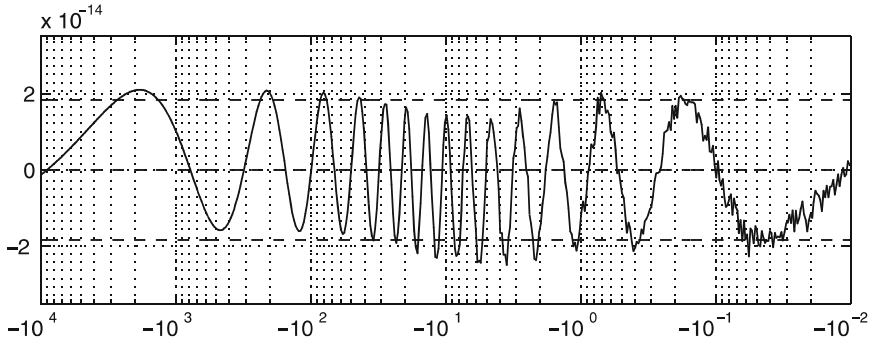

Figure 8.7: Value of $|e^z - r^*(z)|$ with $N = 14$. Figure taken from Ref. [5]

Table 8.1: Poles and Residues for the best rational approximation to the exponential with $N = 14$. For this function, $r^*(\infty) \approx 0$

k	z_k	$c_k/100$
1	5.623151880088747 + 1.194068309420004i	-0.278754565727894 - 1.021482174078080i
3	5.089353593691644 + 3.588821962583661i	0.469337296545605 + 0.456439548888464i
5	3.993376923428209 + 6.004285841369451	-0.234984158551045 - 0.058083433458861i
7	2.269789514323265 + 8.461734043748510i	0.048071353323537 - 0.013210030313639i
9	-0.208754946413353 +10.991254996068200i	-0.003763599179114 + 0.003351864962866i
11	-3.703276086329081 +13.656363257468552i	0.000094388997996 - 0.000171848578807i
13	-8.897786521056833 +16.630973240336562i	-0.000000715408253 + 0.000001436094999i

The form we write this best approximation is

(8.37)

where $r^*(z)$ the best rational approximation of order (N, N). There are algorithms available to compute $r^*(z)$, both with fun names, the Remes algorithm and the Carathéodory-Fejér algorithm[2]. A version of the CF algorithm is given for Matlab in Ref. [5]. This code is used to compute the residues, c_k, and poles, z_k, for the $N = 14$ case.

Using the these points we can compute the matrix exponential as in Figure 8.6, except that now the z_k and c_k are from this table.

8.5 Transmutation Trajectory Analysis

The method known as Transmutation Trajectory Analysis (TTA) solves the decay equations by looking at the decay and transmutation reactions and writes

[2]The CF algorithm is approximate, but the errors are $O(56^{-N})$.

the reaction networks as a set of linear chains. The population of each of these chains can be independently solved and then combined to get the total population of nuclides in the system. The resulting algorithm then only needs to solve linear chains, which can be done analytically in principle. In practice, when a branch in a chain occurs one then treats each branch as an independent linear chain. Difficulties can arise when chains are cyclic, i.e., the same nuclide appears multiple times in a chain as happens when an (n,2n) reaction is followed by radiative capture. As we will see, it is possible to treat this with a simple damping factor to terminate the chain after some number of cycles.

Consider a linear chain where only the first nuclide, n_1, has a nonzero initial concentration. Bateman, in 1910, gave the solution for the lth nuclide in a chain as

(8.38)

where

(8.39)

and

(8.40)

Notice that this solution is undefined when the effective decay constants for two nuclides are equal. This will clearly happen if the chain is cyclic, but can also happen if there is a large number of nuclides. In practice this is treated by making the adjustment

(8.41)

A typical value of ϵ is 10^{-5} and the condition $j > i$ means that we can adjust the decay constants as we progress down the chain.

