2016

Modeling of Structural Relaxation By A Variable-Order Fractional Differential Equation

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by

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Bachelor of Science
University of Science and Technology of China, 2013

Submitted in Partial Fulfillment of the Requirements

for the Degree of Master of Science in

Mathematics

College of Arts and Sciences

University of South Carolina

2016

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Acknowledgments

Gratitude is the memory of the heart and I feel very grateful that many people have offered me valuable help for my master's thesis, including my advisors, friends and parents.

Firstly, I want to express my sincerest gratitude to my advisor professor Hong Wang, who has given me much help by offering me necessary materials, advice of modifying algorithm and inspiration of new ideas with great patience and consistent encouragement. I could not correct many mistakes and accomplish an excellent thesis without his help. Moreover, I appreciate professor Lili Ju a lot for his advice not only in academic but also in my life.

Then I would like to express my sincere grateful to professor Rui Xiao, my collaborator. I can't finish my thesis without the experimental data he has offered to me. And he also illustrated the physical background of structural relaxation and shape-memory behavior to me, which provided me a general idea of these two physical processes.

Furthermore, I want to acknowledge my parents. It is really a long process from preparing materials to finishing the thesis. I feel very happiness that my parents can accompany with me all the time. Their help really benefited me a lot.

At last, I would like to express my gratitude to my supporter. This work was supported in part by the National Science Foundation under Grants EAR-0934747 and DMS-1216923, and by the OSD/ARO MURI Grant W911NF-15-1-0562.

Abstract

In physical point of view, relaxation usually describes the return from a perturbed system into equilibrium and each process has its own characteristic relaxation time. In 1946, Tool first formulated the notion of fictive temperature to characterize the structure of a glass-forming melt. Since then, people used to simulate structural relaxation by first order model. Since fractional-based models have not widely applied in modeling the fictive temperature, I want to explore the the possibility of modeling structural relaxation by fractional differential equation.

In this thesis, I will first introduce the definitions of two different kinds of fractional derivatives: Riemann-Liouville fractional derivative and Caputo fractional derivative briefly, and then show several existing and newly proposed models for structural relaxation and shape-memory behavior. Finally, I will illustrate the numerical scheme for each model and show some related numerical experiments.

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Chapter 1

BACKGROUND

In the field of physics, the first order evolution equation is the most widely adopted model to describe many physical processes. It owns many advantages but at the same time, there are many shortcomings which make the first order model not simulate some processes well. Nowadays, as the rapidly development of fractional calculus, more and more scholars realize that the fractional model owns advantages in simulating processes with algebra decay.

In this chapter, I will instruct some general ideas of two typical processes respectively, structural relaxation process and shape-memory behavior, which are usually modeled by first order evolution equation previously.

1.1 classic model for structural relaxation

In physical point of view, relaxation is generally considered as the return of a perturbed system into equilibrium and each relaxation process owns characteristic with a relaxation time t. The structural relaxation describes the relaxation in amorphous solids.

The structural relaxation model[**1**] describes the transition process of glass forming materials under fitted temperature. Since transition process of structure is instantaneous when the temperature is higher than the softening temperature of the glass forming material, the material always maintains in equilibrium state. When the temperature is lower than the transition temperature, the transition process takes

place quite slowly which resulting in the non-equilibrium state of glass. When the temperature lies between the softening temperature and transition temperature, the non-equilibrium state trends to approach to equilibrium state as the time increasing. The time dependent transition process of structure at particular temperature can be described as structural relaxation. In 1946, Tool introduced the fictive temperature to describe properties of glass forming materials inside and below the glass transition region. Tool illustrated fictive temperature of a material in a non-equilibrium state as the real temperature of the identical material in the equilibrium state whose structure resembles to that of the non-equilibrium material.

The first order evolution equation of fictive temperature is the most widely used one to model structural relaxation

$$\frac{dT_f}{dt} = -\frac{T_f - T}{\tau} \tag{1.1}$$

where τ is the structural relaxation time and can be calculated as

$$\tau(T, T_f) = \tau^g \exp\Big[-\frac{C_1}{\log e}\Big(\frac{C_2(T - T_f) + T(T_f - T_g)}{T(C_2 + T_f - T_g)}\Big)\Big]$$

where τ^g is the characteristic structural relaxation time at the transition temperature T_g, C_1, C_2 are all constants.

1.2 A FRACTIONAL MODEL FOR STRUCTURAL RELAXATION

Since the fractional-based models have been already used in modeling viscoelastic, diffusion problem but not throughly studied in modeling structural relaxation, our collaborator proposed a fractional model to simulate the structural relaxation of amorphous solids.

$$\frac{d^\alpha T_f}{dt^\alpha} = -\frac{T_f - T}{\tau^\alpha} \quad 0 < \alpha < 1 \tag{1.2}$$

where τ is the structural relaxation time and can be calculated as

$$\tau(T, T_f) = \tau^g \exp\Big[- \frac{C_1}{\log e}\Big(\frac{C_2(T - T_f) + T(T_f - T_g)}{T(C_2 + T_f - T_g)}\Big)\Big]$$

where τ^g is the characteristic structural relaxation time at the transition temperature T_g, C_1, C_2 are all constants.

1.3 A MODIFIED FRACTIONAL MODEL FOR STRUCTURAL RELAXATION

In previous section, we have discussed two existing models. In this section, we are going to present a new modified fractional model to describe the structural relaxation. Comparing the existing fractional model in which there is only one unknown α, we introduce a new modified model in which two parameters, α, β, are all needed to be determined. The modified model can be expressed as

$$\frac{d^\alpha T_f}{dt^\alpha} = -\frac{T_f - T}{\tau^\beta} \quad 0 < \alpha < 1, 0 < \beta < 1 \tag{1.3}$$

1.4 CLASSIC MODEL FOR SHAPE-MEMORY BEHAVIOR

Shape-memory polymers are particular materials which can recover to their original state from a deformed state caused by the outer stimulation factors such as the changing of temperature. The shape-memory behavior is introduced to describe this kind of property.

The Zener model is widely used to describe the shape-memory property. Figure 1.1 presents a general Zener model.

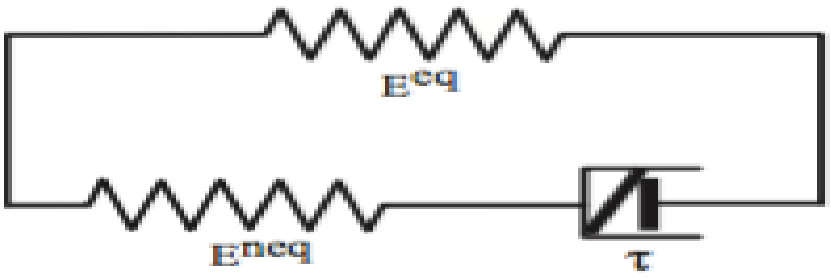

figure 1.1 representative of Zener model

Kinematics:

$$\epsilon = \epsilon^e + \epsilon^v \tag{1.4}$$

Constitutive relationship:

$$\sigma = E^{eq}\epsilon + E^{neq}\epsilon^e \tag{1.5}$$

Evolution equation of internal variable:

$$\frac{d\epsilon^v}{dt} = \frac{\epsilon - \epsilon^v}{\tau} \tag{1.6}$$

Combine (1.4),(1.5),(1.6), we get a first order ODE

$$\frac{d\epsilon^v}{dt} = \frac{\sigma(t) - E^{eq}\epsilon^v}{(E^{neq} + E^{eq})\tau} \tag{1.7}$$

where τ is a temperature-dependent relaxation time and σ is the load.

