A Doctor Thesis

博士論文

High Accuracy Numerical Computational Methods for Fractional Differential Equations

(非整数階微分方程式に対する高精度数値計算法)

by

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ABSTRACT

In many areas, many formulae which contain fractional derivatives and integrals have been proposed. Fractional calculus is the field which treats non-integer order calculus. This fractional calculus is an extended version of integer order calculus, and fractional calculus has the potential to be utilized in fields which employ integer order calculus. Actually, fractional calculus is applied to many models which cannot be represented by integer order calculus, for example, viscosity model, diffusion process, control system, finance and fractal. This thesis contributes to mainly two models. One is the simulation of diffusion process which is formulated by using fractional partial differential equations. This fractional diffusion process appears in the diffusion phenomenon of radioactive materials, and fractional calculus is used in the prediction of diffusion of materials which is spilt from Fukushima nuclear power plant. Therefore, there is a need to develop high accurate numerical computational method to predict where radioactive materials spread with highly accuracy. The other model is the simulation of control systems. Control systems include robotics and electronic systems, and fractional calculus enables simulations of those systems which perform a behavior which integer order calculus cannot simulate. Hence, by having accurate method, simulations of control systems using fractional calculus can be done precisely and many control systems will utilize fractional calculus for more appropriate modeling.

For fractional partial differential equations, the finite difference method which seems to be first order accuracy has been proposed by Mark M. Meerschaert and Charles Tadjeran, but the accuracy of the method has not been proven. They also have proposed a second order accuracy method, but that method means the extrapolation of a first order accuracy finite difference method and does not employ computational method with second order accuracy formula. For fractional ordinary differential equations, explicit computational method which applies the predictor corrector method has been proposed by Kai Diethelm. However, the global accuracy of this method is less than second order accuracy, and the local accuracy around initial point is lower than the local accuracy around terminal point. In addition to explicit computational method, implicit computational method using Gaussian quadrature has been proposed by Seyadahmad Beheshti, Hassan Khosravian-Arab and Iman Zare, but that method assumes that solution function must be represented with nondifferentiable function at an initial point. This assumption does not include the solution function which is represented with differentiable functions, and the accuracy for differentiable function is not guaranteed.

In this thesis, the author discusses the both of partial differential and ordinary differential, and proposes highly accurate numerical computational methods for parabolic fractional partial differential equations and fractional ordinary differential equations.

Firstly, the author proposes a second order accuracy finite difference method for one dimensional parabolic fractional partial differential equations, and analyzes its accuracy and stability. The author shows that the stability of the proposed finite difference methods depends on some parameters which are coefficients appeared in the scheme, and proves the condition of stability by using Gerschgorin's theorem. Next, the author represents the accuracy of the proposed finite difference method is conditionally second order accuracy, and if the analytical solution function is not differentiable on boundaries, the accuracy around boundaries decays. In addition, this thesis discusses how much accuracy will be lost depending on the analytical solution. The author also develops numerical solutions in the form of polynomial expansion for homogeneous parabolic fractional partial differential equations to investigate the stability in more detail and to find whether the analytical solution function has a property which is the condition of accuracy decaying.

Secondly, the author proposes two new numerical computational methods for fractional ordinary differential equations. One is a high accuracy explicit difference method with predictor-corrector schemes. The accuracy of this method is third order accuracy and higher than the existing methods. The other computational method is an implicit method using Gaussian quadrature and Lagrange polynomials. Since the proposed implicit method assumes the solution functions consist of polynomials and can be expanded to a series around the initial point, this method can compute such differential equations with a few nodes more accurately than existing methods.

Experimental results indicate the proposed second order accuracy finite difference method for fractional partial differential equations is actually second order accuracy and conditionally stable, and the author observes the condition to cause the accuracy decaying from the numerical experiments. In addition, by developing the numerical solutions in the form of polynomial expansion for homogeneous fractional partial differential equations, it is observed that the solution cannot be expressed with Fourier series, and the analytical solution function satisfies the condition of the accuracy decaying. Experimental results also represent that proposed explicit computational methods for fractional ordinary differential equations have higher accuracy than the existing method proposed by Kai Diethelm. For implicit computational method, the author observes that the proposed method is higher accuracy with a few nodes than the existing method proposed by Seyadahmad Beheshti, Hassan Khosravian-Arab and Iman Zare if the analytical solution can be represented with polynomials.

論文要旨

多くの分野で非整数階微分と積分を含んだ公式が提案されている。”Fractional calculus ”とは非整数階の微積分を取り扱う分野である。この非整数階微積分は整数階微積分の拡張版となっており、非整数階微積分は整数階微積分が用いられている分野で活用されうる可能性がある。現在、非整数階微積分は整数階微積分で表現する事の出来ない多くのモデルに対し応用されており、例えば、粘弾性体や拡散過程、コントロールシステム、ファイナンス、フラクタルなどに応用されている。本論文は主に二つのモデルに対し貢献する。一つは非整数階偏微分方程式で定式化された拡散過程のシミュレーションである。この非整数階拡散過程は放射性物質の拡散現象に現れ、福島原子力発電所から放出された放射性物質の拡散の予測にも非整数階微積分は用いられている。そのため、高精度でどこに放射性物質が広がるのか予測するためには高精度な数値計算法が必要である。また、もう一つのモデルは制御系のシミュレーションである。制御系はロボティクスや電子システムを含み、非整数階微積分によって整数階微積分ではシミュレートできない振る舞いをするシステムのシミュレーションが可能となる。したがって、精度の良い手法があれば、非整数階微積分を使った制御系のシミュレーションが精確に行われ、より最適なモデリングのために多くの制御系システムが非整数階微積分を活用することになるだろう。

非整数階偏微分方程式に対しては、Mark M. Meerschaert と Charles Tadjeran によって一次精度と思われる有限差分法が提案されていたが、それが本当に一次精度かは証明されていなかった。彼らは二次精度の手法も提案しているが、それは一次精度の有限差分法を加速させるという手法であり、二次精度の公式を用いたものではない。また非整数階常微分方程式に対しては、Kai Diethelm によって予測修正子法を応用する陽的な数値計算法が提案されている。しかしながら、その手法の大域誤差は二次精度以下であり、また、初期点周りの局所誤差が終端点周りの局所誤差よりも低かった。陽的な手法に加えガウス求積を用いた陰的な手法も Seyadahmad Beheshti らによって提案されている。しかしその手法は解の関数が初期点で微分不可能な関数で表現されなければいけないことを仮定している。この仮定は微分可能な解の関数を含んでおらず、微分可能な関数に対し精度を保証していない。

本論文で、著者は偏微分と常微分の両方について議論し、非整数階偏微分方程式と常微分方程式に対する高精度数値計算法を提案する。

初めに、著者は一次元非整数階偏微分方程式に対する二次精度有限差分法を提案し、その精度と安定性を解析する。また、提案する有限差分法の安定性はスキームに現れる係数であるパラメータに依存することを示し、安定性条件を Gerschgorin の定理を用いて証明する。次に、提案する有限差分法の精度が条件付きで二次精度であることを示し、もし解析解の関数が境界で微分不可能な場合、境界の周りで精度が劣化することを示す。加えて、本論文は解析解によってどの程度精度が失われるについても議論する。また、安定性についてより詳細を調査し、解析解が精度劣化の条件となる性質を持つかどうか調べるため、非整数階拡散方程式に対する多項式展開の形の数値解を導出する。

次に著者は非整数階常微分方程式に対する二つの新しい数値計算法を提案する。一つは予測子修正子法のスキームを備えた陽的差分法である。この手法の精度は三次精度であり、既存手法よりも精度が高い。もう一つの数値計算法はガウス求積とラグランジュ多項式を用いた陰解法である。提案手法は解の関数が多項式で構成されており、初期点周りで展開

されうることを仮定しているため、そのような微分方程式を少ないノードで既存の手法より高精度に計算できる。

実験結果より、非整数階偏微分方程式に対して提案する二次精度有限差分法は実際に二次精度で条件付きで安定であることが示され、精度劣化を引き起こす条件が判明した。加えて、非整数階拡散方程式に対する多項式展開の形での数値解を導出することで、解はフーリエ級数で表現不可能であり、精度劣化の条件を満たすことが示された。また、実験結果から非整数階常微分方程式に対する提案する陽的計算法は Kai Diethelm によって提案された既存の手法よりも高精度であることが判明した。陰的計算法に対しては解析解が多項式で表現できる場合、Seyadahmad Beheshti らによって提案された既存手法よりも少ないノードでより精度良く計算できることが確認できた。

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Chapter 1

Introduction

Calculus has a long history. Newton and Leibniz developed it in 17th century, and since then calculus is widely used in many fields. Fractional calculus also has a history, but it is a comparatively new field especially in computer science. It is said that Abel is the first person who introduces the idea of fractional calculus, and fractional calculus has firstly appeared in the following Abel's integral equation,

$$f(x) = \int_a^x \frac{\phi(y)}{\sqrt{x-y}} dy,$$

where f is a known function and ϕ is an unknown function. In this equation, x and a denote the height of a starting point and a terminal point respectively, and $f(x)$ is the time that an object slips down from x to a without friction or air resistance. The function ϕ is the shape of the slope, and this problem means, given the time which an object slips down on a slope, what shape is the slope. This problem is also an application of fractional calculus, and the integral of this equation is 0.5 order integral. Since this discovery by Abel, many applications of fractional calculus have been proposed.

Because fractional calculus is the extended version of integer order calculus, there is a potential to be utilized in the area which utilizes integer order calculus. Actually, after Abel's research, fractional calculus is applied to various models which it is difficult to represent by using integer order calculus, for example, diffusion process, finance, control system, viscosity model, image processing, Schrödinger equations, chaos system and fractal.

In this thesis, the author mainly contributes to two applications. One is diffusion process which is represented with fractional partial differential equations. This diffusion process appears in the phenomenon which the radioactive materials spread in the air or soil, and the fractional calculus is also used for the prediction of diffusion of radioactive materials which is spilt from Fukushima nuclear power plant. This thesis contributes to high accuracy prediction by developing high accuracy and high stability finite difference methods for fractional partial differential equations. Actually, Y. Hatano made simulations for the diffusion phenomena of Cs-137 produced by the nuclear meltdown at Chernobyl by using the author's proposed finite difference method. As related works, R. Metzler and J. Klafter have proposed the fractional dynamics to anomalous diffusion based on fractional calculus[42, 43]. E. Barkai, R. Metzler and J. Klafter have shown the fractional Fokker-Plank equations describing anomalous diffusion[41, 3]. The relation between fractional diffusion and Levy stable process has been discussed by B.J. West, P. Grigolini, R. Metzler and T.F. Nonnenmacher[62, 9]. Fractional diffusion is also related to porous medium equation[11]. As an application of fractional diffusion, finance has been also proposed[52, 34]. The price dynamics is represented with a random walk. Finance model using fractional calculus is based on continuous-time random walk and Levy flight models.