We decide when to stop a chain by looking at the passage, $P_l(t)$, which is the fraction of the initial concentration of the first nuclide that has passed through

the first l nuclides in the chain. The passage is calculated via the formula

(8.42)

In this equation m is the total number of nuclides in the chain. It is possible that B_i is a small number, so that the second means of calculating the passage in Eq. (8.42) is not numerically stable. It, however, is possible to compute the passage as one moves along the chain by recognizing that the passage is equal to the ratio of the concentration of the next nuclide in the chain assuming that it does not decay to the initial nuclide:

(8.43)

The passage is used to terminate chains if the remaining nuclides are negligibly small. For instance one could cut chains when

(8.44)

for some cutoff value δ. Common values of δ are 10^{-15} and 10^{-20}.

8.5.1 Example of TTA

We will demonstrate the TTA approach and the Bateman solution using the depleted uranium example from before. To begin we look at all the linear chains in the system. In Figure 8.8 the entire transmutation network is shown. Examining this figure one can break the entire network into three chains, shown in Figures 8.9 through 8.11. Each of these chains has the same beginning, ^{238}U to ^{239}U by radiative capture. To compute the solution for this network, we first compute the concentration of ^{238}U and ^{239}U as a function of time using the Bateman solution in Eq. (8.38). Then for each of the three chains we compute the solution for the remaining members of the chain and add the solution together for each nuclide because some nuclides appear in multiple chains. We do not need to consider the passage cutoff for these chains because they are short and not cyclic.

We could also complicate matters by adding an $(n, 2n)$ reaction to the chain to make it cyclic. In Figure 8.12 there is now a cycle between ^{239}U and ^{238}U. Now for the calculation we have an additional chain that is the cycle between these

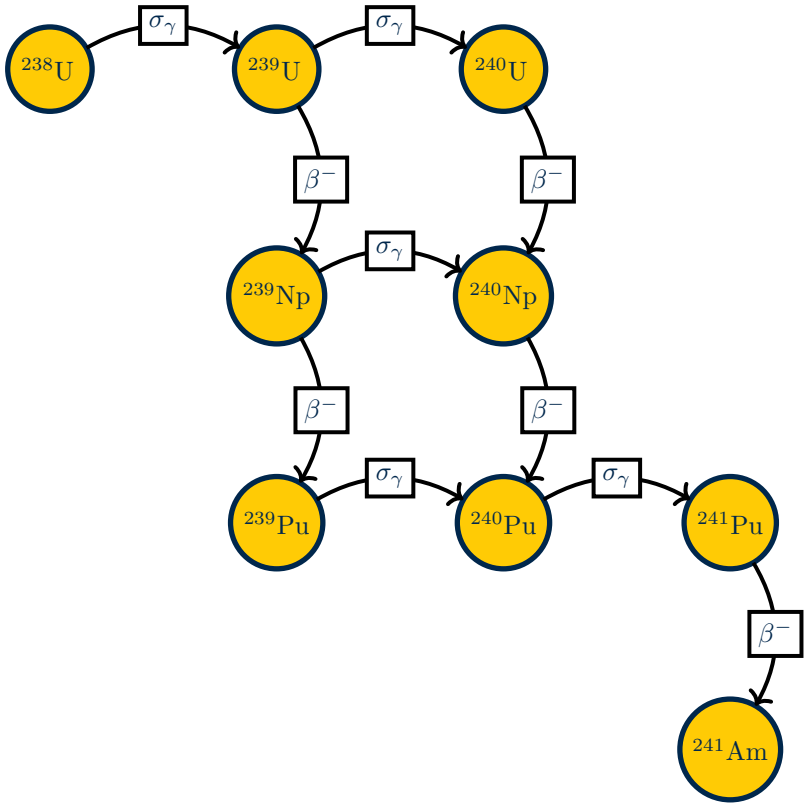

Figure 8.8: A transmutation network for ^{238}U.

