First & Second Order Approximations to Stage Numbers in Multi-component Enrichment Cascades

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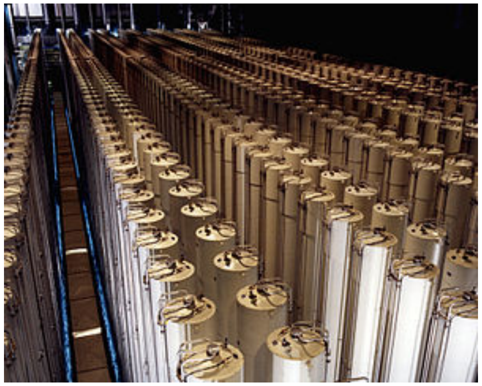
Enrichment

This talk describes a novel and fast method for computing the Matched Abunance Ratio Cascade (MARC) equations.

It is also about the tradeoffs needed to make this method fast.



Problem Description

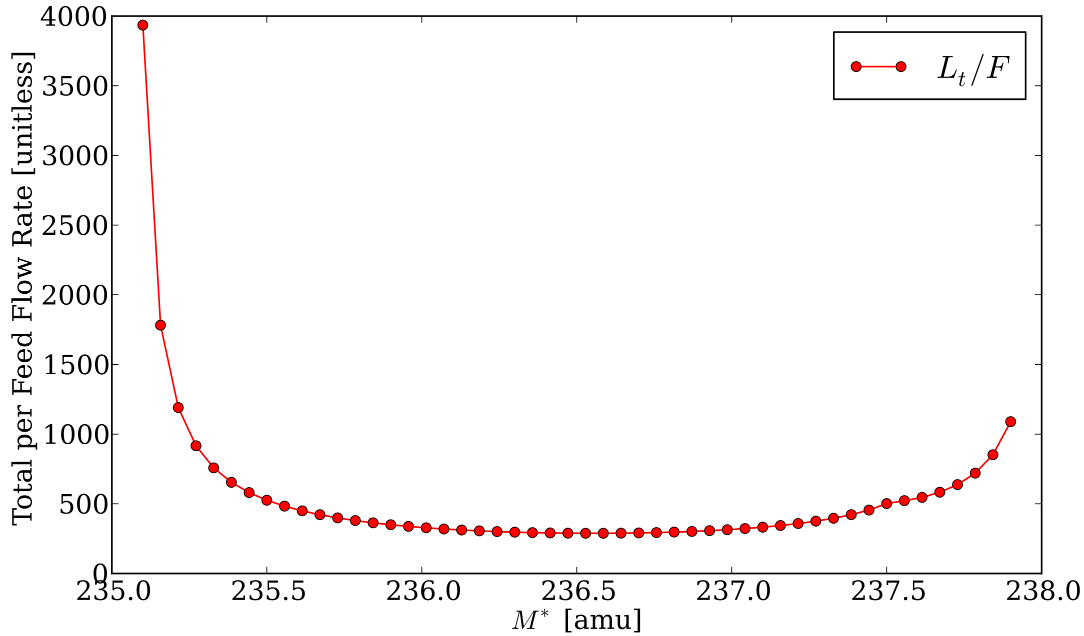


Figure 1: Enrichment Optimization [1]

Terminology

Symbol	Description
F, P, T, L	Feed, Product, Tails, and Total Flow Rates
i, j, and k subscripts	i-th component nuclide and first and second key components
0 subscript	Initial conditions value guess
x_i	Mass fraction of i-th component
$\backslash alpha, \backslash beta_i$	Overall and nuclide stage separation factors
N	Number of Stages
M	Molecular Weight [amu]
M^*	Optimization parameter

MARC Equations

The total flow rate normaizled by the feed flow rate may be computed from,

$$\frac{L}{F} = \sum_i^I \frac{\frac{P}{F} x_i^P \ln\left(\frac{x_j^P}{x_k^P}\right) + \frac{T}{F} x_i^T \ln\left(\frac{x_j^T}{x_k^T}\right) - x_i^F \ln\left(\frac{x_j^F}{x_k^F}\right)}{\ln(\beta_j) \frac{\beta_i - 1.0}{\beta_i + 1.0}}$$

MARC Equations

The following MARC constraints equations must then be solved for N_P, N_T, and M^*.