In this section, I just instruct the physical background of structural relaxation and shape-memory behavior and their corresponding first order ODE model respectively. However, although these first order models are widely used, the accuracy of these models are not so satisfactory. In the following section, I will introduce some fractional models from which we attempt to receive better numerical solutions.

1.5 A FRACTIONAL MODEL FOR SHAPE-MEMORY BEHAVIOR

Since fractional differential equations simulate the heavy tail problem very well, we try to come up with a fractional model to simulate this process.

$$\frac{d^\alpha\epsilon^v}{dt^\alpha} = \frac{\sigma(t) - E^{eq}\epsilon^v}{(E^{neq} + E^{eq})\tau^\alpha} \tag{1.8}$$

where τ is a temperature-dependent relaxation time and σ is the load.

1.6 A MODIFIED FRACTIONAL MODEL FOR SHAPE-MEMORY BEHAVIOR

In order to simulate the shape-memory behavior more accurate, we come up with a modified fractional model in which we use piecewise function to replace the unified

function on the entire domain. The main idea is to divide the time domain [0,T] in to pieces and use different fractional model to describe the property of shape-memory behavior in each piece. In this particular problem, I just divide the entire domain into two pieces [0,T'] and [T',T].

The fractional model can be expressed as

$$\frac{d\epsilon^v}{dt} = \frac{\sigma(t) - E^{eq}\epsilon^v}{(E^{neq} + E^{eq})\tau} \quad 0 < t < T' \tag{1.9}$$

$$\frac{d^\alpha\epsilon^v}{dt^\alpha} = \frac{\sigma(t) - E^{eq}\epsilon^v}{(E^{neq} + E^{eq})\tau^\alpha} \quad T' < t < T \tag{1.10}$$

1.7 SUMMARY

In this chapter, I mainly discuss the first order ODE models and there corresponding fractional models. In chapter 3, I will illustrate the inaccuracy of these first order models and fractional models which carry out better numerical solution. Before that, I will mainly discuss the numerical scheme for each model in chapter 2.

Chapter 2

NUMERICAL SCHEME

In this chapter, I will successively introduce the numerical scheme for first order model and existing fractional model for structural relaxation and shape-memory behavior. At the end of this chapter, I will introduce two modified fractional models which we find match the experimental data very well for structural relaxation and shape-memory behavior respectively. Let's begin with the first order model for structural relaxation.

2.1 FIRST ORDER MODEL FOR STRUCTURAL RELAXATION

Let's first recall the first order model in chapter 1. The fictive temperature can be expressed as

$$\frac{dT_f}{dt} = -\frac{T_f - T}{\tau} \tag{2.1}$$

where τ is the structural relaxation time and can be calculated as

$$\tau(T, T_f) = \tau^g \exp\Big[- \frac{C_1}{\log e}\Big(\frac{C_2(T - T_f) + T(T_f - T_g)}{T(C_2 + T_f - T_g)}\Big)\Big]$$

From backward difference

$$\frac{dT_f^n}{dt} = \frac{T_f^n - T_f^{n-1}}{\Delta t}, \Delta t \to 0 \tag{2.2}$$

Let's combine (2.1) with (2.2), we can easily compute T_f^n by

$$T_f^n = \frac{\Delta h T - \tau T_f^{n-1}}{\Delta t + \tau} \tag{2.3}$$

2.2 FIRST ORDER MODEL FOR SHAPE-MEMORY BEHAVIOR

In chapter 1, we have mentioned the first order model (1.7) for shape-memory behavior as

$$\frac{d\epsilon^v}{dt} = \frac{\sigma(t) - E^{eq}\epsilon^v}{(E^{neq} + E^{eq})\tau} \tag{2.4}$$

By using backward difference, we can easily get the recursive formula

$$\epsilon_n^v = \frac{\Delta t\sigma(t_n) + (E^{eq} + E^{neq})\tau\epsilon_{n-1}^v}{(E^{eq} + E^{neq})\tau + E^{eq}\Delta t} \tag{2.5}$$

2.3 A FIRST ORDER NUMERICAL APPROACHES FOR CAPUTO FRACTIONAL DERIVATIVE

Generally speaking, we used to solve a time-fractional diffusion equation with Caputo fractional derivative. In previous chapter, the two models we mentioned are all time-fractional models. In order to achieve the numerical solution of these equations, we are going to instruct the discrete approximation of Caputo fractional derivative.

From formula (A.2) in appendix A, we know the definition of Caputo fractional derivative. Then we can do the following deduction [**2**]:

$$\begin{aligned}
\frac{d^\alpha T_f^n}{dt^\alpha} &= \frac{1}{\Gamma(1-\alpha)}\int_0^{t_n} \frac{dT_f^n}{dt}(t_n - s)^{-\alpha}ds \\
&= \frac{1}{\Gamma(1-\alpha)}\sum_{j=1}^{n}\int_{(j-1)k}^{jk}[\frac{T_f^j - T_f^{j-1}}{k} + O(k)](nk - s)^{-\alpha}ds \\
&= \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\sum_{j=1}^{n}\{[\frac{T_f^j - T_f^{j-1}}{k} + O(k)][(n-j+1)^{1-\alpha} - (n-j)^{1-\alpha}]\}k^{1-\alpha} \\
&\approx \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\frac{1}{k^\alpha}\sum_{j=1}^{n}(T_f^n - T_f^{n-1})[(n-j+1)^{1-\alpha} - (n-j)^{1-\alpha}]
\end{aligned}$$

Let's assume

$$\sigma_{\alpha,k} = \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\frac{1}{k^\alpha} \text{ and } \omega_j = j^{1-\alpha} - (j-1)^{1-\alpha}$$

Then we finally have the first order approximation of Caputo fractional derivative

$$\frac{d^\alpha T_f^n}{dt^\alpha} = \sigma_{\alpha,k} \sum_{j=1}^{n} \omega_j (T_f^{n-j+1} - T_f^{n-j}) + O(k) \tag{2.6}$$

2.4 A FRACTIONAL MODEL FOR STRUCTURAL RELAXATION

In previous section, we have already deduced the numerical format for Caputo fractional derivative. Let's put it back to (1.2), we will get

$$\sigma_{\alpha,k} \textstyle\sum_{j=1}^{n} \omega_j (T_f^{n-j+1} - T_f^{n-j}) = -\frac{T_f^n - T}{\tau^\alpha}$$
$$\tau^\alpha \sigma_{\alpha,k} \textstyle\sum_{j=1}^{n} \omega_j (T_f^{n-j+1} - T_f^{n-j}) = -(T_f^n - T)$$