This thesis also contributes to the simulation of control systems. The control system is used in robotics or electronic systems, and requires fractional calculus to simulate more various behavior and to deal with various situations than using only integer order calculus[73, 31, 10, 50, 51]. For fractional order control systems, L. Dorcak has proposed the simulation methods by approximations using integer order control systems[18]. X. Cai and F. Liu have proposed the numerical simulation methods using difference methods[6]. To the simulation of fractional order controller, this thesis contribute by developing high accuracy numerical computational methods for fractional ordinary differential equation. Given high accuracy numerical methods, many controllers employ fractional order control systems, and more optimal modeling will be done for every systems.

Viscosity models are based on Maxwell material using springs and dashpots[35, 61]. The reason why viscosity models employ fractional calculus is fractional differentiation depends on the past information unlike integer order differentiation. Integer order differentiation has only the local meaning, but in fractional differentiation the present condition is influenced by the past condition. This property expresses well the behavior of viscosity models. In viscosity models, fractional calculus is widely used, and numerical computational methods have been proposed by H. Nasuno and N. Shimizu[74, 75]. W. Zhang and N. Shimizu also have proposed the numerical algorithm for viscosity models[64]. The research of viscosity models are used in the development of dampers or impact absorbers.

In image processing, some studies employ fractional calculus. J. Uozumi and H. Izumi have used fractional differentiation to emphasize the edge of images[71]. R. Marazzato and A.C. Sparavigna also have proposed the tool for astronomical image analysis[37]. Fractional differentiation enable detection of edges and faint objects, so this property is useful for observation of the image about galaxy.

Fractional calculus is utilized also in Schrödinger equations. N. Laskin has mentioned fractional quantum mechanics derived from the fractality of the Levy flight, and this is related to fractional Schrödinger equations[24, 26, 25]. M. Naber has proposed time fractional Schrödinger equation by applying the nonlocality of fractional differentiation[47]. Not only time fractional but also both space and time fractional Schrödinger equation also has been proposed[60, 19, 17]. Fractional Hamiltonian also has been proposed by S.I. Muslih, D. Baleanu and E. Rabei[46]. In addition, S.I. Muslih, O.P. Agrawal and D. Baleanu have suggested the solution of fractional Schrödinger equations in the form of Mittag-Leffler function[45]. D. Baleanu, Alireza K. Golmankhaneh and Ali K. Golmankhaneh have proposed the solution in the form of rapidly convergent infinite series[2].

Fractional calculus also appears in chaos systems and fractal. H. Takayasu has discussed the connection between fractional differentiation and fractal[72]. In his book, he pointed out that the fractional Brownian motion which B.B Mandelbrot and J. W. Van Ness have proposed[36] is related with fractional differentiation.

As mentioned above, recently various application of fractional calculus are proposed in many fields. Then, what is fractional calculus? Fractional calculus has some definitions, and every definition is an extended version of integer order calculus. Some definitions extends the calculus order to a complex number. The following Riemann-Liouville definition is the most widely used in fractional calculus,

$$
{}_aD_x^q f(x) = \frac{1}{\Gamma(-q)} \int_a^x \frac{f(u)}{(x-u)^{1+q}} du, \qquad q < 0
$$

$$
{}_aD_x^q f(x) = \left[\frac{d}{dx}\right]^{\lceil q \rceil} \frac{1}{\Gamma(\lceil q \rceil - q)} \int_a^x \frac{f(u)}{(x-u)^{1+q-\lceil q \rceil}} du, \qquad q > 0.
$$

There are three significant properties of this definition of fractional calculus comparing to integer order calculus. One is the singularity of the integral kernel. Second property is that fractional differentiation also needs an interval like integral. This character means that fractional differentiation is not local phenomenon, and the calculation of fractional derivative needs the past information. This property fits the property of viscosity models. Third property is to give a singularity to a differentiated function. These three properties make the numerical computation of fractional calculus difficult. Therefore, because of these difficulties, a few research of fractional calculus has been done in the field of numerical computational methods comparing to integer order calculus.

The computation of fractional differential and integral is more difficult than that of integer order calculus. However, it is not impossible to calculate numerically. For fractional differentiation and integration, K.B. Oldham has proposed the difference method with seemingly second order accuracy[49]. This method is based on Grunwald-Letnikov definition, but the author has proved its accuracy can be lower than the second order accuracy in his master thesis[57]. In addition, the author develops second order and fourth order accuracy difference methods and proves the accuracy of those methods and first order accuracy difference method in his master thesis. These high accuracy finite difference methods are employed also in this thesis, so the author introduce the outline of those methods in Chapter 4. In addition to finite difference formula, T. Okayama and S. Murashige have proposed a numerical computational method using automatic differentiation and double exponential formula[69]. However, there is a few paper about the numerical computational methods for fractional differentiation and integration. Because, the idea of fractional calculus comes from mainly applications or engineering fields, not mathematical or computational science. Therefore, there are more papers about the numerical computational methods for fractional differential equations which are near to applications than fractional differentiation and integration.

For space-fractional partial differential equations, M.M Meerschaert and C. Tadjeran have proposed finite difference methods[39, 40, 38, 56]. They have proposed first order accuracy finite difference methods, but the accuracy of the method has not been proved. In addition, they also propose the second order accuracy finite difference method. This method does not employ second order accuracy difference formula, but improves the accuracy by using extrapolation methods. Y. Zhang also has proposed a finite difference method, and analyzes the stability and convergence of his method[65]. E. Sousa has analyzed the stability of finite difference methods by using Von Neumann stability analysis[54]. Stability conditions of finite difference methods have been also discussed by R. Scherer, S.L. Kalla, L. Boyadjiev and B. Al-Saqabi[53]. As another numerical solving method, matrix transform method has been proposed by M. Ilic, F. Liu, I. Turner and V. Anh[21, 22]. This method is based on Fourier expansion, and is compared with finite difference method[63, 23]. In addition to space-fractional differential equations, time-fractional differential equations have been studied[20, 29]. Those papers treats the analytical solutions, but P. Zhuang and F. Liu have proposed finite difference methods for time-fractional differential equations[67]. D.A. Murio also has proposed a finite difference method and shows that his method is first order accuracy[44]. Y. Lin and C. Xu have proposed scheme using spectral method in space and finite difference formula in time with $O(h^{2-\alpha})$ where α is fractional calculus order[28]. Here, numerical solving methods for fractional partial differential equations are introduced, but the analytical solution is also discussed. O.P. Agrawal has expressed the analytical solution in bounded domain by using sine function and Mittag-Leffler function[1]. In contrast, F. Mainardi has considered the analytical solution in unbounded domain[32, 33]. The analytical solution in infinite domain is introduced mainly by Laplase transform and Green function.

For fractional ordinary differential equations, various numerical solving methods are proposed. As explicit numerical computational methods, predictor corrector method has been proposed by K. Diethelm, N.J. Ford, A.D. Freed and Y. Luchko[13, 14, 15, 12]. This method is stable for various conditions, but the accuracy is less than second order accuracy. To improve the accuracy, the method using Gauss-Jacobi quadrature has been proposed by L. Zhao and W. Deng[66]. Another numerical solving method is linear multi-step method. C. Lubich has introduced linear multi-step methods to Volterra integral equations[30], which can be used also for fractional ordinary differential equations. R. Lin and F. Liu also have proposed linear multi-step methods and have analyzed their stability[27]. For fractional ordinary differential equations, implicit numerical computational methods have been also proposed. S. Beheshti, H. Khosravian-Arab and I. Zare propose an implicit method using Jacobi polynomial which is a kind of orthogonal polynomials[4]. This method assumes that the analytical solution is represented by non-differentiable function around an initial point. Because of that, the accuracy for a differentiable function is not better than other methods. T. Okayama has proposed the method using double exponential transform[48]. However, this method assumes only linear equations and does not consider the case of non-linear equations. Moreover, the experimental results of this method are not shown.

In this thesis, the author discusses fractional partial and ordinary differential equations, and proposes high accuracy numerical computational methods for those two equations.

Firstly, the author proposes second order accuracy finite difference methods for one-dimensional and two-dimensional fractional partial differential equations, and analyzes the accuracy and stability. The proposed finite difference methods have a parameter in the schemes, and it is proved that the stability depends on the value of the parameter. In addition, the author proves the optimal value of the parameter. The stability analysis of the proposed scheme is done by using Gerschgorin's theorem. Therefore, proposed schemes do not impose any assumption to the analytical solution of fractional partial differential equations like Von Neumann stability analysis. Next, the author shows that the proposed finite difference methods have second order accuracy, and if the analytical solution can be expanded with low degree polynomials around boundaries, the accuracy will decay. The author also shows this accuracy decaying is caused by the approximations to fractional differential with one point difference formula. In addition, the author discusses how much the accuracy will be lost depending the analytical solution, and shows how the accuracy decaying occurs with some examples. Lastly, the author develops the numerical solutions in the form of polynomial expansion for homogeneous parabolic fractional partial differential equations to investigate what shape the analytical solution is and how much the accuracy decaying happens. Moreover, the author shows that the analytical solution for homogeneous parabolic fractional partial differential equations also can be expanded with orthogonal functions as the analytical solution for integer order partial differential equations are expanded with sine and cosine functions in Fourier expansion.

For fractional ordinary differential equations, the author proposes new high accuracy explicit numerical methods like Runge-Kutta methods. This proposed methods are higher accuracy than existing numerical computational methods, and can calculate with any order accuracy by approximating high degree terms. Moreover, the author analyzes the stability of these methods. In addition to explicit methods, the author also proposes an implicit numerical computational method using Lagrange polynomials, and try experiments of a method using double exponential transform. The method using double exponential transform has higher accuracy than any existing methods with the same number of discretized points, and the method using Lagrange polynomials employs Gauss-Jacobi quadrature and computes high accuracy with a few number of discretized points for the analytical solution which is represented with low degree polynomials.

