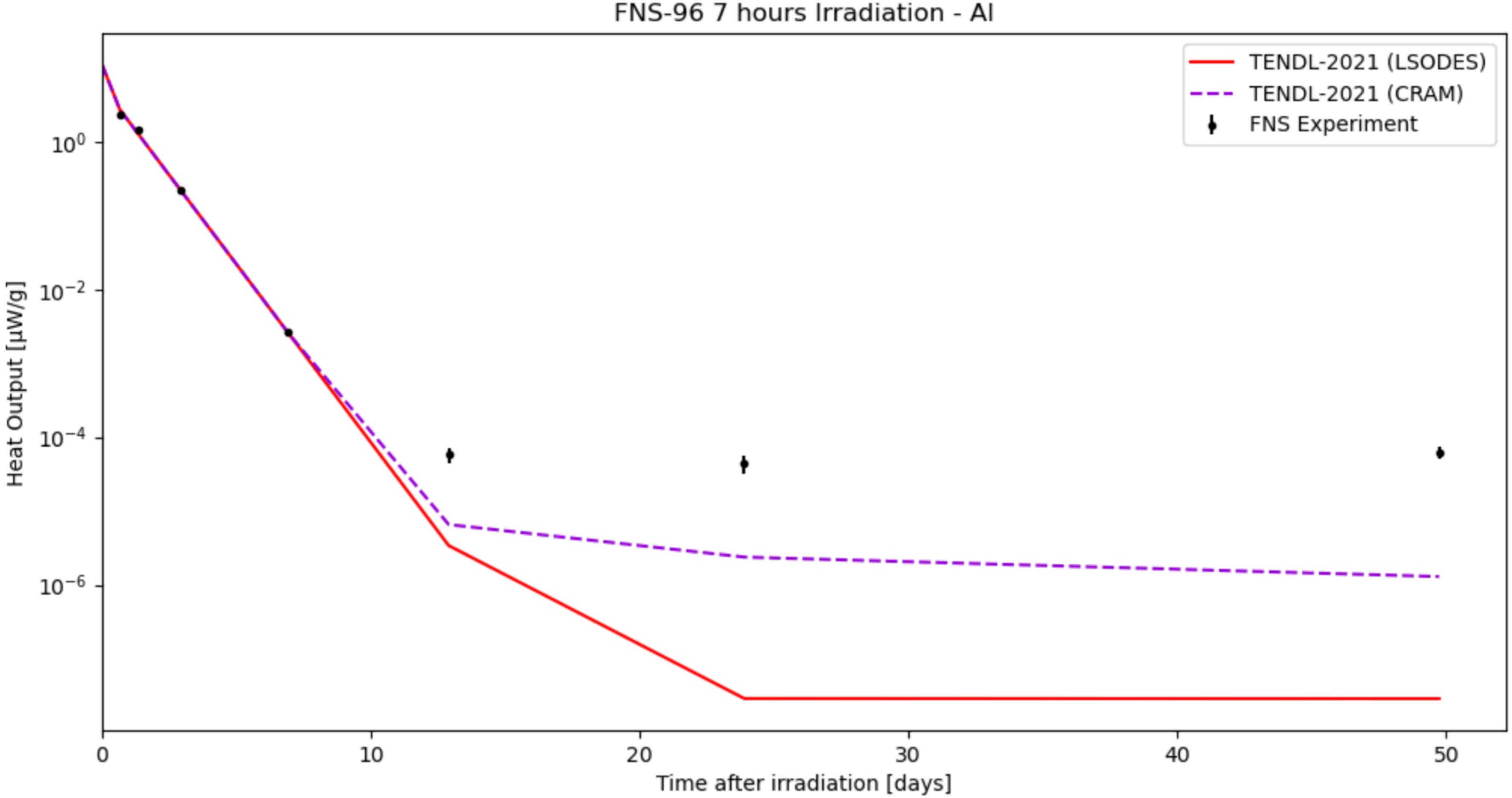


FISPACT CRAM Florine



- 2 peaks under 10 mins, due to the brief presence of Be12 (interesting to compare to the smooth 2000 experiment which has the same initial conditions but different cooling steps)