Then we can get the numerical approximation for T_f^n as following.

$$T_f^n = \begin{cases} \dfrac{T + \tau^\alpha \sigma_{\alpha,k} \omega_1 T_f^1}{\tau^\alpha \sigma_{\alpha,k} \omega_1 + 1} & n = 2 \\ \dfrac{T + \tau^\alpha \sigma_{\alpha,k} T_f^{n-1} - \tau^\alpha \sigma_{\alpha,k} \sum_{j=2}^{n} \omega_j (T_f^{n-j+1} - T_f^{n-j})}{\tau^\alpha \sigma_{\alpha,k} \omega_1 + 1} & n > 2 \end{cases} \tag{2.7}$$

2.5 A MODIFIED FRACTIONAL ORDER MODEL FOR STRUCTURAL RELAXATION

From the numerical scheme (2.7), we can easily get the numerical scheme for the modified model

$$T_f^n = \begin{cases} \dfrac{T + \tau^\beta \sigma_{\alpha,k} \omega_1 T_f^1}{\tau^\beta \sigma_{\alpha,k} \omega_1 + 1} & n = 2 \\ \dfrac{T + \tau^\beta \sigma_{\alpha,k} T_f^{n-1} - \tau^\beta \sigma_{\alpha,k} \sum_{j=2}^{n} \omega_j (T_f^{n-j+1} - T_f^{n-j})}{\tau^\beta \sigma_{\alpha,k} \omega_1 + 1} & n > 2 \end{cases} \tag{2.8}$$

2.6 A FRACTIONAL MODEL FOR SHAPE-MEMORY BEHAVIOR

By the formula (2.6), we can get the recursive formula

$$\epsilon_n^v = \begin{cases} \dfrac{\sigma(t_n) + \tau^\alpha \sigma_{\alpha,k}\omega_1 \epsilon_1^v}{\tau^\alpha \sigma_{\alpha,k}\omega_1 + E^{eq}} & n = 2 \\ \dfrac{\sigma(t_n) + \tau^\alpha \sigma_{\alpha,k}\epsilon_{n-1}^v - \tau^\alpha \sigma_{\alpha,k} \sum_{j=2}^{n} \omega_j (\epsilon_{n-j+1}^v - \epsilon_{n-j}^v)}{\tau^\alpha \sigma_{\alpha,k}\omega_1 + E^{eq}} & n > 2 \end{cases} \tag{2.9}$$

2.7 A MODIFIED FRACTIONAL MODEL FOR SHAPE-MEMORY BEHAVIOR

As we mentioned in chapter 1, we use piecewise function to describe shape-memory behavior. We first divide the domain of t,[0,T], into $[0, t_k]$ and $[t_k, T]$, where t_k is some grid point. Then use first order model simulate the first piece and model with order α to model the second piece. The expression of ϵ_n^v can be written as

$$\epsilon_n^v = \frac{\Delta t \sigma(t_n) + (E^{eq} + E^{neq})\tau \epsilon_{n-1}^v}{(E^{eq} + E^{neq})\tau + E^{eq}\Delta t} \quad 0 < n \leq k$$

$$\epsilon_n^v = \begin{cases} \dfrac{\sigma(t_n) + \tau^\alpha \sigma_{\alpha,k}\omega_1 \epsilon_1^v}{\tau^\alpha \sigma_{\alpha,k}\omega_1 + E^{eq}} & n = k+1 \\ \dfrac{\sigma(t_n) + \tau^\alpha \sigma_{\alpha,k}\epsilon_{n-1}^v - \tau^\alpha \sigma_{\alpha,k} \sum_{j=2}^{n} \omega_j (\epsilon_{n-j+1}^v - \epsilon_{n-j}^v)}{\tau^\alpha \sigma_{\alpha,k}\omega_1 + E^{eq}} & n > k+1 \end{cases} \tag{2.10}$$

2.8 SUMMARY

In this chapter, we expound how to deduce the numerical scheme of Caputo fractional derivative. And in the following chapter, I am going to give some numerical experiments to explain how to use the the numerical scheme to solve fractional models and how to determine the order of a fractional model with given experimental data.

Chapter 3

NUMERICAL EXPERIMENTS

In this chapter, I will give some numerical examples to illustrate why the first order model does not match the experimental data very well and then check whether existing fractional models have better results in modeling structural relaxation and shape-memory behavior. After that, I will present numerical investigation of modified fractional models which may be more accurate than current fractional models.

3.1 STRUCTURAL RELAXATION

Let's first recall the first order model in chapter 1. The fictive temperature can be expressed as

$$\frac{dT_f}{dt} = -\frac{T_f - T}{\tau} \tag{3.1}$$

where τ is the structural relaxation time and can be calculated as

$$\tau(T, T_f) = \tau^g \exp\big[- \frac{C_1}{\log e}\big(\frac{C_2(T - T_f) + T(T_f - T_g)}{T(C_2 + T_f - T_g)}\big)\big]$$

The parameters are chosen as $C_1 = 13.76, C_2 = 32.46, \tau = 900, T_g = 309K$. Now let's further define 1/N as the grid size in time, where N is an integer. Then the grid points in the time interval [0,T] are labled $t_n = nk, n = 0, 1, 2, ..., T \times N$, where k=1/N.

From (2.3), we can compute the numerical solution by iteration.

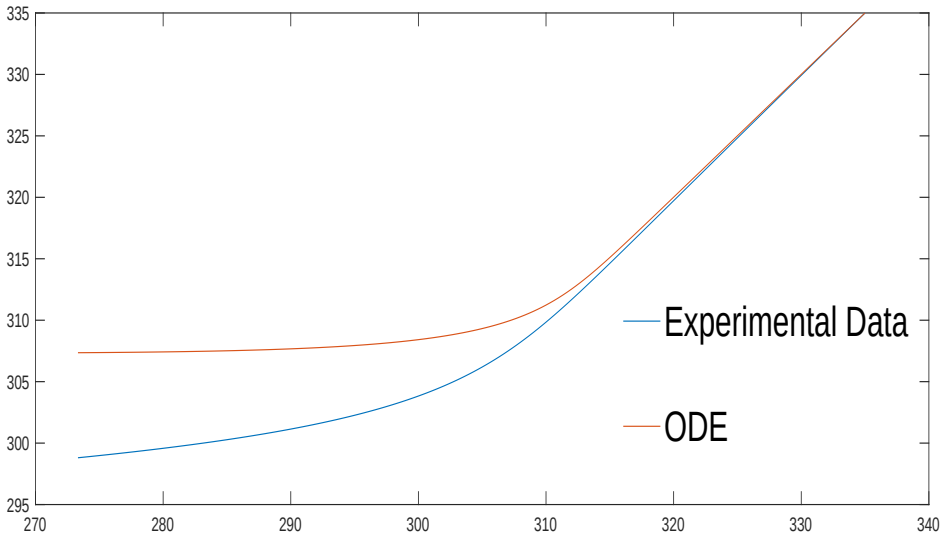

figure 3.1 Simulation by first order ODE

From figure 3.1, we can clearly see that the first order ODE model does not simulate the experimental data very well. Then let's take a look at fractional model. In chapter 1, we have mentioned that the fractional model can be expressed as

$$\frac{d^\alpha T_f}{dt^\alpha} = -\frac{T_f - T}{\tau^\alpha} \qquad 0 < \alpha < 1 \tag{3.2}$$

We can also achieve the numerical solution by iteration. Without loss of generality, we pick $\alpha = 0.2, \alpha = 0.5, \alpha = 0.8$ respectively and observe their accuracy by compute thing normalized error $\|T_f^\alpha - T_f^e\|_{L^2}$ by the following formula

$$\|T_f^\alpha - T_f\|_{L^2} = \frac{\sqrt{\sum_{j=0}^{N}(T_f^j - T_f^e(j))^2}}{N}$$

where $T_f^e(j)$ is the experimental data at time t=jk.