The organization of this thesis is as follows. This thesis states preliminaries after introduction. In Chapter 2, definitions of fractional calculus are introduced and some properties of fractional calculus are shown with examples. Additionally, the author develops the fractional partial differential equations from Levy flight model. Also in preliminary, the author establishes the problems which this thesis treats. In Chapter 3 about related work, the author introduces six studies relating to this thesis. Six studies are explained in detail in order to compare to the author's research. In Chapter 4, our proposed difference formulae for fractional differentiation and integration are explained with examples and numerical experiments. In Chapter 5, finite difference methods for fractional partial differential equations are discussed. This chapter includes the explanation how to apply difference formulae to finite difference methods, and the stability analysis is also represented in this chapter. Next, the numerical solutions in the form of polynomial expansion are introduced. In this Chapter 6, the author suggests new numerical computational methods for homogeneous parabolic fractional partial differential equations by using fractional sine and cosine. Chapter 7 treats numerical computational methods for fractional ordinary differential equations. This chapter includes both the explicit and the implicit methods. In the last chapter of conclusion, the author summarizes his research, and discusses the future tasks.

Chapter 2

Preliminary

2.1 Gamma function and some properties

Gamma function is an extension of factorial. Fractional calculus utilizes this property to connect integer to fractional number. Gamma function is defined by

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt.$$

Gamma function has three significant properties for fractional calculus and for this thesis. First property is given by

$$\Gamma(x) = (x-1)\Gamma(x-1).$$

From this property, the factorial of integer is computed. Second property is the summation of ratios of gamma functions, which is given by

$$\sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} = -\frac{1}{q}\frac{\Gamma(N-q)}{\Gamma(N)}$$

where q is an arbitrary real number. This expression is used in order to compute the accuracy order of our proposed methods. One of the definitions of fractional calculus contains this summation of ratios of gamma functions, so this appears often in the expressions about fractional calculus. Third property is asymptotic expansion of gamma functions[58]. For $N \to \infty$, this is given by

$$\begin{aligned} \frac{\Gamma(N-q)}{\Gamma(N)} &= N^{-q}\left[1 + \frac{q(q+1)}{2N} + \frac{q(q+1)(q+2)(3q+1)}{24N^2} \right. \\ &\quad \left. + \frac{q^2(q+1)^2(q+2)(q+3)}{48N^3} + O\left(\frac{1}{N^4}\right)\right]. \\ \frac{\Gamma(N+\alpha)}{\Gamma(N+\beta)} &= N^{\alpha-\beta}\left[1 + \frac{(\alpha-\beta)(\alpha+\beta-1)}{2N} + O\left(\frac{1}{N^2}\right)\right] \end{aligned}$$

where q, α and β are arbitrary real numbers. By using this property, we can exchange the exponent number and a ratio of gamma functions for the limit $N \to \infty$. Therefore, these expressions also often appear in the proof about our proposed formulae.

2.2 Definition of fractional calculus

Fractional differentiation and integration have several definitions, and this section introduces definitions which are used in this thesis. Let q be the differential and integral order. The fractional calculus operator means differential for $q > 0$ and integral for $q < 0$. In addition, $q = 0$ means identity transform. Then, the fractional integral operator is defined as

$$ {}_aD_x^q f(x) = \frac{1}{\Gamma(-q)} \int_a^x \frac{f(u)}{(x-u)^{1+q}} du, \qquad q < 0 $$

where a is a constant. However, fractional differential is defined with two ways. The most general definition is the following Riemann-Liouville definition which is also introduced in Chapter 1,

$$ {}_a^{\mathrm{R}}D_x^q f(x) = \left[\frac{d}{dx}\right]^{\lceil q \rceil} \frac{1}{\Gamma(\lceil q \rceil - q)} \int_a^x \frac{f(u)}{(x-u)^{1+q-\lceil q \rceil}} du, \qquad q > 0. $$

Note that R in the above expression is the initial of Riemann-Liouville. This definition indicates that the numerical computation methods of fractional calculus are more difficult than that of integer order calculus. There are three properties about this definition different from integer order calculus. One is singularity of integral kernel. Because of the singularity, the kernel diverges at an end point of integral. This singularity makes it impossible that we use the same methods to that of integer order calculus to calculate integration. In integer order calculus, the rectangular rule or the trapezoidal rule are used, but those methods cannot calculate fractional integral accurately. Second property is that fractional differentiation is defined as an operator on an interval like integral. This means the past information and states affect the present states, and this property is utilized in the simulation of viscosity models. Third property is that the differentiated and integrated function get a singularity by fractional calculus. If fractional differential or integral is applied to the function which is continuous and differentiable, that function is changed to the function having a non-differentiable point. Actually, by applying fractional differential to a constant function $f(x) = C$, we have

$$ \begin{aligned} {}_a^{\mathrm{R}}D_x^q C &= \left[\frac{d}{dx}\right]^{\lceil q \rceil} \frac{1}{\Gamma(\lceil q \rceil - q)} \int_a^x \frac{C}{(x-u)^{1+q-\lceil q \rceil}} du \\ &= \left[\frac{d}{dx}\right]^{\lceil q \rceil} \frac{1}{\Gamma(\lceil q \rceil - q)} \frac{C(x-a)^{\lceil q \rceil - q}}{\lceil q \rceil - q} \\ &= \frac{C(x-a)^{-q}}{\Gamma(1-q)}. \end{aligned} $$

As we see, the differentiated function has a singularity at the initial point $x = a$. This property makes us to treat not only polynomials but real number degree functions like $f(x) = (x-a)^p$ where p is arbitrary real number.

Next definition is the following Caputo definition as

$$ {}_a^{\mathrm{C}}D_x^q f(x) = \frac{1}{\Gamma(\lceil q \rceil - q)} \int_a^x \frac{f^{(\lceil q \rceil)}(u)}{(x-u)^{1+q-\lceil q \rceil}} du, q > 0. $$

Note that the C in the above expression denotes that this operator is Caputo definition. Caputo definition is defined as operating fractional integral after integer order differential. The difference between Riemann-Liouville definition and Caputo definition appears for the function $f(x) = C$. That is, ${}_a^{\mathrm{R}}D_x^q C = C(x-a)^{-q}/\Gamma(1-q)$ and ${}_a^{\mathrm{C}}D_x^q C = 0$. However, Caputo definition also gives a singularity to a function, for example, $f(x) = (x-a)^p$ for $p > q$. From these defintions, we have convenient formulae as

$$\begin{aligned} {}_a^{\mathrm{R}}D_x^q f(x) &= D^{\lceil q \rceil}\ {}_aD_x^{q-\lceil q \rceil} f(x), \\ {}_a^{\mathrm{C}}D_x^q f(x) &= {}_aD_x^{q-\lceil q \rceil}\ D^{\lceil q \rceil} f(x). \end{aligned}$$

This means that Riemann-Liouville definition and Caputo definition are given by exchanging the order of calculus, and the properties of these two definitions are really alike. The integrals included in these two definitions are integrated from left to right in x axis, but there are definitions which integrate from right to left. This left side fractional integral is defined as

$${}_xD_b^q f(x) = \frac{1}{\Gamma(-q)} \int_x^b \frac{f(u)}{(u-x)^{1+q}} du.$$

Moreover, left side fractional differentials are also defined as

$$\begin{aligned} {}_x^{\mathrm{R}}D_b^q f(x) &= D^{\lceil q \rceil}\ {}_xD_b^{q-\lceil q \rceil} f(x) \\ {}_x^{\mathrm{C}}D_b^q f(x) &= {}_xD_b^{q-\lceil q \rceil}\ D^{\lceil q \rceil} f(x) \end{aligned}$$

These left side operators are also utilized in applications, and especially fractional partial differential equations which are introduced later in this thesis employ these operators. Last definition is Grunwald-Letnikov definition as

$${}_a^{\mathrm{G}}D_x^q f(x) = \lim_{N\to\infty} \frac{h^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-jh)$$

where $h = (x-a)/N$. Note that G in the above expression denotes this operator is Grunwald-Letnikov definition. This definition has the same form between integral and differential, and expresses both fractional integral and differential in one formula. This definition is given by the generalization of the definition of integer order derivative. Actually, first, second and n-th order derivatives are defined as

$$\begin{aligned} f'(x) &= \lim_{h\to 0} \frac{f(x) - f(x-h)}{h} \\ f''(x) &= \lim_{h\to 0} \frac{f(x) - 2f(x-h) + f(x-2h)}{h^2} \\ f'''(x) &= \lim_{h\to 0} \frac{f(x) - 3f(x-h) + 3f(x-2h) - f(x-3h)}{h^3} \\ &\vdots \\ f^{(n)}(x) &= \lim_{h\to 0} \frac{1}{\Gamma(-n)h^n} \sum_{j=0}^{n} \frac{\Gamma(j-n)}{\Gamma(j+1)} f(x-jh). \end{aligned}$$

Here, we put $h = (x-a)/N$. Because the values of $\Gamma(j-n)/\left(\Gamma(-n)\Gamma(j+1)\right)$ equal to 0 for $j \le n+1$, we have

$$f^{(n)}(x) = \lim_{N\to\infty} \frac{h^{-n}}{\Gamma(-n)} \sum_{j=0}^{N-1} \frac{\Gamma(j-n)}{\Gamma(j+1)} f(x-jh).$$

By generalizing n to real number q, the above formula equals to Grunwald-Letnikov defitnition. In addition, K.B. Oldham has been proved that Grunwald-Letnikov definition and Riemann-Liouville definition are the same[49]. Left side Grunwald-Letnikov definition is defined as

$${}_x^{\mathrm{G}}D_b^q f(x) = \lim_{N\to\infty} \frac{h^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x+jh)$$

where $h = (b - x)/N$.