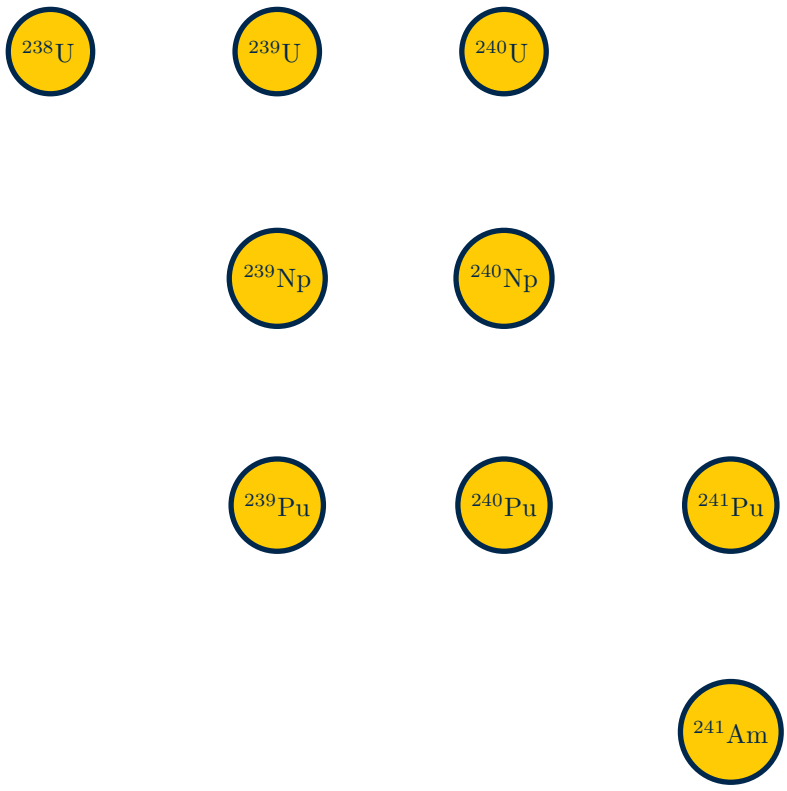

Figure 8.9: First of three linear chains for the ^{238}U transmutation network.

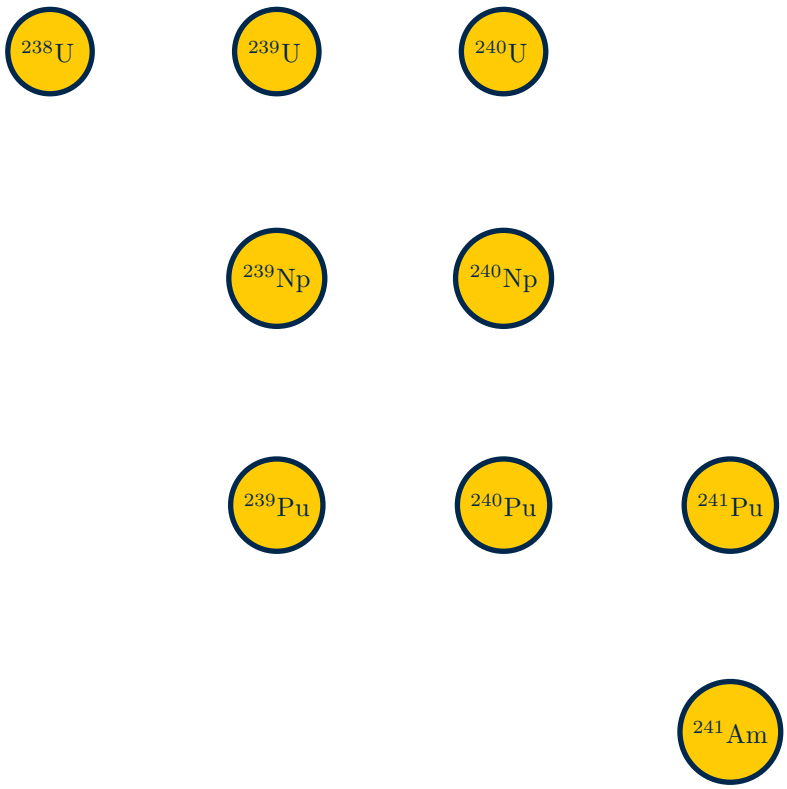

Figure 8.10: Second of three linear chains for the ^{238}U transmutation network.