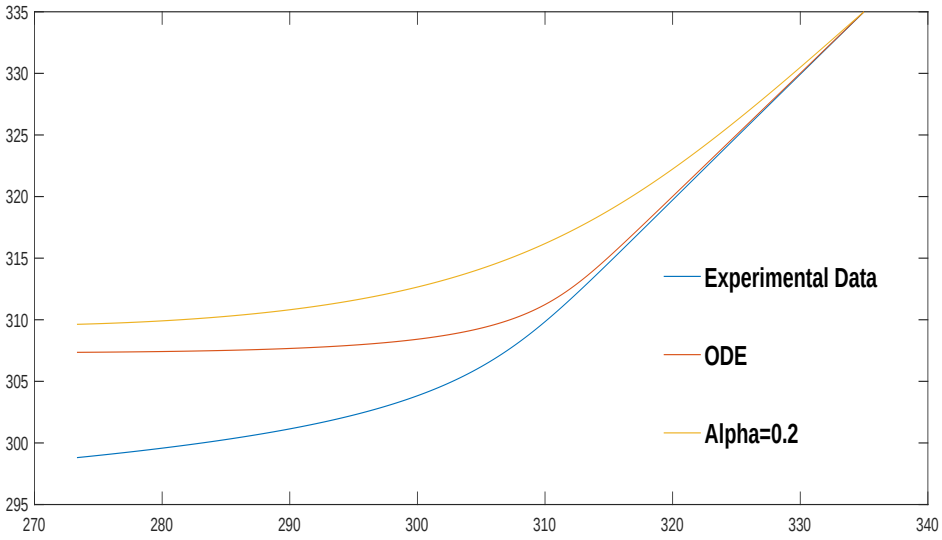

figure 3.2 Simulation by fractional model with $\alpha = 0.2$

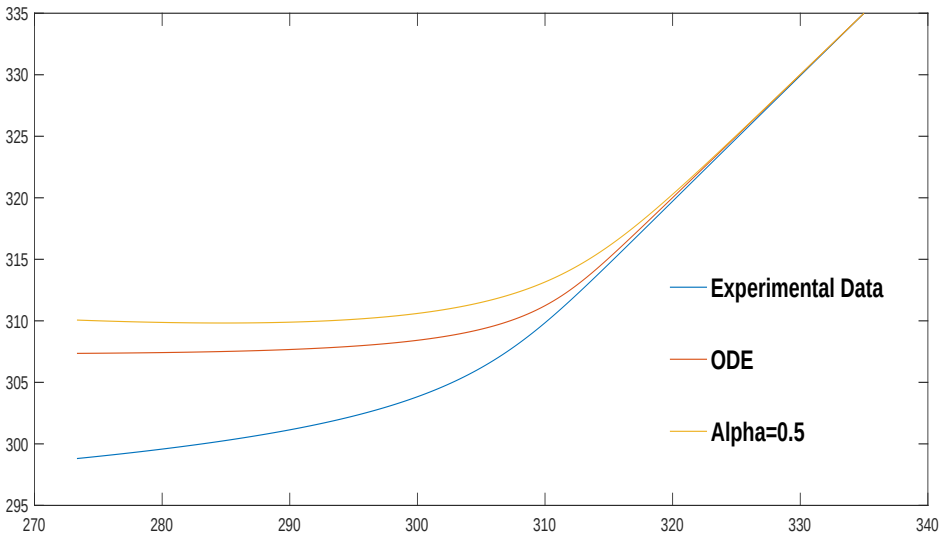

figure 3.3 Simulation by fractional model with $\alpha = 0.5$

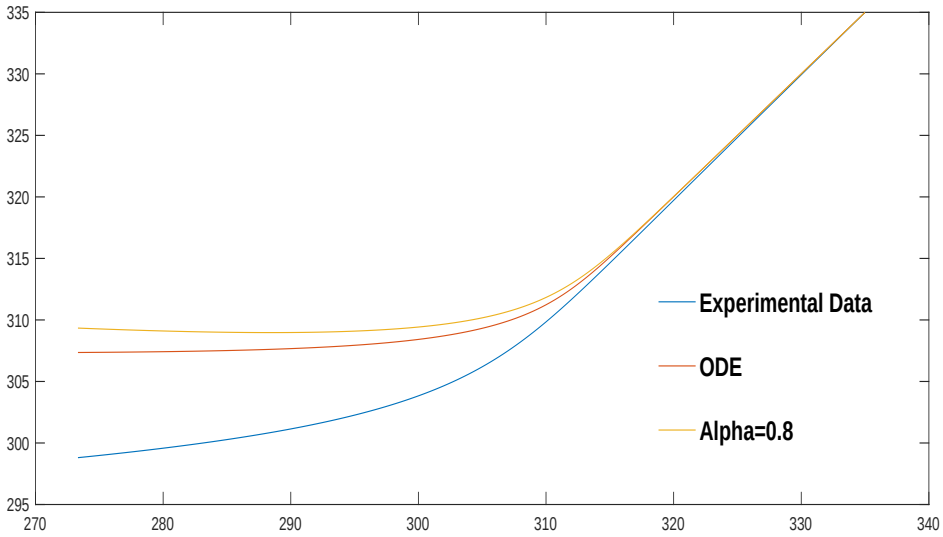

figure 3.4 Simulation by fractional model with $\alpha = 0.8$

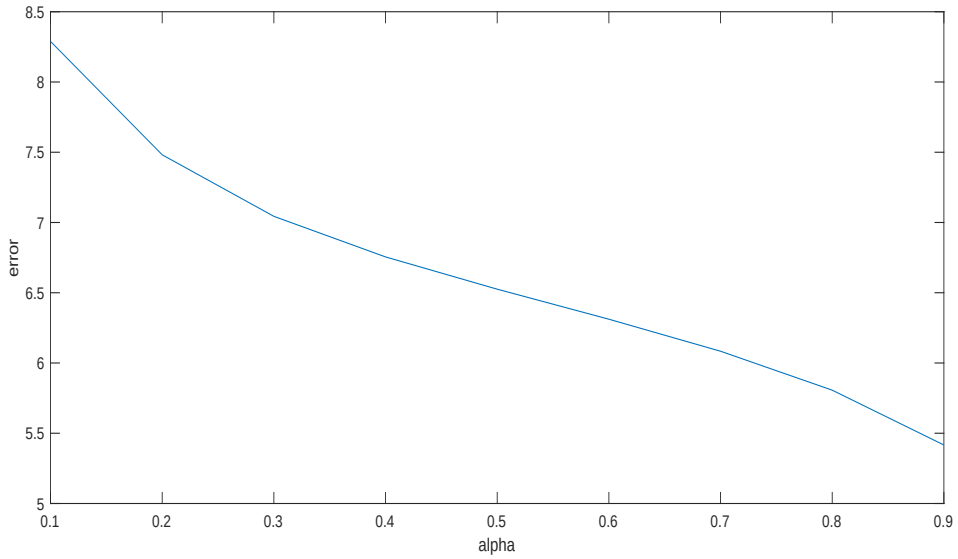

figure 3.5 The relationship between error and α

From figure 3.2, 3.3, 3.4, 3.5, it seems that as α approaches to 1, the fractional model approaches the first order model and the error also becomes smaller and smaller as well. To confirm this conclusion, let's pick $\alpha = 0.999$.