2.3 The basic properties of fractional calculus

This section explains basic properties of fractional calculus. Firstly, the author shows the fractional derivative of exponentiation functions. By Riemann-Liouville definition, power functions are differentiated as

$$ {}_a^{\mathrm{R}}D_x^q (x-a)^p = \left[\frac{d}{dx}\right]^{\lceil q\rceil} \frac{1}{\Gamma(\lceil q\rceil - q)} \int_a^x \frac{(u-a)^p}{(x-u)^{1+q-\lceil q\rceil}} du, $$

where $p > -1$. By applying changing variables for $v = (u-a)/(x-a)$, we have

$$ = \left[\frac{d}{dx}\right]^{\lceil q\rceil} \frac{1}{\Gamma(\lceil q\rceil - q)} \int_0^1 (x-a) \frac{v^p (x-a)^p}{(x-a)^{1+q-\lceil q\rceil}(1-v)^{1+q-\lceil q\rceil}} dv. $$

This integral is a beta function, and it holds

$$ = \left[\frac{d}{dx}\right]^{\lceil q\rceil} \frac{1}{\Gamma(\lceil q\rceil - q)} (x-a)^{p-q+\lceil q\rceil} \frac{\Gamma(p+1)\Gamma(\lceil q\rceil - q)}{\Gamma(p+1+\lceil q\rceil - q)}. $$

Therefore, we have

$$ {}_a^{\mathrm{R}}D_x^q (x-a)^p = \frac{\Gamma(p+1)}{\Gamma(p+1-q)} (x-a)^{p-q}. $$

This formula holds for fractional integral $q < 0$ in the same way. In addition, the derivative to $f(x) = (x-a)^{q-1}$ becomes 0 as

$$ {}_a^{\mathrm{R}}D_x^q (x-a)^{q-1} = 0. $$

Therefore, the following function is identity to fractional derivatives ${}_0^{\mathrm{R}}D_x^q$,

$$ f(x) = \frac{x^{q-1}}{\Gamma(q)} + \frac{x^{2q-1}}{\Gamma(2q)} + \frac{x^{3q-1}}{\Gamma(3q)} + \cdots . $$

Next, let us consider the fractional integral operator ${}_{-\infty}D_x^q$ for $q < 0$. By operating this fractional integral to an exponential function, we find the common point to integer order calculus as

$$ {}_{-\infty}D_x^q e^{ax} = \frac{1}{\Gamma(-q)} \int_{-\infty}^x \frac{e^{au}}{(x-u)^{1+q}} du. $$

By applying changing variables $v = x - u$, we have

$$ = \frac{1}{\Gamma(-q)} \int_0^\infty \frac{e^{ax-av}}{v^{1+q}} du. $$

This is Laplace transform, and it holds

$$ \begin{aligned} &= \frac{e^{ax}}{\Gamma(-q)} \frac{\Gamma(-q)}{a^{-q}} \\ &= a^q e^{ax}. \end{aligned} $$

In the same way, it holds for fractional derivative, and $f(x) = e^x$ is the identity function to the fractional calculus operator ${}_{-\infty}^{\mathrm{R}}D_x^q$ and ${}_{-\infty}^{\mathrm{C}}D_x^q$ for arbitrary q. This result indicates that the continuity of fractional calculus and integer order calculus for exponential functions, and the effectivity of functional transform for fractional calculus operator. In fact, Fourier transform and Mellin transform are used to analyze fractional calculus. Lastly, we check the additivity of fractional calculus operator. Generally, it does not hold the additivity,

$$\begin{aligned} {}^{\mathrm{R}}_{a}D^{p}_{x}\,{}^{\mathrm{R}}_{a}D^{q}_{x}f(x) &\neq {}^{\mathrm{R}}_{a}D^{p+q}f(x), \\ {}^{\mathrm{C}}_{a}D^{p}_{x}\,{}^{\mathrm{C}}_{a}D^{q}_{x}f(x) &\neq {}^{\mathrm{C}}_{a}D^{p+q}f(x) \end{aligned}$$

for some $f(x)$ and $p, q > 0$. For example, the additivity does not hold for the function $f(x) = x^{q-1}$ in first formula, and does not hold for the function $f(x) = 1$ in second formula. This property is also big difference from integer order calculus.

Lastly, the author shows two important rules. One is the additivity of fractional integral. As mentioned above, the additivity for fractional derivative does not hold in general, but the additivity for fractional integral holds.

Theorem 2.3.1 *For arbitrary negative real numbers $p, q < 0$, it holds*

$$ {}_{a}D^{p}_{x}\,{}_{a}D^{q}_{x}f(x) = {}_{a}D^{p+q}_{x}f(x). $$

Next, the author shows the exchange rule between Riemann-Liouvillde definition and Caputo definition.

Theorem 2.3.2 *For an arbitrary real number $q > 0$, it holds*

$$ {}^{\mathrm{R}}_{a}D^{q}_{x}f(x) = \sum_{n=0}^{\lceil q\rceil-1} \frac{f^{(n)}(a)}{\Gamma(1-q+n)}(x-a)^{n-q} + {}^{\mathrm{C}}_{a}D^{q}_{x}f(x). $$

Proof
By applying integration by parts, we have

$$\begin{aligned} & {}^{\mathrm{R}}_{a}D^{q}_{x}f(x) \\ = & \left[\frac{d}{dx}\right]^{\lceil q\rceil} \frac{1}{\Gamma(\lceil q\rceil-q)} \int_a^x \frac{f(u)}{(x-u)^{1+q-\lceil q\rceil}}du \\ = & \left[\frac{d}{dx}\right]^{\lceil q\rceil} \left\{ \frac{1}{\Gamma(\lceil q\rceil-q)} \left[-f(u)\frac{(x-u)^{\lceil q\rceil-q}}{\lceil q\rceil-q} \right]_a^x + \frac{1}{\Gamma(\lceil q\rceil-q)} \int_a^x f'(u)\frac{(x-u)^{\lceil q\rceil-q}}{\lceil q\rceil-q}du \right\} \\ = & \left[\frac{d}{dx}\right]^{\lceil q\rceil} \left\{ \frac{1}{\Gamma(\lceil q\rceil-q)} f(a)\frac{(x-a)^{\lceil q\rceil-q}}{\lceil q\rceil-q} + \frac{1}{\Gamma(\lceil q\rceil-q)} \int_a^x f'(u)\frac{(x-u)^{\lceil q\rceil-q}}{\lceil q\rceil-q}du \right\} \end{aligned}$$

By applying Leibniz integral rule which is given by

$$ \frac{d}{dx}\int_{a(x)}^{b(x)} g(x,u)du = \int_{a(x)}^{b(x)} \frac{\partial g(x,u)}{\partial x}du + b'(x)g(x,b(x)) - a'(x)g(x,a(x)), $$

we obtain

$$ = \left[\frac{d}{dx}\right]^{\lceil q\rceil-1} \left\{ \frac{f(a)}{\Gamma(\lceil q\rceil-q)}(x-a)^{\lceil q\rceil-q-1} + \frac{1}{\Gamma(\lceil q\rceil-q)} \int_a^x f'(u)(x-u)^{\lceil q\rceil-q-1}du \right\}. $$

By repeating this, we have

$$ {}^{\mathrm{R}}_{a}D^{q}_{x}f(x) = \sum_{n=0}^{\lceil q\rceil-1} \frac{f^{(n)}(a)}{\Gamma(1-q+n)}(x-a)^{n-q} + {}^{\mathrm{C}}_{a}D^{q}_{x}f(x). $$

□

2.4 Derivation of fractional partial differential equations

2.4.1 Fourier transform for tempered distributions

In this subsection, suppose the Fourier transform to fractional differentiation and integration operators. Fourier transform to fractional operator is the essential to develop fractional partial differential equations from heavy tailed probabilistic distribution. By having Fourier transform to fractional operator, fractional partial differential equations are developed from a probability density function like diffusion equations. To know how to get equations is important to know how to apply equations to physical phenomena. However, there is no paper including the detail of Fourier transform to fractional operator and how to develop equations. Therefore, in this subsection let us consider how to obtain Fourier transform to fractional operator. This Fourier transform is not the same to Fourier transform in general meaning, because fractional operator includes a non-integral function. However, if the function is tempered distribution, Fourier transform can be applied to it. Firstly, Fourier transform is defined with the following notations as

$$F\left\{f(x);w\right\} = \hat{f}(w) = \int_{-\infty}^{\infty} f(x)e^{-ixw}dx.$$

Then, Fourier transform to fractional operator is shown by the following theorem.

Theorem 2.4.1 *For arbitrary $q>0$, it holds*

$$\begin{aligned} F\left\{{}^{\mathrm{C}}_{-\infty}D^q_x f(x);w\right\} = \left\{{}^{\mathrm{R}}_{-\infty}D^q_x f(x);w\right\} = (iw)^q\hat{f}(w), \\ F\left\{{}^{\mathrm{C}}_{x}D^q_\infty f(x);w\right\} = \left\{{}^{\mathrm{R}}_{x}D^q_\infty f(x);w\right\} = (-1)^{\lceil q\rceil}(-iw)^q\hat{f}(w). \end{aligned}$$

Proof
Firstly, we prove that $F\left\{{}^{\mathrm{C}}_{\infty}D^q_x f(x);w\right\} = (iw)^q\hat{f}(w)$. Let $g(x)$ be

$$g(x) = \begin{cases} \frac{x^{\lceil q\rceil-1-q}}{\Gamma(\lceil q\rceil-q)}, & x>0 \\ 0, & x\le 0. \end{cases}$$

Then, from the convolution of Fourier transform, we have

$$\begin{aligned} & F\left\{{}^{\mathrm{C}}_{-\infty}D^q_x f(x);w\right\} \\ = & F\left\{\frac{1}{\lceil q\rceil - q}\int_{-\infty}^{x}\frac{f^{(\lceil q\rceil)}(u)}{(x-u)^{1+q-\lceil q\rceil}}du;w\right\} \\ = & F\left\{\int_{-\infty}^{\infty} f^{(\lceil q\rceil)}(u)g(x-u)du;w\right\} \\ = & (iw)^{\lceil q\rceil}\hat{f}(w)\cdot\hat{g}(w). \end{aligned}$$

Here, in general Fourier transform, to transform a function, the function must be integrable as

$$\int_{-\infty}^{\infty}|f(x)|dx < M$$

where M is a constant. However, the function g is not integrable in the above sense. Therefore, we have to consider Fourier transform in the meaning of distributions or generalized functions. To apply Fourier transform to the function g, we introduce three ideas of functions[70, 55]. One is the rapidly decreasing function which is introduced in the following definition.

Definition 2.4.2 *If a function f satisfies the following conditions, the function f is a rapidly decreasing function,*

$$\begin{aligned} & f \in C^{\infty}(\mathbb{R}) \\ & \sup_x |x^m D^n f(x)| < \infty \end{aligned}$$

where m, n are arbitrary positive integers.

Next, we define semi-norm for a rapidly decreasing function f as

Definition 2.4.3

$$p_m(f) = \sum_{\alpha+k \leq m} \sup_x (1+|x|^2)^k |D^{\alpha} f(x)|$$

where k, α are arbitrary positive integer.

Lastly, we define tempered distribution as

Definition 2.4.4 *If a function f satisfies the following two conditions, the function f is tempered distribution.*

1. $$\int_{-\infty}^{\infty} f(x) c\phi(x) dx = c \int_{-\infty}^{\infty} f(x)\phi(x) dx,$$
   $$\int_{-\infty}^{\infty} f(x)(\phi(x)+\psi(x)) dx = \int_{-\infty}^{\infty} f(x)\phi(x) dx + \int_{-\infty}^{\infty} f(x)\psi(x) dx,$$
2. $$\left| \int_{-\infty}^{\infty} f(x)\phi(x) dx \right| \leq C p_m(\phi)$$

where c is a constant, ϕ and ψ are rapidly decreasing functions, and $C > 0$.