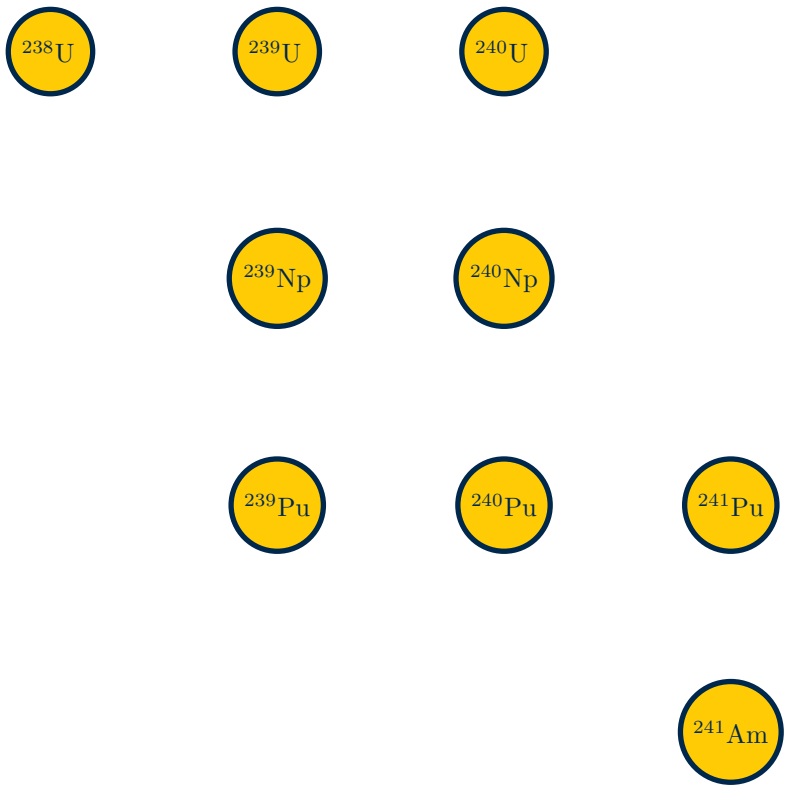

Figure 8.11: Third of three linear chains for the ^{238}U transmutation network.

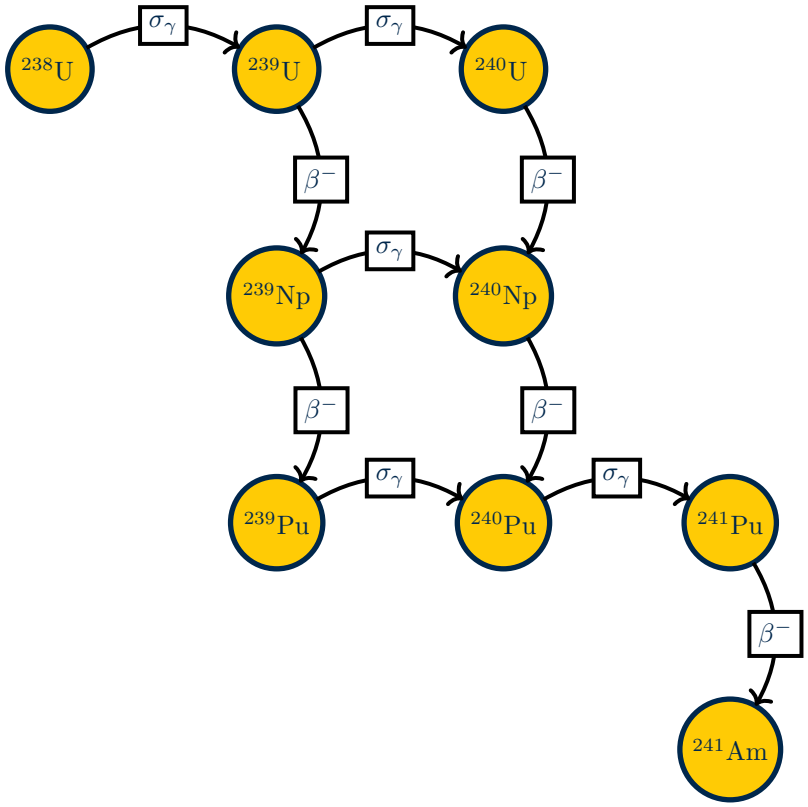

Figure 8.12: A transmutation network for ^{238}U with a cycle.