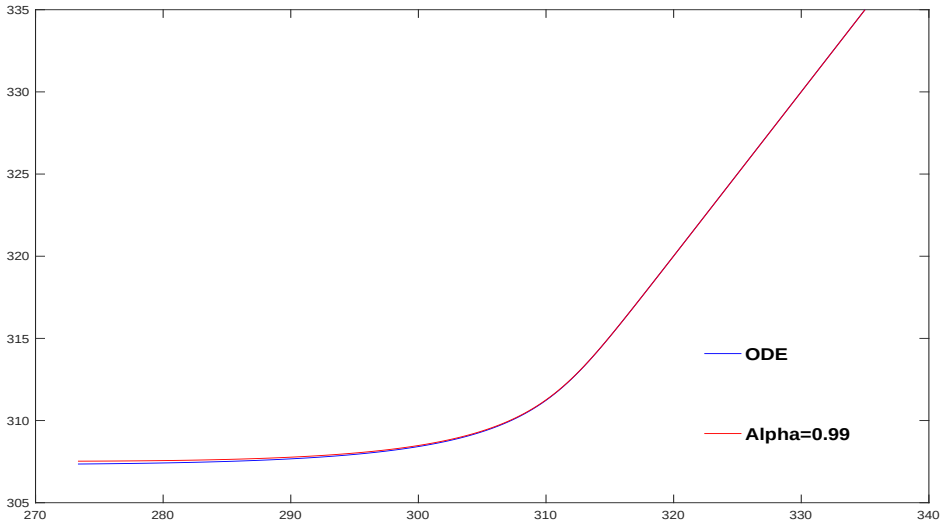

figure 3.6 The comparison between ODE and $\alpha = 0.99$.

Figure 3.6 shows that these two lines are almost overlapping which means the two numerical solutions are almost equal. In another word, the fractional model does not simulate better than the original first order model. Since these two existing models can not accurately simulate the structural relaxation process, we come up with a modified model.

$$\frac{d^{\alpha}T_f}{dt^{\alpha}} = -\frac{T_f - T}{\tau^{\beta}} \qquad 0 < \alpha < 1, 0 < \beta < 1$$

Unlike the former fractional model, in which there is only one unknown parameter, there exist two unknowns α and β this time. In order to determine these two unknowns accurately, I firstly set up the region as $\alpha = [0.1, 0.9]$ and $\beta = [0.1, 0.9]$. I want to find the minimum value of the error and its corresponding pair of α and β. Firstly, we chose $\alpha \times \beta = [0.1, 0.9] \times [0.1, 0.9]$ and 0.1×0.1 as the grid density. Then we can obtain a 3-D figure with X-axis α, Y-axis β and Z-axis error.

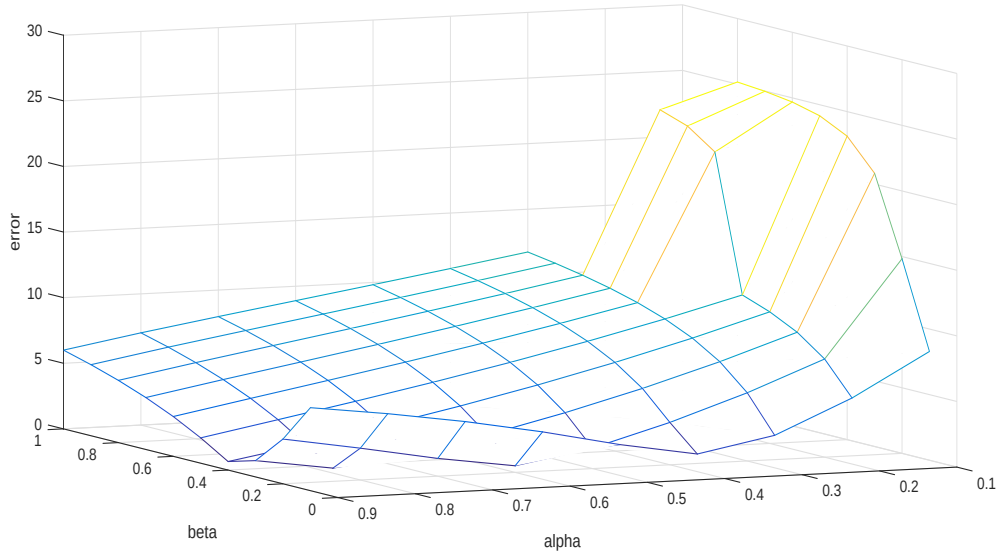

figure 3.7 The relationship between α, β and error.

Figure 3.7 shows that the minimum value of error drops in $\alpha \times \beta = [0.6, 0.8] \times [0.2, 0.4]$. Then we dense the grid in this region from 0.1×0.1 to 0.01×0.01. Then we obtain another 3-D figure as following.

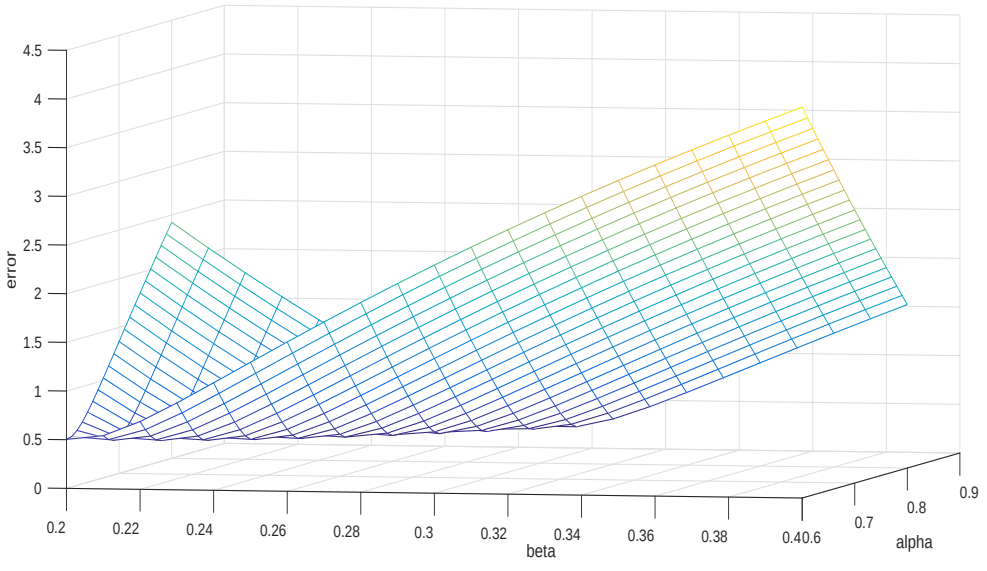

figure 3.8 The relationship between α, β and error.