By using the above definitions, it is indicated that the function g is a tempered distribution. To suppose the inner product between the function g and a rapidly decreasing function ϕ, we have

$$\begin{aligned} & \int_{-\infty}^{\infty} \frac{x^{\lceil q \rceil - 1 - q}}{\Gamma(\lceil q \rceil - q)} \phi(x) dx \\ = & \lim_{\epsilon \to 0} \int_{\epsilon}^{\infty} \frac{x^{\lceil q \rceil - 1 - q}}{\Gamma(\lceil q \rceil - q)} \phi(x) dx. \end{aligned}$$

Here, apparently, the above formula satisfies the condition 1. Since $\lim_{x\to\infty} \phi(x) = 0$, by applying integral by part, we have

$$= - \int_0^{\infty} \frac{x^{\lceil q \rceil - q}}{\Gamma(\lceil q \rceil + 1 - q)} \phi'(x) dx.$$

Then, by taking absolute values and dividing the integral into two parts, the first integral is

$$\begin{aligned} & \left| \int_1^{\infty} \frac{x^{\lceil q \rceil - q}}{\Gamma(\lceil q \rceil + 1 - q)} \phi'(x) dx \right| \\ \leq & \int_1^{\infty} \frac{(1+x^2)}{\Gamma(\lceil q \rceil + 1 - q)} \phi'(x) dx \\ = & \int_1^{\infty} \frac{1}{(1+x^2)} \frac{(1+x^2)^2}{\Gamma(\lceil q \rceil + 1 - q)} \phi'(x) dx \\ \leq & \frac{\pi}{\Gamma(\lceil q \rceil + 1 - q)} \sup_x (1+x^2)^2 \phi'(x). \end{aligned}$$

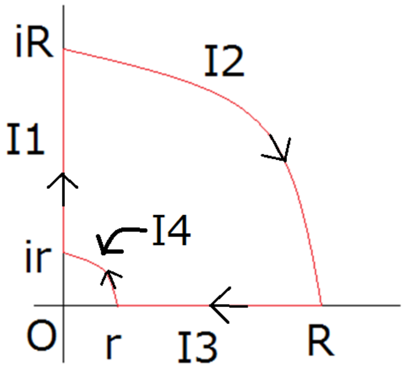


Figure 2.1: Complex integral

The second integral is

$$
\begin{aligned}
& \left| \int_0^1 \frac{x^{\lceil q \rceil - q}}{\Gamma(\lceil q \rceil + 1 - q)} \phi'(x) dx \right| \\
\leq & \int_0^1 \frac{1}{\Gamma(\lceil q \rceil + 1 - q)} \phi'(x) dx \\
\leq & \frac{1}{\Gamma(\lceil q \rceil + 1 - q)} \sup_x \phi'(x).
\end{aligned}
$$

Therefore, it is proved that the function g is a tempered distribution. Then, the function g is not integrable, but applicable to Fourier transform in the meaning of distribution as the following theorem[70, 55].

Theorem 2.4.5 *Fourier transform to a tempered function $f(x)$ is defined as*

$$\int_{-\infty}^{\infty} F\{f(x); w\} \phi(w) dw = \int_{-\infty}^{\infty} f(x) F\{\phi(w); x\} dx$$

where ϕ is a rapidly decreasing function.

This theorem is proved by using Fubini's theorem. Since Fourier transform to tempered functions is defined, let us apply it to the function g. Given a rapidly decreasing function $\phi(x)$, we have

$$
\begin{aligned}
& \int_{-\infty}^{\infty} F\{g(x); w\} \phi(w) dw \\
= & \int_{-\infty}^{\infty} \phi(w) \int_0^{\infty} e^{-iwx} \frac{x^{\lceil q \rceil - 1 - q}}{\Gamma(\lceil q \rceil - q)} dx dw.
\end{aligned}
$$

By changing variable for $iwx = y$, we have

$$= \int_{-\infty}^{\infty} \frac{\phi(w)}{\Gamma(\lceil q \rceil - q)} (iw)^{q-n} \lim_{R \to \infty} \int_0^{iR} e^{-y} y^{\lceil q \rceil - 1 - q} dy dw. \tag{2.1}$$

Here, we make complex integral as Figure 2.1. By changing variables for $y = re^{i\theta}$, the integrals I_1, I_2, I_3, I_4 are computed as

$$\begin{aligned}
I_1 &= \lim_{R\to\infty} \int_0^{iR} e^{-y} y^{\lceil q\rceil -1-q} dy \\
I_2 &= \lim_{R\to\infty} i\int_{\pi/2}^{0} \exp(-Re^{i\theta})(Re^{i\theta})^{\lceil q\rceil -q} d\theta = 0 \\
I_3 &= \lim_{R\to\infty} \int_R^{0} e^{-y} y^{\lceil q\rceil -1-q} dy = -\Gamma(\lceil q\rceil - q) \\
I_4 &= \lim_{r\to 0} i\int_0^{\pi/2} \exp(-re^{i\theta})(re^{i\theta})^{\lceil q\rceil -q} d\theta = 0.
\end{aligned}$$

Since exponential functions $\exp(-R)$ decrease more rapidly than the increase of $R^{\lceil q\rceil - q}$ for $R \to \infty$, it holds $I_2 = 0$. I_3 can be calculated from the definition of gamma functions, and we have $I_3 = -\Gamma(\lceil q\rceil - q)$. In addition, it holds $I_4 = 0$ for $r \to 0$. Then, there is no residue inside of the integral circuit. Therefore, it gets $I_1 + I_2 + I_3 + I_4 = 0$, and we have $I_1 = \Gamma(\lceil q\rceil - q)$. By putting the value of the integral I_1 to Formula (2.1), Fourier transform to the function g is given as

$$\begin{aligned}
& \int_{-\infty}^{\infty} F\left\{g(x);w\right\}\phi(w)dw = \int_{-\infty}^{\infty} \phi(w)(iw)^{q-\lceil q\rceil} dw \\
\Rightarrow\quad & F\left\{g(x);w\right\} = (iw)^{q-\lceil q\rceil}.
\end{aligned}$$

Consequently, Fourier transform to fractional operator is obtained as

$$\begin{aligned}
F\left\{{}_{-\infty}^{\mathrm{C}}D_x^q f(x);w\right\} &= (iw)^{\lceil q\rceil}\hat{f}(w)(iw)^{q-\lceil q\rceil} \\
&= (iw)^q \hat{f}(w).
\end{aligned}$$

The other also can be proved in a similar way.

Fourier transform to fractional operator is defined as above. In the next subsection, we develop fractional partial differential equations from a probability density function by using Fourier transform.

2.4.2 Heavy tailed distribution and fractional partial differential equations

Many papers introduce that the fractional partial differential equations are coming from heavy tailed distribution[68, 9, 8], but none of papers actually shows how equations are developed from the distribution. The author explains how equations are obtained from heavy tailed distribution by using Fourier transform. Firstly, let $f(x)$ be an even function as $f(x) = f(-x)$ and be a probability density function satisfying

$$\int_{-\infty}^{\infty} f(x)dx = 1.$$

This probability density function expresses the probability which a particle moves from 0 to x. That is, the probability which a particle moves from 0 to 1 is $f(1)$. Next, let $P(x,t)$ denote the number of particles at position x and time t. Then, after tiime dt, the distribution of particles changes as

$$P(x, t+dt) = \int_{-\infty}^{\infty} f(x-y)P(y,t)dy.$$

Then, let the function $P(x,t)$ be analytical and we apply Taylor expansion to $P(x,t)$ and changing variables as,

$$\begin{aligned}
& P(x,t) + dt\frac{\partial P(x,t)}{\partial t} + \frac{(dt)^2}{2}\frac{\partial^2 P(x,t)}{\partial t^2} + \cdots \\
= & \int_{-\infty}^{\infty} f(u)P(x-u,t)dy \\
= & \int_{-\infty}^{\infty} f(u)\left\{P(x,t) - u\frac{\partial P(x,t)}{\partial x} + \frac{u^2}{2!}\frac{\partial^2 P(x,t)}{\partial x^2} - \frac{u^3}{3!}\frac{\partial^2 P(x,t)}{\partial x^2} + \cdots\right\} du \\
= & P(x,t) + \frac{1}{2!}\frac{\partial^2 P(x,t)}{\partial x^2}\int_{-\infty}^{\infty} u^2 f(u)du + \frac{1}{4!}\frac{\partial^4 P(x,t)}{\partial x^4}\int_{-\infty}^{\infty} u^4 f(u)du + \cdots .
\end{aligned}$$

Here, the integral of the second term in the last expression denotes the second moment or the variance of $f(x)$, and the integral of the third term denotes the fourth moment or the kurtosis of $f(x)$. If $2 \cdot n$-th moment of $f(x)$ is proportional to $(dx)^n$, the above formulae equal to diffusion equations for $dt \to 0$. However, some probability density function has the infinite variance, for example, Cauchy distribution. For such a probability density function whose variance is infinite, the behavior of particles are represented by fractional partial equations. Let us consider the following probability density function

$$f(x) = \frac{q \cdot dt}{2}\left((dt)^{\frac{1}{q}} + |x|\right)^{-1-q}, 0 < q < 2.$$

This function is heavy tailed and integrable as

$$\begin{aligned}
& \int_{-\infty}^{\infty} f(x)dx \\
= & \frac{q \cdot dt}{2}\int_{-\infty}^{0}\left((dt)^{\frac{1}{q}} - x\right)^{-1-q} dx + \frac{q \cdot dt}{2}\int_{0}^{\infty}\left((dt)^{\frac{1}{q}} + x\right)^{-1-q} dx \\
= & \frac{q \cdot dt}{2}\left[\frac{1}{q}\left((dt)^{\frac{1}{q}} - x\right)^{-q}\right]_{-\infty}^{0} + \frac{q \cdot dt}{2}\left[\frac{-1}{q}\left((dt)^{\frac{1}{q}} + x\right)^{-q}\right]_{0}^{\infty} \\
= & 1.
\end{aligned}$$

Its variance is infinite as

$$\begin{aligned}
& \int_{-\infty}^{\infty} x^2 f(x)dx \\
= & \int_{-\infty}^{0} x^2\frac{q \cdot dt}{2}\left((dt)^{\frac{1}{q}} - x\right)^{-1-q} dx + \int_{0}^{\infty} x^2\frac{q \cdot dt}{2}\left((dt)^{\frac{1}{q}} + x\right)^{-1-q} dx.
\end{aligned}$$

