SOLUTION OF 3 COMPONENT DECAY

Computer Project 1 of NPRE 247

Hao Xiong

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UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

I INTRODUCTION

1.1 BACKGROUNDS

Radioactive decays obey to the radioactive decay law: the decay probability of an unstable nucleus is independent of the past history and is the same for all radionuclides of the same type.

$$\frac{dN}{dt} = -\lambda N \tag{1.1}$$

The number of atoms of a particular radionuclide depends on three aspects: (1) rates of production and decay, (2) initial values of it and its parents, (3) the rate at which it escapes from the sample. In this computer project, we consider a decay chain of three components, where A decays to B with decay constant λ_A, B decays to C with decay constant λ_B and C is stable.

$$A \xrightarrow{\lambda_A} B \xrightarrow{\lambda_B} C$$

We denote the number of these three types of particles at time t as $N_A(t), N_B(t), N_C(t)$, and decay constant of particle A, B as λ_A, λ_B. The differential decay equations for these particles are

$$\begin{aligned}
\frac{dN_A(t)}{dt} &= -\lambda_A N_A(t) \\
\frac{dN_B(t)}{dt} &= -\lambda_B N_B(t) + \lambda_A N_A(t) \\
\frac{dN_C(t)}{dt} &= \lambda_B N_B(t)
\end{aligned} \tag{1.2}$$

1.2 ANALYTICAL SOLUTIONS

The analytical solutions of the equations above can be attained through this way: Integrate the first equation we can get $N_A(t)$; Plug it into the second equation and integrate, we can get $N_B(t)$; Plug it into the third equation and integrate, we can get $N_C(t)$. Thus, the solutions are

$$\begin{aligned}
N_A(t) &= N_A(0)e^{-\lambda_A t} \\
N_B(t) &= N_B(0)e^{-\lambda_B t} + \frac{\lambda_A N_A(0)}{\lambda_B - \lambda_A}\left[e^{-\lambda_A t} - e^{-\lambda_B t}\right] \\
N_C(t) &= N_C(0) + N_B(0)\left[1 - e^{-\lambda_B t}\right] + \frac{N_A(0)}{\lambda_B - \lambda_A}\left[\lambda_B(1 - e^{-\lambda_A t}) - \lambda_A(1 - e^{-\lambda_B t})\right]
\end{aligned} \tag{1.3}$$

To obtain the time of maximal N_B, we can let $\frac{dN_B(t)}{dt} = -\lambda_B N_B(t) + \lambda_A N_A(t) = 0$, which yields

$$\lambda_B N_B(t) = \lambda_A N_A(t) \tag{1.4}$$

$$\lambda_B\left(N_B(0)e^{-\lambda_B t} + \frac{\lambda_A N_A(0)}{\lambda_B - \lambda_A}\left[e^{-\lambda_A t} - e^{-\lambda_B t}\right]\right) = \lambda_A N_A(0)e^{-\lambda_A t} \tag{1.5}$$

Its solution is

$$t = \frac{1}{\lambda_B - \lambda_A} \log(\frac{\lambda_A\lambda_B N_A(0) + \lambda_A\lambda_B N_B(0) - \lambda_B^2 N_B(0)}{\lambda_A^2 N_A(0)}) \tag{1.6}$$

Note that, to make the above solution meaningful, these following conditions should be satisfied,

$$\begin{aligned} &\lambda_A\lambda_B N_A(0) + \lambda_A\lambda_B N_B(0) - \lambda_B^2 N_B(0) > 0 \\ &\lambda_B - \lambda_A \quad \lambda_A\lambda_B N_A(0) + \lambda_A\lambda_B N_B(0) - \lambda_B^2 N_B(0) - \lambda_A^2 N_A(0) \;\; > 0 \end{aligned} \tag{1.7}$$

They can be simplified as

$$\lambda_A N_A(0) > \lambda_B N_B(0) \tag{1.8}$$

which means, the number of particle B should increase at first. So the time of maximal N_B is

$$t = \begin{cases} \frac{1}{\lambda_B - \lambda_A} \log(\frac{\lambda_A\lambda_B N_A(0) + \lambda_A\lambda_B N_B(0) - \lambda_B^2 N_B(0)}{\lambda_A^2 N_A(0)}) & \text{for } \lambda_A N_A(0) > \lambda_B N_B(0) \\ 0 & \text{for } \lambda_A N_A(0) \le \lambda_B N_B(0) \end{cases} \tag{1.9}$$