$$\frac{x_j^P}{x_j^F} \cdot \frac{P}{F} - \frac{\beta_j^{N_T+1} - 1}{\beta_j^{N_T+1} - \beta_j^{-N_P}} = 0$$

$$\left(\frac{x_j^F}{\frac{T}{F}} \cdot \frac{1 - \beta_i^{-N_P}}{\beta_j^{N_T+1} - \beta_j^{-N_P}} \right) - \left(x_j^T \cdot \sum_i^I x_i^T \right) = 0$$

$$\min\left[\frac{L}{F} \right] \rightarrow \frac{d}{dM^*} \frac{L}{F} = 0$$

Problem Statement

In PyNE, we wanted to build a very fast solver for this system (more or this later). One major speed up is to reduce the system from 3 equations and 3 unknowns to 1 equation and 1 unknown -- namely M^*.

Table I. Feed flow concentrations for a four component uranium re-enrichment cascade.

Nuclide	**VISION x^F [2]**
U-234	0.00018
U-235	0.00819
U-236	0.00611
U-238	0.98552

Elimination of N_T

Luckily, there is an analytic solution to $N_T(N_P, M^*)$

$$
\begin{aligned}
N_T \quad = \quad & \left[M^\star \log\left(\alpha\right) - M_j \log\left(\alpha\right) + \log\left(x^T_j\right) + \log\left(\frac{-1.0 + \frac{x^P\_j}{x^F\_j}}{x^P\_j - x^T_j}\right)\right. \\
& \left. - \log\left(\frac{\alpha^{N_P\left(-M^\star + M_j\right)}\left(x^F\_j x^P\_j - x^P\_j x^T\_j\right)}{-x^F_j x^P_j + x^F\_j x^T_j} + 1\right)\right] \times \frac{1}{\left(-M^\star + M\_j\right)\log\left(\alpha\right)}
\end{aligned}
$$

Elimination of N_T

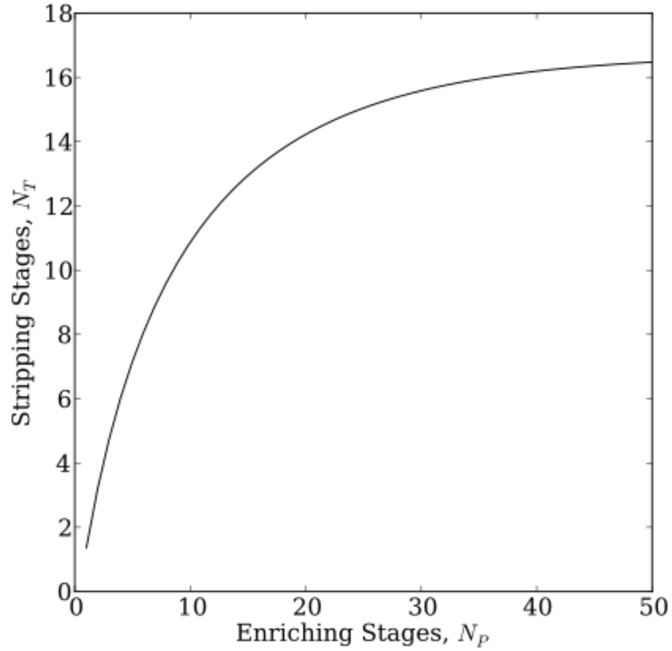


Figure 2: $N_T(N_P, M^*)$ for a four component uranium re-enrichment cascade with $N_P \in [1, 50]$ and $M^* = 236.547$.

Elimination of N_P

Call f,

$$f(N_P, M^*) = \left(\frac{x_j^F}{\frac{T}{F}} \cdot \frac{1 - \beta_i^{-N_P}}{\beta_j^{N_T(N_P, M^*)+1} - \beta_j^{-N_P}} \right) - \left(x_j^T \cdot \sum_i^I x_i^T \right) \equiv 0$$

Unfortunately, solving for $N\_P(M^\star)$ from $f(N\_P, M^\star)$ or $\min\left[\frac{L}{F}\right]$ is impossible.