By applying changing variables, it holds

$$\begin{aligned}
= & \frac{q \cdot dt}{2}\int_{(dt)^{1/q}}^{\infty}\left((dt)^{\frac{1}{q}} - u^2\right)^2 u^{-1-q}du + \frac{q \cdot dt}{2}\int_{(dt)^{1/q}}^{\infty}\left((dt)^{\frac{1}{q}} - v\right)^2 v^{-1-q}dv \\
= & q \cdot dt\int_{(dt)^{1/q}}^{\infty} (dt)^{\frac{2}{q}}u^{-1-q} - 2(dt)^{\frac{1}{q}}u^{-q} + u^{1-q}du \\
= & \infty.
\end{aligned}$$

Therefore, the behavior of particles which moves on this distribution cannot be represented by diffusion equations. Then, in the same way to diffusion equations, let $P(x,t)$ be the number of particles at x and t, and we have

$$P(x,t+dt) = \int_{-\infty}^{\infty} f(x-y)P(y,t)dy.$$

By taking convolution of Fourier transform, we have

$$\begin{aligned}
& \hat{P}(x,t+dt) \\
= \; & \hat{P}(x,t)\int_{-\infty}^{\infty} e^{-iwx} f(x)dx \\
= \; & \hat{P}(x,t)\left[\int_{-\infty}^{0} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}-x\right)^{-1-q}dx\right. \\
& \left. +\int_{0}^{\infty} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}+x\right)^{-1-q}dx\right]
\end{aligned}$$

As mentioned above, the fractional calculus order is restricted as $0<q<2$, but firstly let us assume that $1<q<2$. By applying integral by part, the first integral is

$$\begin{aligned}
& \int_{-\infty}^{0} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}-x\right)^{-1-q}dx \\
= \; & \left[e^{-iwx}\frac{dt}{2}\left((dt)^{\frac{1}{q}}-x\right)^{-q}\right]_{-\infty}^{0}+(iw)\int_{-\infty}^{0} e^{-iwx}\frac{dt}{2}\left((dt)^{\frac{1}{q}}-x\right)^{-q}dx \\
= \; & \frac{1}{2}+\left[(iw)e^{-iwx}\frac{dt}{2(q-1)}\left((dt)^{\frac{1}{q}}-x\right)^{1-q}\right]_{-\infty}^{0} \\
& +(iw)^2\int_{-\infty}^{0} e^{-iwx}\frac{dt}{2(q-1)}\left((dt)^{\frac{1}{q}}-x\right)^{1-q}dx \\
= \; & \frac{1}{2}+\frac{(iw)}{2(q-1)}+(iw)^2\int_{-\infty}^{0} e^{-iwx}\frac{dt}{2(q-1)}\left((dt)^{\frac{1}{q}}-x\right)^{1-q}dx.
\end{aligned}$$

The second integral can be converted in a similar way as

$$\begin{aligned}
& \int_{0}^{\infty} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}+x\right)^{-1-q}dx \\
= \; & \left[e^{-iwx}\frac{-dt}{2}\left((dt)^{\frac{1}{q}}+x\right)^{-q}\right]_{0}^{\infty}-(iw)\int_{0}^{\infty} e^{-iwx}\frac{dt}{2}\left((dt)^{\frac{1}{q}}+x\right)^{-q}dx \\
= \; & \frac{1}{2}+\left[(iw)e^{-iwx}\frac{dt}{2(q-1)}\left((dt)^{\frac{1}{q}}+x\right)^{1-q}\right]_{0}^{\infty} \\
& +(iw)^2\int_{0}^{\infty} e^{-iwx}\frac{dt}{2(q-1)}\left((dt)^{\frac{1}{q}}+x\right)^{1-q}dx \\
= \; & \frac{1}{2}-\frac{(iw)}{2(q-1)}+(iw)^2\int_{0}^{\infty} e^{-iwx}\frac{dt}{2(q-1)}\left((dt)^{\frac{1}{q}}+x\right)^{1-q}dx.
\end{aligned}$$

Next, we compute the integral as

$$\begin{aligned}
& \int_{-\infty}^{0} e^{-iwx}\left((dt)^{\frac{1}{q}}-x\right)^{1-q}dx \\
= \; & \int_{-\infty}^{(dt)^{1/q}} e^{-iwx}\left((dt)^{\frac{1}{q}}-x\right)^{1-q}dx-\int_{0}^{(dt)^{1/q}} e^{-iwx}\left((dt)^{\frac{1}{q}}-x\right)^{1-q}dx.
\end{aligned}$$

By applying changing variables for $y=(dt)^{1/q}-x$ and using the definition of gamma function, we obtain

$$\begin{aligned}
= \; & \int_{0}^{\infty} e^{iwy-iw(dt)^{1/q}}y^{1-q}dy-\int_{0}^{(dt)^{1/q}} e^{-iwx}\left((dt)^{\frac{1}{q}}-x\right)^{1-q}dx \\
= \; & e^{-iw(dt)^{1/q}}\Gamma(2-q)(-iw)^{q-2}+O\left((dt)^{\frac{2}{q}-1}\right).
\end{aligned}$$

In a similar way, it holds

$$\begin{aligned}
& \int_0^{\infty} e^{-iwx}\left((dt)^{\frac{1}{q}}+x\right)^{1-q} dx \\
= \quad & e^{-iw(dt)^{1/q}}\Gamma(2-q)(iw)^{q-2}+O\left((dt)^{\frac{2}{q}-1}\right).
\end{aligned}$$

Therefore, we have

$$\begin{aligned}
& \hat{P}(x,t+dt) \\
= \quad & \hat{P}(x,t)+dt\frac{\partial \hat{P}(x,t)}{\partial t}+\frac{(dt)^2}{2!}\frac{\partial^2 \hat{P}(x,t)}{\partial t^2}+\cdots \\
= \quad & \hat{P}(x,t)\left[1+\frac{(iw)^2 dt}{2(q-1)}\left\{e^{-iw(dt)^{1/q}}\Gamma(2-q)(-iw)^{q-2}\right.\right. \\
& \left.\left. +e^{-iw(dt)^{1/q}}\Gamma(2-q)(iw)^{q-2}+O\left((dt)^{\frac{2}{q}-1}\right)\right\}\right].
\end{aligned}$$

Then, by taking $dt \to 0$, it holds

$$\frac{\partial \hat{P}(x,t)}{\partial t}=\hat{P}(x,t)\frac{-\Gamma(1-q)}{2}\left\{(-iw)^q+(iw)^q\right\}.$$

Fractional partial differential equation for $1<q<2$ is obtained by applying inverse Fourier transform as

$$\frac{\partial P(x,t)}{\partial t}=\frac{-\Gamma(1-q)}{2}\left\{{}_{-\infty}D_x^q P(x,t)+{}_xD_{\infty}^q P(x.t)\right\}.$$

Here, $\Gamma(1-q)/2$ is a positive value. Next, let us consider for $0<q<1$. In a similar way, by applying Fourier transform, we have

$$\begin{aligned}
& \hat{P}(x,t+dt) \\
= \quad & \hat{P}(x,t)\int_{-\infty}^{\infty} e^{-iwx} f(x)dx \\
= \quad & \hat{P}(x,t)\left[\int_{-\infty}^{0} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}-x\right)^{-1-q} dx\right. \\
& \left. +\int_0^{\infty} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}+x\right)^{-1-q} dx\right].
\end{aligned}$$

By taking integral by part, the first integral is

$$\begin{aligned}
& \int_{-\infty}^{0} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}-x\right)^{-1-q} dx \\
= \quad & \frac{1}{2}-(-iw)\int_{-\infty}^{0} e^{-iwx}\frac{dt}{2}\left((dt)^{\frac{1}{q}}-x\right)^{-q} dx.
\end{aligned}$$

The second integral is computed as

$$\begin{aligned}
& \int_0^{\infty} e^{-iwx}\frac{q\cdot dt}{2}\left((dt)^{\frac{1}{q}}+x\right)^{-1-q} dx \\
= \quad & \frac{1}{2}-(iw)\int_0^{\infty} e^{-iwx}\frac{dt}{2}\left((dt)^{\frac{1}{q}}+x\right)^{-q} dx.
\end{aligned}$$

In a similar way to the case $1<q<2$, we have

$$\begin{aligned}
& \int_{-\infty}^{0} e^{-iwx}\left((dt)^{\frac{1}{q}}-x\right)^{-q} dx \\
= \quad & e^{-iw(dt)^{1/q}}\Gamma(1-q)(-iw)^{q-1}+O\left((dt)^{\frac{1}{q}-1}\right),
\end{aligned}$$

and we have

$$\begin{aligned}&\int_0^\infty e^{-iwx}\left((dt)^{\frac{1}{q}}+x\right)^{-q}dx\\ =\ & e^{-iw(dt)^{1/q}}\Gamma(1-q)(iw)^{q-1}+O\left((dt)^{\frac{1}{q}-1}\right).\end{aligned}$$

Therefore, we have

$$\begin{aligned}&\hat{P}(x,t+dt)\\ =\ &\hat{P}(x,t)+dt\frac{\partial\hat{P}(x,t)}{\partial t}+\frac{(dt)^2}{2!}\frac{\partial^2\hat{P}(x,t)}{\partial t^2}+\cdots\\ =\ &\hat{P}(x,t)\left[1-\frac{dt}{2}\left\{e^{-iw(dt)^{1/q}}\Gamma(1-q)(-iw)^q\right.\right.\\ &\left.\left.+e^{-iw(dt)^{1/q}}\Gamma(1-q)(iw)^q+O\left((dt)^{\frac{1}{q}-1}\right)\right\}\right].\end{aligned}$$

By taking $dt\to 0$, it holds

$$\frac{\partial\hat{P}(x,t)}{\partial t}=\hat{P}(x,t)\frac{-\Gamma(1-q)}{2}\left\{(-iw)^q+(iw)^q\right\}.$$

Fractional partial differential equation for $0<q<1$ is also obtained by applying inverse Fourier transform as

$$\frac{\partial P(x,t)}{\partial t}=\frac{-\Gamma(1-q)}{2}\left\{{}_{-\infty}D_x^q P(x,t)+{}_xD_\infty^q P(x.t)\right\}.$$

In contrast to the fractional partial differential equations for $1<q<2$, $\Gamma(1-q)/2$ is a negative value. This means that this equation is more similar to advection equations than diffusion equations.