two. The cycle will be terminated by adjusting the decay constant and having a passage cutoff. For completion we show a reaction network that includes a fission product in Figure 8.13. This adds another chain to the system that will have to be handled. At this point, it is probably clear that developing the reaction networks and linear chains for a full-blown depletion calculation is a straightforward, though not simple, endeavor.

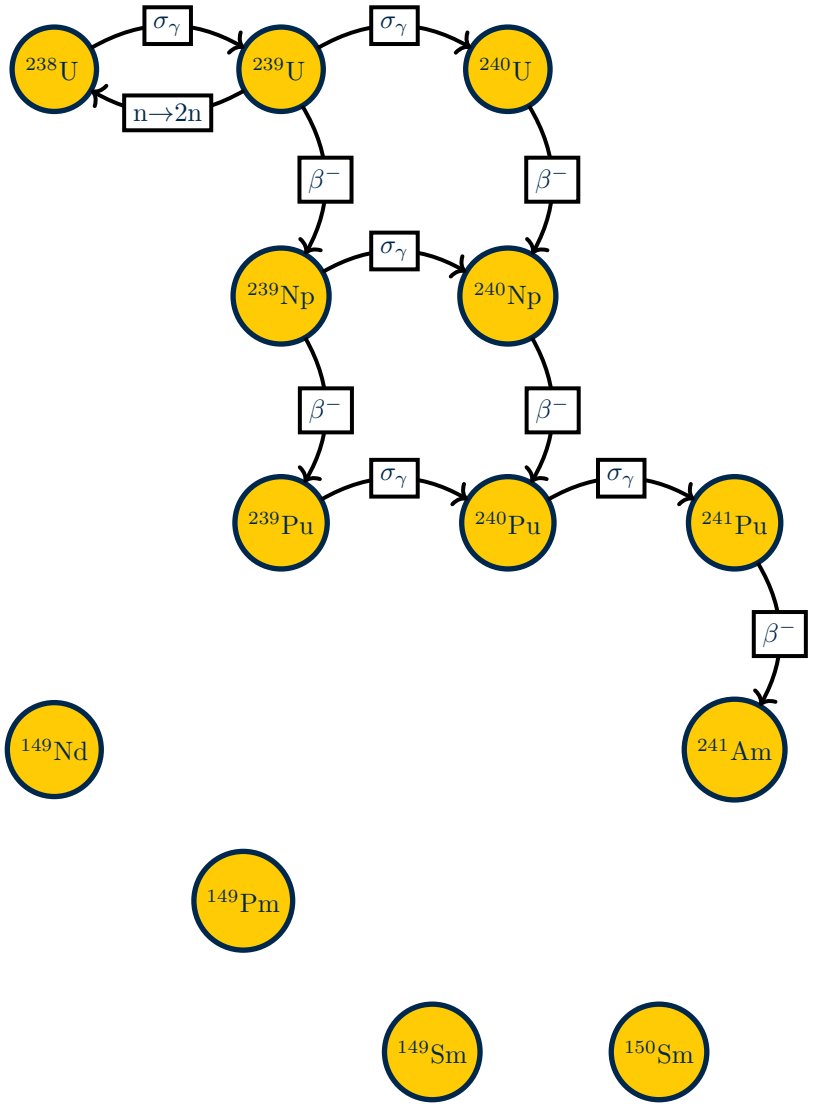

Figure 8.13: A transmutation network for ^{238}U with a fission product.