1.3 NUMBERICAL METHODS

In this section we show how to numerically solve the differential equations above with a forward difference approximation. For $\frac{dN_i(t)}{dt}$, we can approximate it as $\frac{N_i(t+\Delta t) - N_i(t)}{\Delta t}$.If we denote the initial number of paritcle i as $N_i^1 = N_i(0)$, and denote the number after time $(j-1)\Delta t$ as N_i^j, then we can approximate $\frac{dN_i(t)}{dt}$ as $\frac{N_i^{j+1} - N_i^j}{\Delta t}$ for time $t = (j-1)\Delta t, j = 1,2,3,\ldots$. Thus, the differential equations can be converted into the equations below,

$$\begin{aligned} N_A^{j+1} &= N_A^j + (-\lambda_A N_A^j)\Delta t \\ N_B^{j+1} &= N_B^j + (-\lambda_B N_B^j + \lambda_A N_A^j)\Delta t \\ N_C^{j+1} &= N_C^j + (\lambda_B N_B^j)\Delta t \end{aligned} \tag{1.10}$$

If we give the initial number of these three types of particles N_1^1, N_2^1, N_3^1, then we can get N_A^2, N_B^2, N_C^2 using the above equations, and so on. Thus, by repeating this process, we can get the numbers at any time $t = (j-1)\Delta t, j = 1,2,3,\ldots$, with a time resolution of Δt.

To use the numerical solutions above, we also need these initial values: (1) half life time $T_{1/2}$ or decay constant λ of particle A and B; (2) initial numbers of A, B and C; (3) time resolution Δt used to calculate; (4) final time t_{final}, which is the end time of calculation.

In practice, the given Δt may yields a coarse solution, which is not stable enough. Thus, we may have to decrease Δt by half until the solution does not change significantly with further decreasing of Δt.

1.4 FILE FORMAT DESCRIPTION

There are four output files for every decay chain, they are

(1) Coarse numbers of A, B and C;

(2) Medium numbers of A, B and C;

(3) Stable numbers of A, B and C;

(4) Time of maximal N_B vs. $1/\triangle t$.

The first three files have the following format,

(First line) $T_{1/2A}$ $T_{1/2B}$ N_{A0} N_{B0} N_{C0} $\triangle t_{\text{initial}}$ t_{final}

(Second line) $\triangle t_{\text{used}}$ 'Length of the data'

(Third line) data.

The fourth file has the following format,

(First line) $T_{1/2A}$ $T_{1/2B}$ N_{A0} N_{B0} N_{C0} $\triangle t_{\text{initial}}$ t_{final}

(Second line) $t_{\max}$ calculated by analytical solution; 'length of the data'

(Third line) data.

II DECAY CHAIN 1

In this section, we consider a given decay chain with the following initial values:

Table 2.1 Initial values of decay chain 1

$t_{1/2A}$	$t_{1/2B}$	$t_{1/2C}$	N_{A0}	N_{B0}	N_{C0}	$\triangle t$	t_{final}
1h	10h	stable	100	0	0	1h	50h

Here, $t_{1/2A}$ and $t_{1/2B}$ are half life time of A and B; *C* is stable. N_{A0}, N_{B0}, N_{C0} are initial numbers of A, B and C. $\triangle t$ is the given initial time interval used for calculation. t_{final} is the end time of calculation.

With equations (1.3) and (1.10) in section I, we could get the analytical and numerical solutions. Here, we assume that if the maximal difference of numbers between results calculated from $\triangle t$ and $\triangle t/2$ is 0.01, the numerical solution is stable. This value could be smaller if needed.

The numerical solution shows: when $\triangle t = 1h$, it gives a coarse solution; when $\triangle t = 0.5002h$, it gives a medium solution; when $\triangle t = 0.00049h$, it gives a stable solution, which means the change of numbers with further smaller $\triangle t$ is within 0.01. These three situations and the analytical solution are shown in Fig. 2.1.

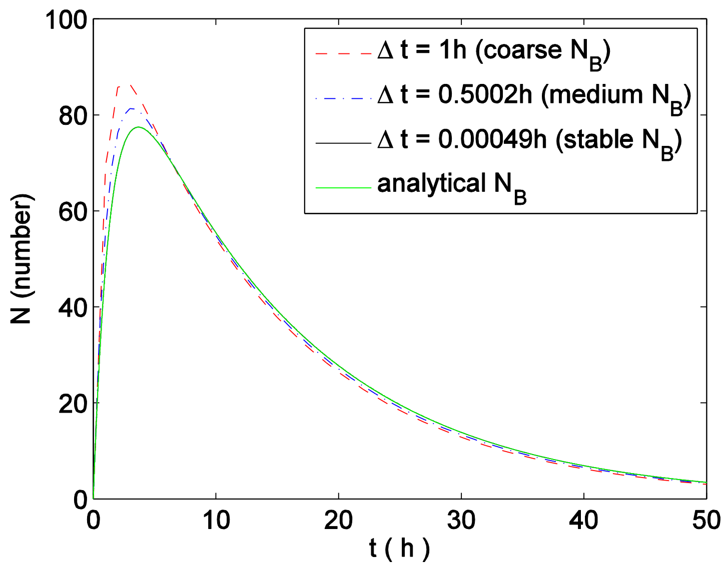

Fig. 2.1 Coarse, medium and stable number of N_B.