2.5 Integer order diffusion equations and Von Neumann stability analysis

The idea of stability is really important for finite difference methods. If a finite difference method is unstable, the error of numerical solution diverges and numerical solution does not converge. Von Neumann stability analysis is one of methods to analyze the stability of finite difference methods for partial differential equations, and it appears in later chapter. In this section, the author introduces the integer order diffusion equations and how to analyze its stability by using Von Neumann stability analysis. Firstly, the following equation is the diffusion equation

$$\frac{\partial u(x,t)}{\partial t}=C\frac{\partial^2 u(x,t)}{\partial x^2},\quad 0\le x\le L,\quad 0\le t\le T$$

where C is a diffusion coefficient. Let us consider to solve the above diffusion equation with an initial condition $u(x,0)=u_0(x)$ and boundary conditions $u(0,t)=a, u(L,t)=b$. Here, we approximate time derivative with forward difference and space derivative with central difference. Then, we have

$$\frac{u(x,t+h_t)-u(x,t)}{h_t}=C\frac{u(x-h_x,t)-2u(x,t)+u(x+h_x,t)}{h_x^2}$$

where h_t,h_x are grid sizes for time and space respectively. Let N_x and N_t be the numbers of grids, and satisfy $h_x=L/N_x$ and $h_t=T/N_t$. By approximation as $u(j\cdot h_x,m\cdot h_t)\simeq U_j^m$, we have the following difference equations as

$$U_j^{m+1}-U_j^m=r\left\{U_{j-1}^m-2U_j^m+U_{j+1}^m\right\}\tag{2.2}$$

where $r = Ch_t/h_x^2$. In the matrix form, the above formulae are represented with matrices as

$$\begin{pmatrix} 1 & & & & \\ r & 1-2r & r & & \\ & \ddots & \ddots & \ddots & \\ & & r & 1-2r & r \\ & & & & 1 \end{pmatrix} \begin{pmatrix} U_0^m \\ U_1^m \\ \vdots \\ U_{N_x-1}^m \\ U_{N_x}^m \end{pmatrix} = \begin{pmatrix} U_0^{m+1} \\ U_1^{m+1} \\ \vdots \\ U_{N_x-1}^{m+1} \\ U_{N_x}^{m+1} \end{pmatrix}.$$

Here, Von Neumann stability analysis assume the special solution of Fourier series as

$$U_j^m = \kappa^m \exp(i\xi j h_x) \tag{2.3}$$

where ξ is the wave number and κ is the amplifier factor. For $|\kappa| \leq 1$, this scheme is stable. By substituting the expression (2.3) to the difference equations (2.2), we have

$$\begin{aligned} \kappa &= 1 + r\left\{\exp(-i\xi h_x) - 2 + \exp(i\xi h_x)\right\} \\ &= 1 + r\left\{2\cos(\xi h_x) - 2\right\} \\ &= 1 - 4r\sin^2\left(\frac{\xi h_x}{2}\right). \end{aligned}$$

For arbitrary wave number ξ, it holds $0 \leq \sin^2(\xi h_x/2) \leq 1$. Therefore, from $|\kappa| \leq 1$, we have

$$r \leq \frac{1}{2}.$$

This is the stability condition of the scheme (2.2). In a similar way, it is observed that the following implicit scheme is unconditionally stable,

$$U_j^m - U_j^{m-1} = r\left\{U_{j-1}^m - 2U_j^m + U_{j+1}^m\right\}.$$

2.6 Gerschgorin's theorem

Gerschgorin's theorem is a method to estimate the area where the eigenvalues exist[59]. The author introduces the Gerschgorin's theorem in the following theorem.

Theorem 2.6.1 *Let $a_{i,j}$ be the elements of any square matrix A, and let λ be any eigenvalue of the matrix A. Then, there is a positive integer i such that*

$$|\lambda - a_{i,i}| \leq \sum_{j \neq i} |a_{i,j}|.$$

This theorem holds by exchanging the column and row as

$$|\lambda - a_{i,i}| \leq \sum_{j \neq i} |a_{j,i}|.$$

This Gerschgorin's theorem is used in the matrix method which analyzes the stability of finite difference methods. The author also uses it to analyze his proposed methods.

2.7 Jacobi polynomials and Gauss-Jacobi quadrature

Jacobi polynomials have a similarity to fractional calculus. Actually, some papers propose numerical methods using Jacobi polynomials and Gauss-Jacobi quadrature. This section introduces the definitions of Jacobi polynomials and Gauss-Jacobi quadrature. The Jacobi polynomials $P_n^{(a,b)}$, $n = 0, 1, \ldots$ are given by

$$P_i^{(a,b)}(x) = \sum_{m=0}^{i} \frac{(-1)^{i-m}(1+b)_i(1+a+b)_i}{m!(i-m)!(1+b)_m(1+b+a)_i} \left(\frac{x+1}{2}\right)^m,$$

where

$$(a)_k = a(a+1)\ldots(a+k-1), (a)_0 = 1.$$

These Jacobi polynomials are orthogonal polynomials, and for $a, b > -1$ it holds

$$\begin{aligned} &\int_{-1}^{1} (1-x)^a(1+x)^b P_m^{(a,b)}(x) P_n^{(a,b)}(x) dx \\ = &\begin{cases} 0 & m \neq n \\ \frac{2^{a+b+1}}{n!(2n+a+b+1)} \frac{\Gamma(n+a+1)\Gamma(n+b+1)}{\Gamma(n+a+b+1)} & m = n. \end{cases} \end{aligned}$$

From this orthogonality, Jacobi polynomials are used to numerically compute integrals as Gauss-Jacobi quadrature. Let $\xi_i^{(a,b)}$, $i = 1, \ldots, n$ be the i-th root of Jacobi polynomial $P_n^{(a,b)}$, then Gauss-Jacobi quadrature is given by

$$\int_{-1}^{1} (1-x)^a(1+x)^b f(x) dx \simeq \sum_{i=1}^{n} \omega_i^{(a,b)} f(\xi_i^{(a,b)})$$

where $\omega_i^{(a,b)}$, $i = 1, \ldots, n$ are Gauss-Jacobi quadrature weights defined as

$$\omega_i^{(a,b)} = -\frac{2n+a+b+2}{n+a+b+1} \frac{\Gamma(n+a+1)\Gamma(n+b+1)}{\Gamma(n+a+b+1)(n+1)!} \frac{2^{a+b}}{P_n^{(a,b)\prime}(\xi_i^{(a,b)}) P_{n+1}^{(a,b)}(\xi_i^{(a,b)})}.$$

This Gauss-Jacobi quadrature has a similar form to fractional calculus operator for $b = 0$. Therefore, the author proposes the implicit numerical methods by using this property.

Chapter 3

Related works

3.1 Exsiting finite difference methods for fractional partial differential equations

For fractional partial differential equations, first order accuracy finite difference method has been already proposed by M.M. Meerschaert and C. Tadjeran. In this section, the present author explains their paper published in 2006 titled "Finite difference approximations for two-sided space-fractional partial differential equations"[40]. To compare to our proposed methods, this section analyzes the methods in their paper. In their paper, they consider about the following fractional partial differential equations,

$$\frac{\partial u(x,t)}{\partial t} = c_+(x,t)\,{}_{L}^{\mathrm{R}}D_x^q u(x,t) + c_-(x,t)\,{}_{x}^{\mathrm{R}}D_R^q u(x,t) + s(x,t)$$

on a finite domain $L < x < R$, $0 \le t \le T$ where functions c_+, c_-, s are known functions. In addition, they consider fractional calculus order q satisfies $1 \le q \le 2$ and the functions $c_+(x,t) \ge 0$ and $c_-(x,t) \ge 0$. They also assume that an initial condition $u(x,0) = F(x)$ and zero Dirichlet boundary conditions as $u(L,t) = u(R,t) = 0$.
Firstly, M.M. Meerschaert and C. Tadjeran analyze only the following left-handed fractional differential equations

$$\frac{\partial u(x,t)}{\partial t} = c(x,t)\,{}_{L}^{\mathrm{R}}D_x^q u(x,t) + s(x,t)$$

where $c(x,t) \ge 0$ and $L \le x \le R$, $0 \le t \le T$. They also define $t_n = n\triangle t$ for $0 \le t_n \le T$, and $\triangle x = h > 0$ is a grid size for spatial domain where $h = (R-L)/K$, $x_i = L + ih$ for $i = 0, \ldots, K$ so that $L \le x \le R$. Next, they let u_i^n be the numerical approximation to $u(x_i, t_n)$, and let c_i^n and s_i^n be $c_i^n = c(x_i, t_n)$, $s_i^n = s(x_i, t_n)$ respectively. In their paper, it is written that the following discretized explicit (Euler) method is unstable

$$\begin{aligned} &\frac{u_i^{n+1} - u_i^n}{\triangle t} \\ = \;& c_i^n \frac{h^{-q}}{\Gamma(-q)} \sum_{k=0}^{i} \frac{\Gamma(k-q)}{\Gamma(k+1)} u_{i-k}^n + s_i^n. \end{aligned}$$

The proof of unstability is written in their paper published in 2004[39].

In their paper, the scheme which is simply discretized by using Grunwald-Letnikov definition is unstable, and they mention that finite difference methods using Grunwald-Letnikov definition to two-sided fractional partial differential equations is also unconditionally unstable. However, their paper introduces a stable scheme which is fixed by using idea of shifted Grunwald-Letnikov definition in the following proposition.

Proposition 3.1.1 ([40]) *The following explicit Euler method is stable if* $\triangle t/h^q \leq 1/(q \cdot c_{max})$*, where* c_{max} *is the maximum value of* $c(x,t)$ *over region* $L \leq x \leq R$*,* $0 \leq t \leq T$*,*

$$u_i^{n+1} - u_i^n = \beta c_i^n \sum_{k=0}^{i+1} \frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)} u_{i-k+1}^n + s_i^n \triangle t.$$

Proof
At each time step, we apply a matrix stability analysis to the linear system of equations, and use the Gerschgorin Theorem to determine a stability condition.