Elimination of N_P

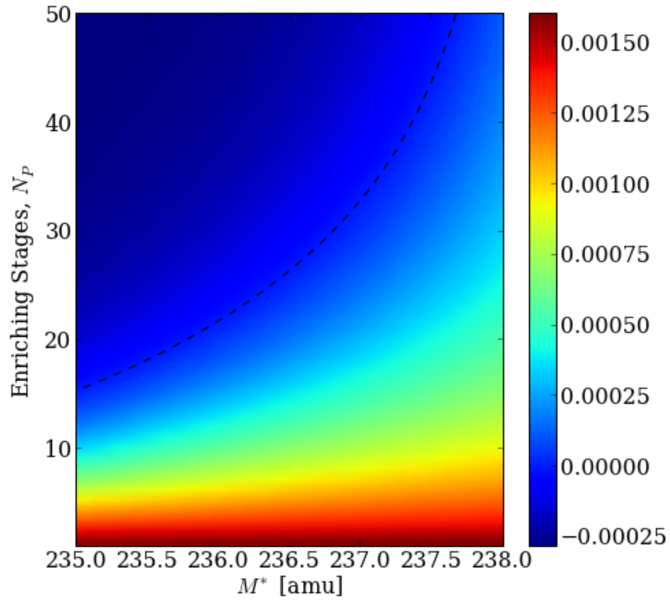


Figure 3: $f(N\_P, M^\star)$ over the range of possible N_P and $M^\star$ values. The black dashed contour line represents $f(N\_P, M^\star) = 0$

Approximation Strategy

- Approximate f with a Taylor series,
- And use this approximation to compute an analytic solution for $N_P(M^*)$.

First Order Approximation

$$f^{(1)}(N_P, M^*) \approx f(N_P^0, M^*) + \left(N_P - N_P^0\right) \frac{df}{dN_P}\Big|_{N_P=N_P^0}$$

yields

$$N_P^{(1)}(M^*) = N_P^0 - \frac{\frac{df}{dN_P}\Big|_{N_P=N_P^0}}{f(N_P^0, M^*)}$$

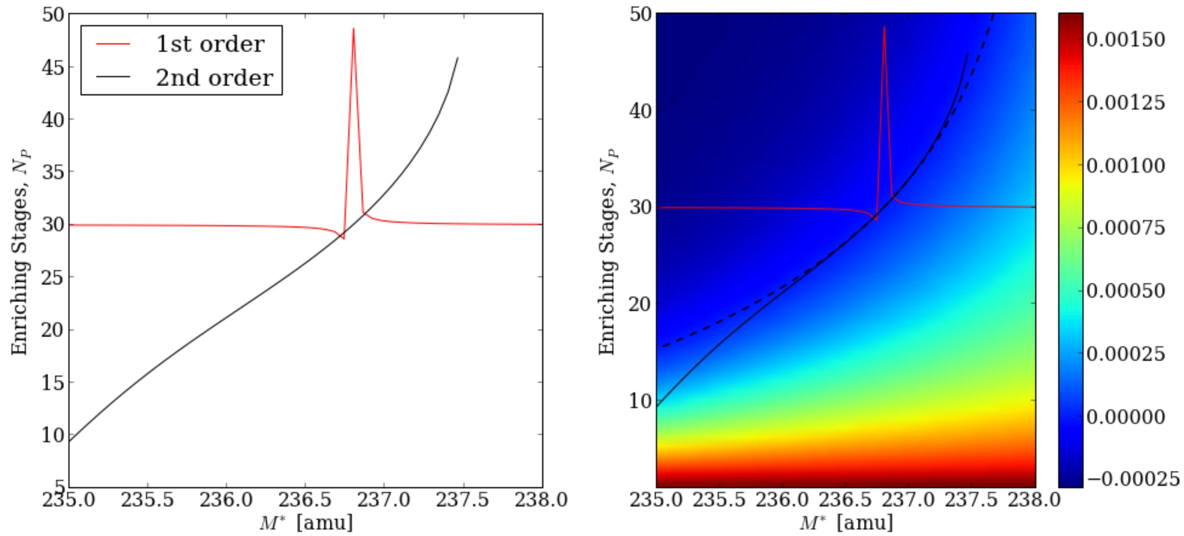
Second Order Approximation

$$
\begin{aligned}
f^{(2)}(N_P, M^*) \quad &\approx \quad f(N_P^0, M^*) \\
&\quad + \left(N_P - N_P^0\right) \frac{df}{dN_P}\bigg|_{N_P = N_P^0} \\
&\quad + \frac{\left(N_P - N_P^0\right)^2}{2} \cdot \frac{d^2 f}{(dN_P)^2}\bigg|_{N_P = N_P^0}
\end{aligned}
$$

yields

$$
\begin{aligned}
f^{(2)}(N_P, M^*) \quad &= \quad a(N_P)^2 + bN_P + c \\
a \quad &= \quad \frac{1}{2} \cdot \frac{d^2 f}{(dN_P)^2} \\
b \quad &= \quad \frac{df}{dN_P}\bigg|_{N_P = N_P^0} - N_P^0 \frac{d^2 f}{(dN_P)^2} \\
c \quad &= \quad f(N_P^0, M^*) - N_P^0 \cdot \frac{df}{dN_P} + \frac{(N_P^0)^2}{2} \frac{d^2 f}{(dN_P)^2} \\
N_P^{(2)}(M^*) \quad &= \quad \frac{-b - \sqrt{b^2 - 4ac}}{2a}
\end{aligned}
$$