We find that when $\alpha = 0.79, \beta = 0.3$ the outcome has the minimum error and the error is 0.3666. To provide how accurate my new model is, I plot the numerical solution of my

new fractional model with the experimental data and the numerical solution of ODE in a same figure.

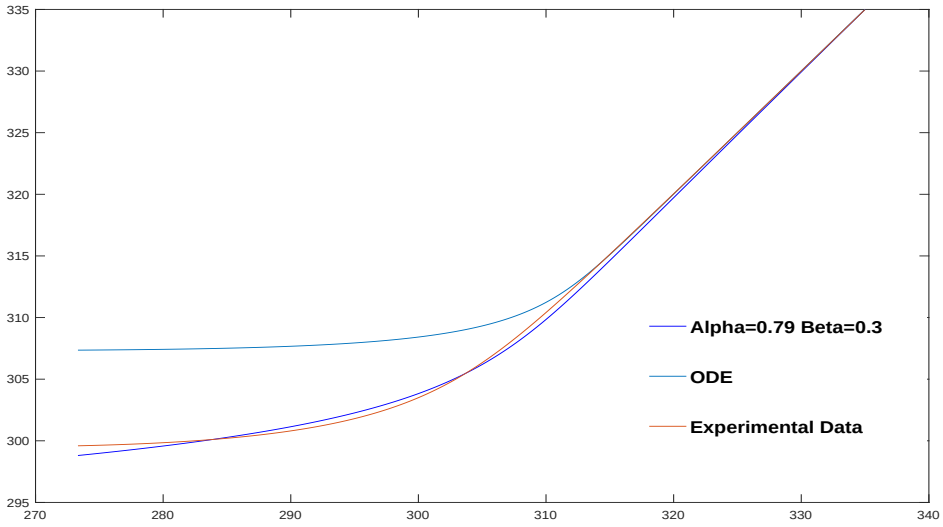

figure 3.9 The comparison of ODE model and our model.

From figure 3.9, we can easily figure out that our new fractional model are much more accurate in fitting the experimental data.

In previous section, we provide a general idea of structural relaxation process discuss the accuracy of the first order ODE model. Since the ODE model does not work very well, we then discuss the probability of a fractional model with one unknown parameter α. After the failure of attempt to set up a fractional model with one parameter, I try to come up with a modified fractional model with two unknownsα, β. By numerical experiments. I make a conclusion that my new model approaches the experimental data well and I determine the value of α, β respectively. In the coming section, I am going to introduce numerical experiments for shape-memory behavior.

Our collaborator offers us the model parameters as following: $C1 = 13.76, C2 = 32.46, T_g = 309, E^{eq} = 1.5, E^{neq} = 1500, A = 15000, \tau^{ref} = 40.$

$$\tau = \begin{cases} \tau^{ref} 10^{-\frac{C_1(T-T_g)}{C_2+T-T_g}} & T \geq T_g \\ \tau^{ref} 10^{A(\frac{1}{T}-\frac{1}{T_g})} & T < T_g \end{cases}$$

The loading condition is chosen as:$\sigma(t) = 0.01 * t, t \leq 300; \sigma(t) = 0.3, 300 < t \leq 980; \sigma(t) = 0.3 - 0.03(t - 980), 980 < t \leq 990; \sigma(t) = 0, t > 990.$

The temperature profile is chosen as:$T(t) = 333, t \leq 330; T(t) = 333-(t-330)/10, 330 < t \leq 930; T(t) = 273, 930 < t \leq 1000; T(t) = 273 + (t - 1000)/20, t > 1000.$

Applying formula (2.5) in chapter 2, we can compute the numerical solution for first order model and fractional model and compare them with experimental data respectively. From figure (3.10) and (3.11), we can conclude that, the first order model simulates every well at the very beginning, but does not match the experimental data as time going on. On contrast, the fractional model.works very well in the decay part but inaccurate in the flat part.

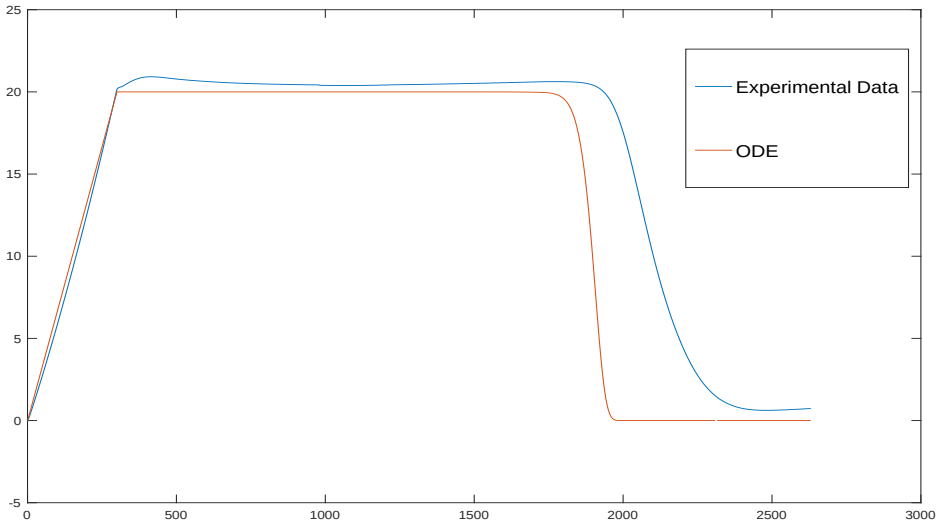

figure 3.10 First order ODE compared with experimental data

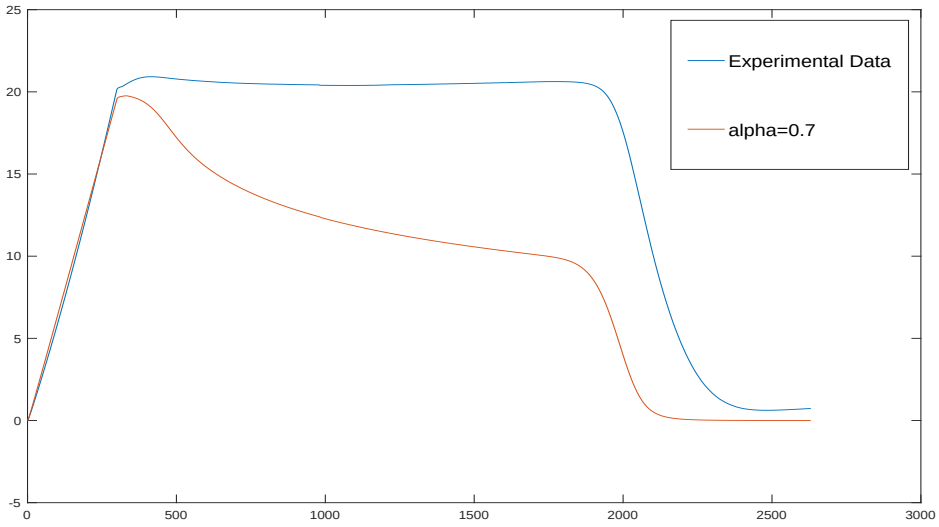

figure 3.11 FDE compared with experimental data

As we mentioned before, we need to divide the domain of t into two parts. For this problem, the domain of t is [0,2630s]. After analysis the value of τ and many tries, I pick the division point as $t_k = 1830s$. Let's utilize the trick mentioned in chapter 2 again to determine the corresponding parameter α, β (we find that the model has the minimum error