The green line indicates the analytical solution.

For stable condition, the numbers of A, B and C and their sum are shown in Fig. 2.2.

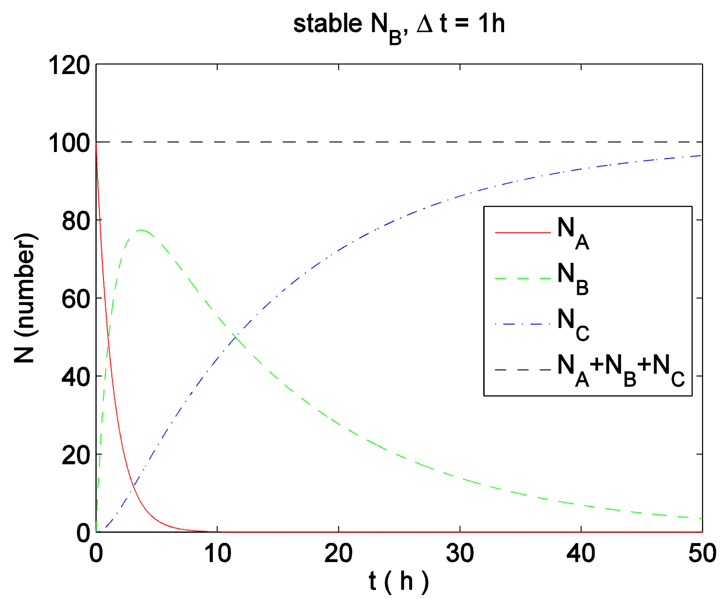

Fig. 2.2 stable numbers of N_A, N_B, N_C. The black dash line indicates their sum, which is always $N_{A0} + N_{B0} + N_{C0}$.

Time of maximal N_B and dependence of $1/\Delta t$ are shown in Fig. 2.3. The time value of the maximal N_B obtained from equation (1.9) is also shown in it.

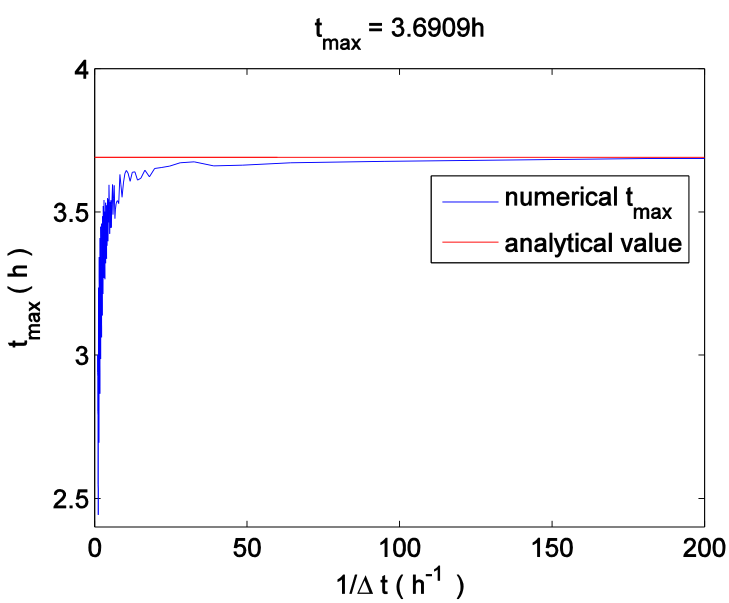

Fig 2.3 The time of maximal N_B vs. $1/\Delta t$

III DECAY CHAIN 2

In this section, we consider a given decay chain with the following initial values:

Table 3.1 Initial values of decay chain 2

$t_{1/2A}$	$t_{1/2B}$	$t_{1/2C}$	N_{A0}	N_{B0}	N_{C0}	$\triangle t$	t_{final}
2min	12s	stable	100	0	0	10s	10min

The symbols used here has the same meaning as those in section II.

The numerical solution shows: when $\triangle t = 10s$, it gives a coarse solution; when $\triangle t = 0.5002h$, it gives a medium solution; when $\triangle t = 0.00049h$, it gives a stable solution, which means the change of numbers with further smaller $\triangle t$ is within 0.01. These three situations and the analytical solution are shown in Fig. 2.1.