Approximation Results



(a) (b)

Figure 4: Approximations to $f(N_P, M^\star)$ over the range of possible N_P and $M^\star$ values.

L / F Results

Having expressions for $N\_T(N\_P, M^\star)$ and $N\_P(M^\star)$, we can substitute these to create an $\frac{L}{F}(M^\star)$.

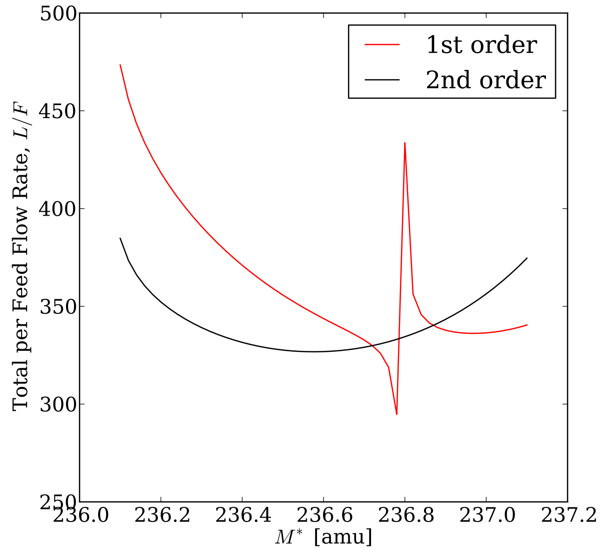


Figure 5: L / F(M^*) over the range of valid M^* values.

L / *F* Scaling

Table II: Number of instances of $M^\star$ and the number of binary operations in $L / F(M^\star)$ for first and second order Taylor series approximations for a four component mixture.

	1st order	2nd order
Number of $M^\star$	6,852	111,012
Number of Operations	57,383	945,575

- Note: these numbers are prior to CSE.

Benchmark

Table III: Table 6: Cascade parameter comparison after L / F minimization

Parameter	Approximation	Exact	Difference
L / F	326.89566	326.89609	-4.3245e-04
M^*	236.58177	236.57897	+2.8000e-03
N_P	27.36549	27.33457	+3.0923e-02
N_T	15.02947	15.05036	-2.0889e-02
x^P U-234	0.00147	0.00147	-2.2165e-07
x^P U-235	0.05500	0.05500	-2.9836e-06
x^P U-236	0.02846	0.02845	+4.8174e-06
x^P U-238	0.91507	0.91507	-1.6122e-06
x^T U-234	0.00003	0.00003	+1.7416e-08
x^T U-235	0.00250	0.00250	+1.7114e-08
x^T U-236	0.00339	0.00339	-7.4989e-07
x^T U-238	0.99408	0.99408	+7.1536e-07