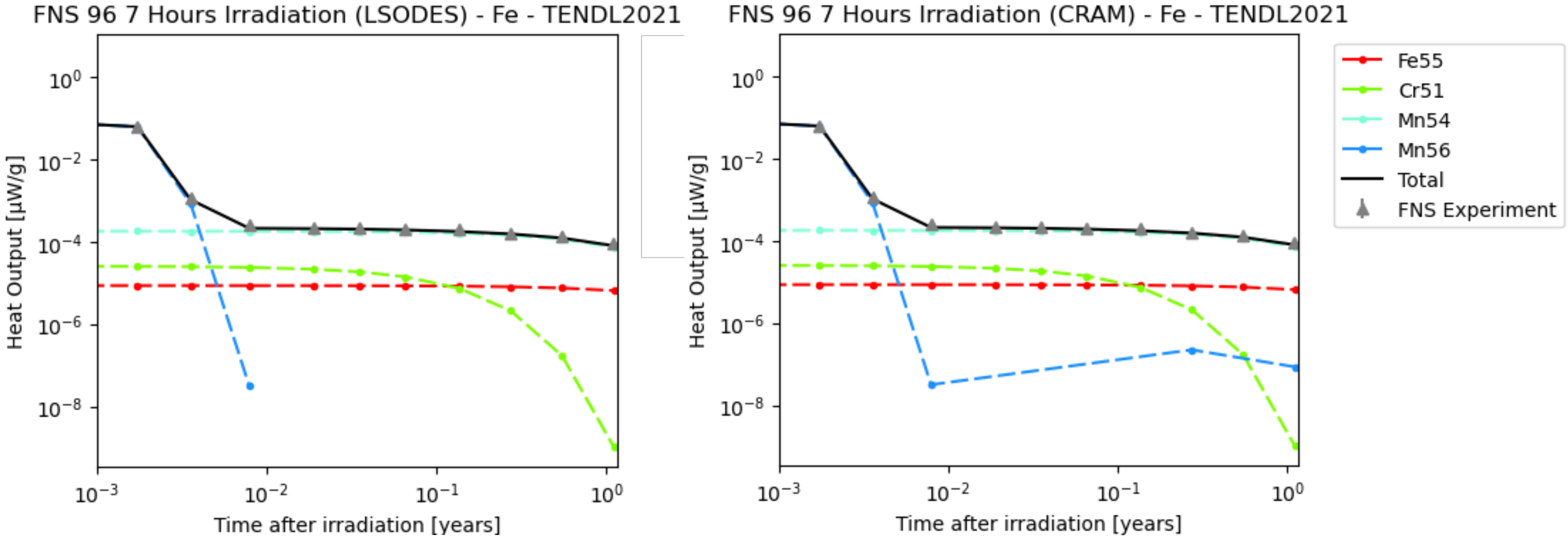
FISPACT CRAM/BDF Aluminum



CRAM improves the heat output past 10 days. However, CRAM includes Mg27 instead for the final three cooling times via Al27(n,p)Mg27

FISPACT CRAM/BDF

Iron



- Mn56 decay is different

Summary

- Investigated the matrix exponential, CRAM and BDF from a graphical
- Nuclear data as a graph
  - CRAM, matrix exponential, and BDF are on the transitive closure
- CRAM FISPACT-II (and further developments)
  - Noted some deviations between CRAM and BDF
  - Small nuclide contribution is not as important for fission as for fusion (waste)
    - CRAM (approximations) have problems with the small nuclide concentrations which are important for fusion
    - CRAM's current lack of truncation error leads to potentially non-physical nuclide concentrations for fusion
- Further investigation
    - Other fits of CRAM – lead by FISPACT-II BDF
    - Error bounds as a function of time

Thank you very much