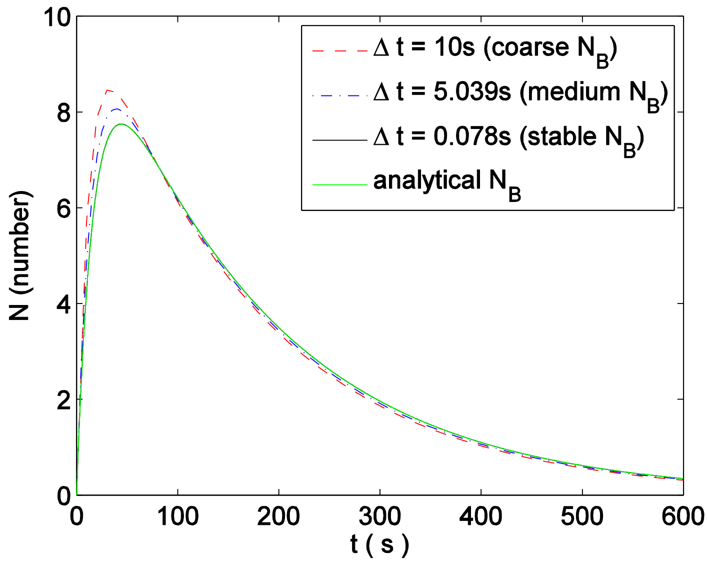

Fig. 3.1 Coarse, medium and stable number of N_B.

The green line indicates the analytical solution.

For stable condition, the numbers of A, B and C and their sum are shown in Fig. 2.2.

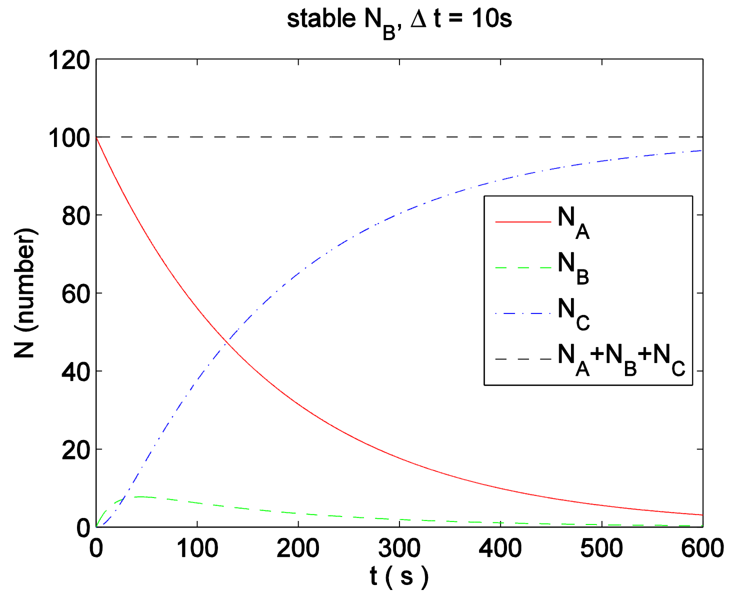

Fig. 3.2 stable numbers of N_A, N_B, N_C. The black dash line indicates their sum, which is always $N_{A0} + N_{B0} + N_{C0}$.

Time of maximal N_B and dependence of $1/\Delta t$ are shown in Fig. 2.3. The time value of the maximal N_B obtained from equation (1.9) is also shown in it.

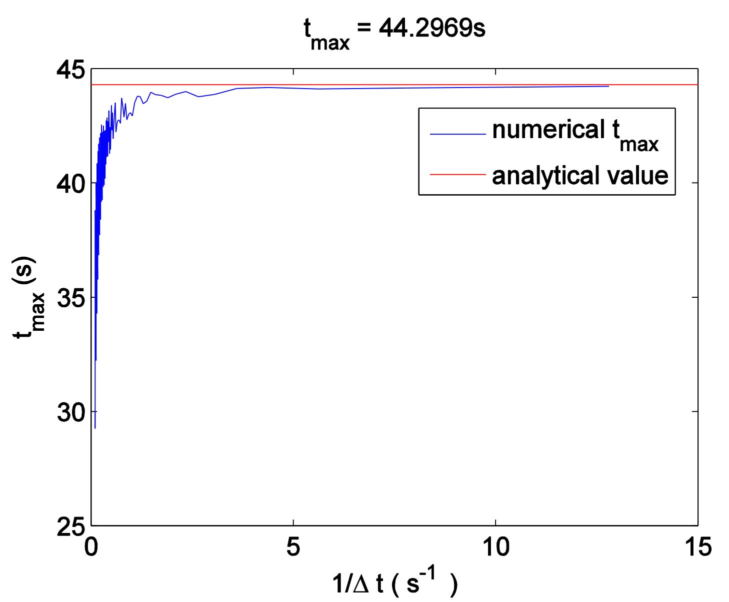

Fig 3.3 The time of maximal N_B vs. $1/\Delta t$