L / *F* Execution Time

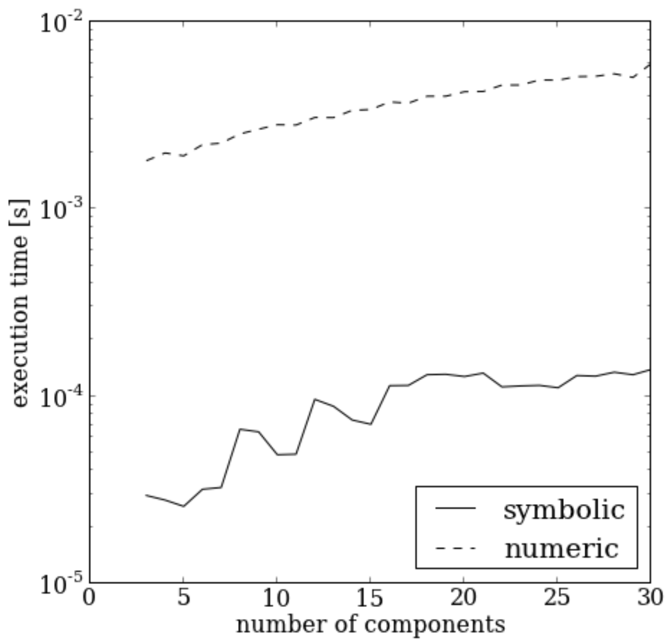
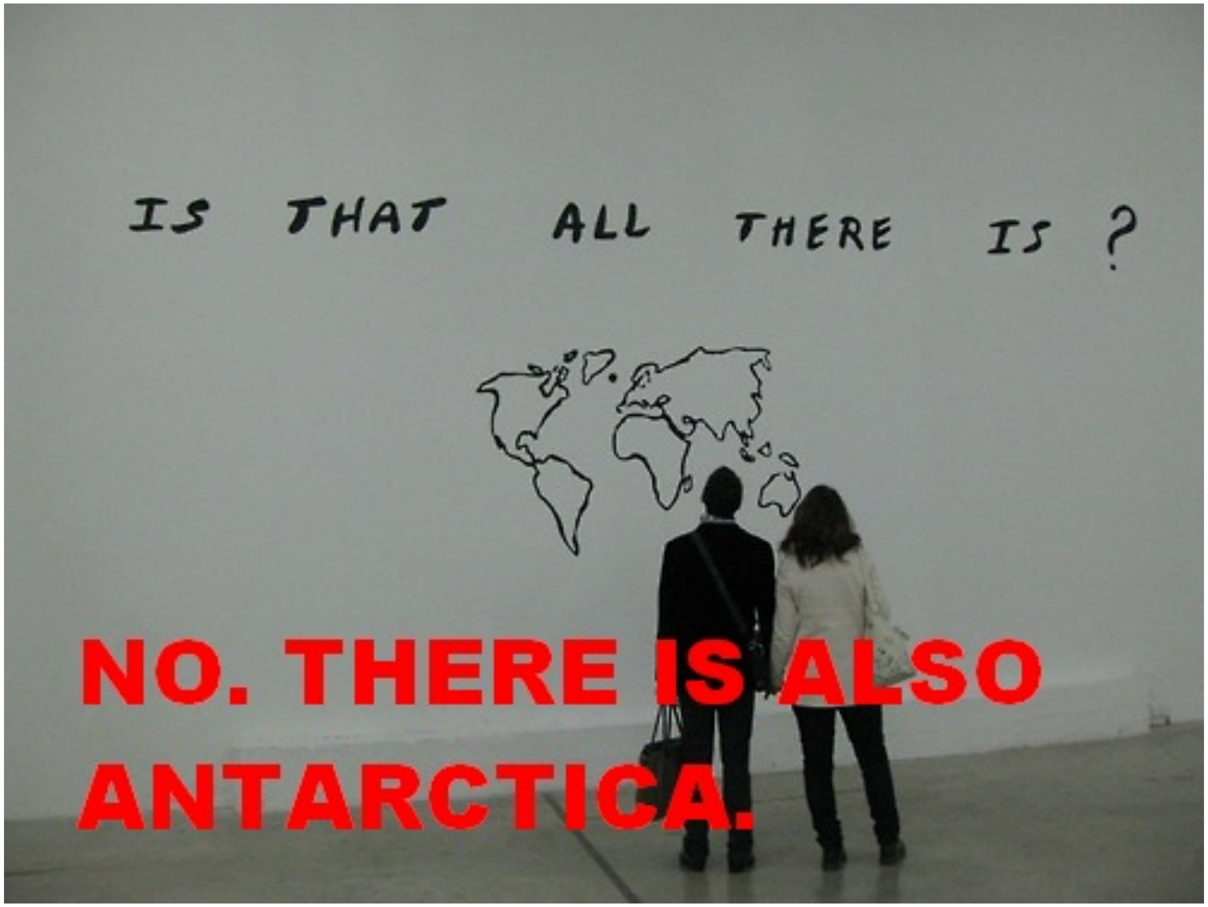


Figure 6: Execution time for L / $F(M^*)$ calculation.

PyNE

http://pynesim.org (http://pynesim.org)

Questions



References

1. Anthony Scopatz, "Erichment: M* vs Flowrate", URL: http://pynesim.org/gallery/enrichment_mstar_vs_flowrate.html
2. J. J. JACOBSON, G. E. MATTHERN, S. J. PIET, and D. E. SHROPSHIRE, “VISION : Verifiable Fuel Cycle Simulation Model Advances in Nuclear Fuel Management,” , Idaho National Laboratory (2009).