when $\alpha = 0.5, \beta = 0.7$). Using formula (2.10), we can compute the numerical solution in each piece respectively.

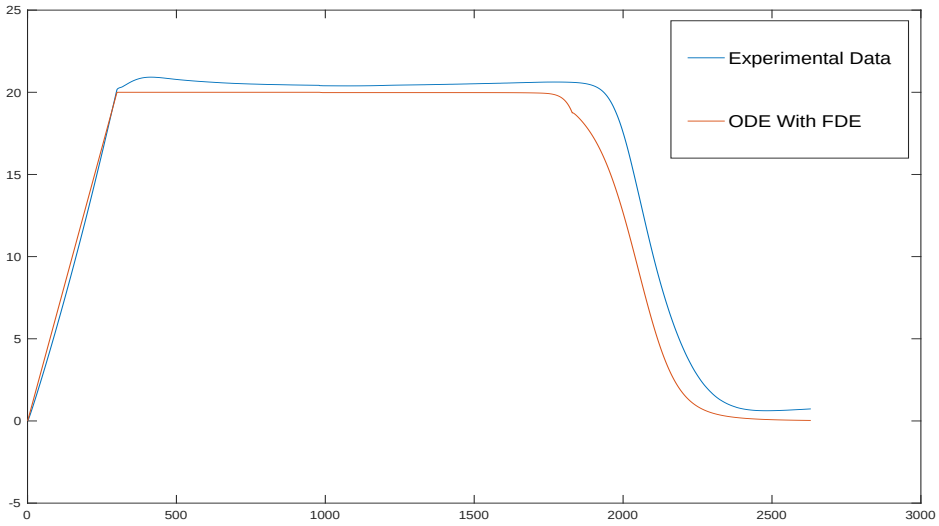

figure 3.12 A new method compared with experimental data

From figure 3.12, we find that our new model works more accurate than the previous models. However, the new model still does not simulate the decaying part very well. So I want to find some ways to improve the accuracy in this part. One way to solve this problem is to divided the decaying part into several pieces and using different fractional model in each piece to simulate. Therefore, in next chapter, I am going to illustrate how to determine the order of FDE model in each piece.

Chapter 4

VARIABLE-ORDER FRACTIONAL DIFFERENTIAL EQUATION

In many applications, it is usually not precise to use only one fractional model with constant order to simulate a given process. In order to improve the accuracy, we need to set up new model with the help of variable-order fractional differential equation. In contract to the fractional equation with constant order, the new model could change with time or space. In this chapter, I will only discuss the model changing with time.

4.1 A VARIABLE-ORDER FRACTIONAL MODEL

In this chapter, we always suppose to use time-fractional differential equation to simulate a process. Let's assume the domain of time to be [0,T] and the fractional model we use in the following form.

$$\frac{d^{\alpha}u}{dt^{\alpha}} = a(t)u + f(t) \tag{4.1}$$

The main idea in this chapter is to divide the whole domain [0,T] into pieces and use the fractional model above to simulate the process in different piece respectively. To simplify the problem, we assume the order of fractional model in each piece is constant. Let N be a positive integer, and $h = 1/N$ be the time step. Then the grid points can be expressed as $t_i = i/N, i = 0, 1, 2, ..., T \times N$. Without loss of generality, let's start with divide the domain into two pieces.$[0, t_k]$ and $[t_k, T]$ and α_1, α_2, the orders of fractional model in each part respectively. Then the model can be described as

$$\frac{d^{\alpha_1}u}{dt^{\alpha_1}} = \frac{\sigma(t) - u}{\tau(t)} \quad 0 \le t \le t_k \tag{4.2}$$

$$\frac{d^{\alpha_2}u}{dt^{\alpha_2}} = \frac{\sigma(t)-u}{\tau(t)} \quad t_k \le t \le T \tag{4.3}$$

In the first piece, we can just need to use (2.6) to get the approximation for Caputo fractional derivative in this piece. The remain problem is how to get a approximation for Caputo fractional derivative in the second piece. Since the fractional derivative is nonlocal, we need to use the value of grid points in the first piece when computing the fractional derivative in the second piece.

$$ {}_0D_{t_i}^{\alpha}u = {}_0D_{t_k}^{\alpha_1}u + {}_{t_k}D_{t_i}^{\alpha_2}u, \quad t_k \le t_i \le T \tag{4.4}$$

Let's compute ${}_0D_{t_k}^{\alpha_1}u$ at grid point $t_i, i > k$ first.

$$\begin{aligned}
{}_0D_{t_k}^{\alpha_1}u &= \frac{1}{\Gamma(1-\alpha_1)}\int_0^{t_k}\frac{du}{dt}(t_i-s)^{-\alpha_1}ds \\
&= \frac{1}{\Gamma(1-\alpha_1)}\sum_{j=1}^{k}\int_{(j-1)h}^{jh}\big[\frac{u_j-u_{j-1}}{h}+O(h)\big](ih-s)^{-\alpha_1}ds \\
&= \frac{1}{\Gamma(1-\alpha_1)}\frac{1}{1-\alpha_1}\sum_{j=1}^{k}\big\{\big[\frac{u_j-u_{j-1}}{h}+O(h)\big][(i-j+1)^{1-\alpha_1}-(i-j)^{1-\alpha_1}]\big\}h^{1-\alpha_1} \\
&\approx \frac{1}{\Gamma(1-\alpha_1)}\frac{1}{1-\alpha_1}\frac{1}{h^{\alpha_1}}\sum_{j=1}^{k}(u_j-u_{j-1})[(i-j)^{1-\alpha_1}-(i-j-1)^{1-\alpha_1}]
\end{aligned}$$

Then we compute ${}_{t_k}D_{t_i}^{\alpha_2}u$

$$\begin{aligned}
{}_{t_k}D_{t_i}^{\alpha_2}u &= \frac{1}{\Gamma(1-\alpha_2)}\int_{t_k}^{t_i}\frac{du}{dt}(t_i-s)^{-\alpha_2}ds \\
&= \frac{1}{\Gamma(1-\alpha_2)}\sum_{j=1}^{i-k}\int_{(j-1)h}^{jh}\big[\frac{u_{k+j+1}-u_{k+j}}{h}+O(h)\big](ih-s)^{-\alpha_2}ds \\
&= \frac{1}{\Gamma(1-\alpha_2)}\frac{1}{1-\alpha_2}\sum_{j=0}^{i-k-1}\big\{\big[\frac{u_{i-j}-u_{i-j-1}}{h}+O(h)\big][(j+1)^{1-\alpha_2}-j^{1-\alpha_2}]\big\}h^{1-\alpha_2} \\
&\approx \frac{1}{\Gamma(1-\alpha_2)}\frac{1}{1-\alpha_2}\frac{1}{h^{\alpha_2}}\sum_{j=0}^{i-k-1}(u_{i-j}-u_{i-j-1})[(j+1)^{1-\alpha_2}-j^{1-\alpha_2}]
\end{aligned}$$

Combining the expression of ${}_0D_{t_k}^{\alpha_1}u$ and ${}_{t_k}D_{t_i}^{\alpha_2}u$ with the formula (4.4), we can get the discrete form

$$\begin{aligned}
{}_0D_{t_i}^{\alpha}u = &\frac{1}{\Gamma(1-\alpha_1)}\frac{1}{1-\alpha_1}\frac{1}{h^{\alpha_1}}\sum_{j=1}^{k}(u_j-u_{j-1})[(i-j)^{1-\alpha_1}-(i-j-1)^{1-\alpha_1}] \\
&+\frac{1}{\Gamma(1-\alpha_2)}\frac{1}{1-\alpha_2}\frac{1}{h^{\alpha_2}}\sum_{j=0}^{i-k-1}(u_{i-j}-u_{i-j-1})[(j+1)^{1-\alpha_2}-j^{1-\alpha_2}]
\end{aligned}$$

Now, Let's put the discrete form back to (4.1)

$$au_i + f(t_i) = \frac{1}{\Gamma(1-\alpha_1)}\frac{1}{1-\alpha_1}\frac{1}{h^{\alpha_1}}\sum_{j=1}^{k}(u_j - u_{j-1})[(i-j)^{1-\alpha_1} - (i-j-1)^{1-\alpha_1}]$$
$$+ \frac{1}{\Gamma(1-\alpha_2)}\frac{1}{1-\alpha_2}\frac{1}{h^{\alpha_2}}\sum_{j=0}^{i-k-1}(u_{i-j} - u_{i-j-1})[(j+1)^{1-\alpha_2} - j^{1-\alpha_2}]$$

We finally deduce the expression of u_i as

$$u_i = [f(t_i) - \sigma_{\alpha_1,h}\sum_{j=1}^{k}(u_j - u_{j-1})[(i-j)^{1-\alpha_1} - (i-j-1)^{1-\alpha_1}]$$
$$- \sigma_{\alpha_2,h}\sum_{j=0}^{i-k-1}(u_{i-j} - u_{i-j-1})[(j+1)^{1-\alpha_2} - j^{1-\alpha_2}] + \sigma_{\alpha_2,h}u_{i-1}]/(\sigma_{\alpha_2,h} - a)$$

where $\sigma_{\alpha_i,h} = \frac{1}{\Gamma(2-\alpha_i)}\frac{1}{h^{\alpha_i}}, i = 1, 2.$

We have already conclude the expression for t_i, when the domain [0,T] is divided into two pieces. To be more general, let consider the condition that [0,T] is divided into n pieces, $[t_0, t_{k_1}], [t_{k_1}, t_{k_2}], ...[t_{k_{n-1}}, t_n]$, where $t_0 = 0, t_n = T$ and t_i drops in the m-th interval $[t_{k_{m-1}}, t_{k_m}]$, $1 \leq m \leq n$. Let's just do some induction, we can easily find that

$$u_i = [f(t_i) - \sum_{n=1}^{m-1}\sigma_{\alpha_n,h}\sum_{j=k_{n-1}}^{k_n}(u_j - u_{j-1})[(i-j)^{1-\alpha_n} - (i-j-1)^{1-\alpha_n}]$$
$$- \sigma_{\alpha_2,h}\sum_{j=0}^{i-k_{m-1}-1}(u_{i-j} - u_{i-j-1})[(j+1)^{1-\alpha_m} - j^{1-\alpha_m}] + \sigma_{\alpha_m,h}u_{i-1}]/(\sigma_{\alpha_m,h} - a)$$

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Appendix A

BASIC KNOWLEDGE OF FRACTIONAL DERIVATIVE

Fractional derivatives are defined via fractional integration. The fractional order integration can date back to the origin of differential calculus itself. The strict research about fractional derivative was first worked out by Liouville in 1837.[**3**]

After unremitting efforts in developing and modifying, various types of fractional derivatives has been studied such as Rieman-Liouville, Caputo, Hadamard, Marchand, Riesz, etc. In the following sections, I am going to pay more attentions on giving a general illustration of Riemann-Liouville fractional derivative and Caputo fractional derivative.

A.1 Riemann-Liouville Fractional derivative

The Riemann-Liouville fractional derivative [**3**] is based on Riemann-Liouville fractional integral operator which is the most widely used when computing fractional integration. Let's start with how to get the fractional integral operator.

Let f(x) be a function with x>0. The definite integral operator can be define as

$$(Jf)(x) = \int_0^x f(t)dt$$

If we repeat the process, we will get

$$(J^2 f)(x) = \int_0^x (Jf)(t)dt = \int_0^x (\int_0^t f(s)ds)dt$$

From Cauchy formula for repeated integration, we have

$$(J^n f)(x) = \frac{1}{(n-1)!}\int_0^x (x-t)^{n-1} f(t)dt$$

Now, let's replace the factorial term by Gamma function, we will get a fractional integral operator.

$$(J^{\alpha}f)(x) = \frac{1}{\Gamma(\alpha)}\int_0^x (x-t)^{\alpha-1}f(t)dt$$

From the deduction above, we already have a rough frame of the Riemann-Liouville integration operator. And the corresponding derivative is calculated as

$$ {}_aD_t^{\alpha}f(t) = \frac{d^n}{dt^n}\,{}_aI_t^{n-\alpha}f(t) = \frac{1}{\Gamma(\alpha)}\int_a^t (t-\tau)^{\alpha-1}f(\tau)d\tau,\ n = \lceil\alpha\rceil \tag{A.1}$$

A.2 Caputo fraction derivative

Another choice for computing fractional derivative is to apply Caputo fractional derivative which was derived by M. Caputo in his paper in 1967. Different from Riemann-Liouville Derivative, the Caputo fractional derivative changes the order of integration operator and derivative operator. The Caputo derivative of fractional order α of function is defined as

$$ {}_0D_t^{\alpha}f(t) = {}_0I_t^{n-\alpha}\frac{d^n}{dt^n}f(t) = \frac{1}{\Gamma(n-\alpha)}\int_0^t (t-\tau)^{(n-\alpha-1)}f^{(n)}(\tau), n = \lfloor\alpha\rfloor \tag{A.2}$$