The proposed scheme with Dirichlet boundary conditions can be represented in a linear system of equations of the form $\underline{U}^{n+1} = \underline{AU}^n + \triangle t \underline{S}^n$ where

$$\begin{aligned} \underline{U}^n &= [u_0^n, u_1^n, u_2^n, \ldots, u_K^n]^T \\ \underline{S}^n &= [0, s_1^n, s_2^n, \ldots, s_{K-1}^n, 0]^T \end{aligned}$$

Here, $\underline{A}$ is the sum of a lower triangular matrix and a diagonal matrix, and this scheme is stable if absolute values of all eigenvalues of $\underline{A}$ are equal or less than 1. The matrix entries $A_{i,j}$ for $i = 1, \ldots, K-1$ and $j = 1, \ldots, K-1$ are defined for $g_i = \Gamma(i-q)/(\Gamma(-q)\Gamma(i+1))$ by

$$A_{i,j} = \begin{cases} 0, & j \geq i+2 \\ 1 + g_1 c_i^n \beta, & j = i \\ g_{i-j+1} c_i^n \beta, & otherwise \end{cases}$$

while $A_{0,0} = 1$, $A_{0,j} = 0$ for $j = 1, \ldots, K$, $A_{K,K} = 1$, $A_{K,j} = 0$ for $j = 0, \ldots, K-1$. Note that for $1 \leq q \leq 2$ and $i \neq 1$ we have $g_i \geq 0$. This is shown by using induction. We also have $-g_1 \geq \sum_{k=0,k\neq 1}^{k=N} g_k$, which follows from the well-known equality $\sum_{k=0}^{\infty} g_k = 0$. According to Gerschgorin Theorem, the eigenvalues μ of the matrix $\underline{A}$ satisfy $|\mu - A_{i,i}| \leq r_i$ where $r_i = \sum_{k=0,k\neq i}^{K} A_{i,k}$. Then, to be stable, the matrix $\underline{A}$ must satisfy two conditions $A_{i,i} + r_i \leq 1$ and $A_{i,i} - r_i \geq -1$. Here, we have $A_{i,i} = 1 - qc_i^n \beta$ and

$$r_i = \sum_{k=0,k\neq i}^{K} A_{i,k} = \sum_{k=0,k\neq i}^{i+1} A_{i,k} = c_i^n \beta \sum_{k=0,k\neq i}^{i+1} g_i \leq qc_i^n \beta$$

and therefore it holds $A_{i,i} + r_i \leq 1$. Then, we also have $A_{i,i} - r_i \geq 1 - 2qc_i^n \beta \geq 1 - 2qc_{max}\beta$. Therefore, the stability condition is represented as

$$\beta = \frac{\triangle t}{h^q} \leq \frac{1}{qc_{max}}.$$

It is proven that their proposed scheme is conditionally stable with the stability condition $\beta \leq\ 1/(qc_{mx})$.

□

Next, they analyze the finite difference methods for two-sided fractional partial differential equations. They propose both implicit and explicit finite difference methods. The implicit finite difference scheme is introduced as

$$\begin{aligned} &\frac{u_i^{n+1}-u_i^n}{\triangle t} \\ = &\frac{1}{h^q}\left[\sum_{k=0}^{i+1}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}c_{+,i}^{n+1}u_{i-k+1}^{n+1}+\sum_{k=0}^{K-i+1}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}c_{-,i}^{n+1}u_{i+k-1}^{n+1}\right] \\ &+s_i^{n+1}. \end{aligned} \tag{3.1}$$

The explicit finite difference scheme is also introduced as

$$\begin{aligned} &\frac{u_i^{n+1}-u_i^n}{\triangle t} \\ = &\frac{1}{h^q}\left[\sum_{k=0}^{i+1}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}c_{+,i}^{n}u_{i-k+1}^{n}+\sum_{k=0}^{K-i+1}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}c_{-,i}^{n}u_{i+k-1}^{n}\right] \\ &+s_i^{n}. \end{aligned} \tag{3.2}$$

They prove that implicit finite difference scheme is unconditionally stable, and explicit scheme is stable with the stability condition. In this thesis, the present author introduces stability analysis only for the explicit scheme. The stability analysis for the implicit scheme is also done in a similar way to explicit scheme. The detail of its stability analysis can be found in [40]. They mention that the scheme (3.2) is stable as the following proposition[40].

Proposition 3.1.2 ([40]) *The explicit Euler method approximation defined by (3.2) with $1 \le q \le 2$ is stable if*

$$\frac{\triangle t}{h^q} \le \frac{1}{q(c_{+max}+c_{-max})}. \tag{3.3}$$

The proof is similar to Proposition 3.1.1.
They also make numerical experiments about the implicit scheme (3.1), and confirm its accuracy. Lastly the present author introduces the experimental results in their paper. Let q be $q = 1.8$, and define $0 < x < 2$ and $0 < t < 1$. Let the coefficient functions $c_+(x,t)$ and $c_-(x,t)$ be

$$\begin{aligned} c_+(x,t) &= \Gamma(1.2)x^{1.8} \\ c_-(x,t) &= \Gamma(1.2)(2-x)^{1.8}, \end{aligned}$$

and let the forcing function $s(x,t)$ be

$$s(x,t) = -32e^{-t}\left[x^2+(2-x)^2-2.5\left(x^3+(2-x)^3\right)+\frac{25}{22}\left(x^4+(2-x)^4\right)\right].$$

The initial condition is $u(x,0) = 4x^2(2-x)^2$, and boundary condition is $u(0,t) = u(2,t) = 0$. In addition, let the analytical solution $u(x,t)$ be $u(x,t) = 4e^{-t}x^2(2-x)^2$. Table 3.1 is the results about maximum errors at $t = 1$ with various parameters. M.M. Meerschaert and C. Tadjeran mention that the results in Tab. 3.1 indicates the error order of the method is $O(\triangle t)+O(\triangle x)$. However, the present author considers these results do not fully show that error order is $O(\triangle t)+O(\triangle x)$. The reason is the similar results may happen if errors e_t derived from time derivative is $O(\triangle t)$ and has a big coefficient like $e_t = 1000\triangle t$, and errors e_x derived

$\triangle t$	$\triangle x$	Maximum Error
0.1000	0.200	0.1417
0.0500	0.100	0.0571
0.0250	0.050	0.0249
0.0125	0.025	0.0113

Table 3.1: Maximum error behavior versus grid size reduction for the example problem

from space is $O(1)$ and has a small coefficient like $e_x = 10^{-10}$. This means that errors having big error order is hidden by errors having small error order. Therefore, the present author suggests we make the experiments for time and space individually. The measurement of error is discussed in Section 5.1.5.

Although it seems that the experiments are not sufficient, this study by M.M. Meerschaert and C. Tadjeran is the first research about finite difference methods for fractional partial differential equations and the stability of schemes is well analyzed. In addition, the stability condition is proven by using Gerschgorin Theorem. The present author's proposed finite difference methods are also analyzed by using Gerschgorin Theorem, and have common points to schemes which are introduced in this section. Later, the present author's experiments are done with comparison to these schemes.

3.2 Another stability analysis using Von Neumann stability analysis

In this section, the present author introduces the paper titled "Finite difference approximations for a fractional advection diffusion problem" by E. Sousa as a related work[54]. That paper also treats finite difference methods for fractional partial differential equations. The biggest difference between that paper and the paper which is introduced in the above section by M.M. Meerschaert and C. Tadjeran is the way to analyze the stability. To analyze stability, E. Sousa uses Von Neumann stability analysis instead of using matrix stability analysis. For comparison with two stability analysis method, let us look at especially how to analyze stability by E. Sousa. Firstly, that paper treats the following fractional partial differential equations

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = A\left(\frac{1}{2}+\frac{\beta}{2}\right)\,_a^R D_x^q + A\left(\frac{1}{2}+\frac{\beta}{2}\right)\,_x^R D_b^q u.$$

where $1 < q \leq 2$ and $-1 \leq \beta \leq 1$. Let U_j^m be the approximation of $u(x_j, t_n)$ at the mesh points

$$x_j = j\triangle x,\ j = -N, \ldots, -2, -1, 0, 1, 2, \ldots, N,$$

and $t_n = n\triangle t$, $n \geq 0$ where $\triangle x$ denotes the space step size and $\triangle t$ is the time step size. In addition, Let μ_q be

$$\mu_q = \frac{A\triangle t}{\triangle x^q}.$$

Then, the proposed finite difference scheme is

$$\begin{aligned} & U_j^{n+1} \\ = \;& U_j^n + \frac{\mu_q}{2}\left[(1+\beta)\sum_{k=0}^{N+j+1}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}U_{j+1-k}^n\right. \\ & \left. +(1-\beta)\sum_{k=0}^{N-j+1}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}U_{j-1+k}^n\right] \end{aligned}$$

where $V = 0$.

Next, we apply Von Neumann stability analysis for the above scheme to give the stability conditions. Then, stability condition is shown by the following proposition[54].

Proposition 3.2.1 ([54]) *Let $-1 \leq \beta \leq 1$ and $1 < q \leq 2$. If the numerical scheme (3.4) is Von Neumann stable, then $\mu_q \leq 2^{1-q}$.*

Proof
If we insert the analytical solution $\kappa^n e^{ij\theta}$ into scheme (3.4), we obtain the following amplification factor

$$\begin{aligned} \kappa(\theta) &= 1 + \frac{\mu_q}{2}\left\{(1+\beta)\sum_{k=0}^{\infty}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}e^{i(1-k)\theta}\right. \\ & \left. +(1-\beta)\sum_{k=0}^{\infty}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}e^{-i(1-k)\theta}\right\}. \end{aligned}$$

Let us consider $\theta = 0$ and $\theta = \pi$. For $\theta = 0$, we have

$$\begin{aligned} & \kappa(0) \\ = \;& 1 + \frac{\mu_q}{2}\left\{(1+\beta)\sum_{k=0}^{\infty}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)} + (1-\beta)\sum_{k=0}^{\infty}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}\right\} \\ = \;& 1. \end{aligned}$$

For $\theta = \pi$, we have

$$\begin{aligned} & \kappa(\pi) \\ = \;& 1 + \frac{\mu_q}{2}\left\{(1+\beta)\sum_{k=0}^{\infty}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}\cos((1-k)\pi)\right. \\ & \left. +(1-\beta)\sum_{k=0}^{\infty}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}\cos((1-k)\pi)\right\}. \end{aligned}$$

Since $cos((1-k)\pi) = (-1)^{k-1}$, it holds

$$\begin{aligned} & \kappa(\pi) \\ = \;& 1 + \frac{\mu_q}{2}\left\{-(1+\beta)\sum_{k=0}^{\infty}\frac{\Gamma(q+1)}{\Gamma(q-k+1)\Gamma(k+1)} - (1-\beta)\sum_{k=0}^{\infty}\frac{\Gamma(q+1)}{\Gamma(q-k+1)\Gamma(k+1)}\right\} \\ = \;& 1 - \mu_q\sum_{k=0}^{\infty}\frac{\Gamma(q+1)}{\Gamma(q-k+1)\Gamma(k+1)}. \end{aligned}$$

Here, the infinite sum is

$$\frac{\Gamma(q+1)}{\Gamma(q-k+1)\Gamma(k+1)} = 2^q,$$

and stability condition $|\kappa| \leq 1$ is equivalent to

$$\mu_q \sum_{k=0}^{\infty} \frac{\Gamma(q+1)}{\Gamma(q-k+1)\Gamma(k+1)} \leq 2.$$

Therefore, we have $\mu_q \leq 2^{1-q}$.

$\square$

This stability analysis is done in infinite domain.

3.3 Another numerical method for fractional partial differential equations

In this section, the present author introduces the matrix transform method as another numerical method for space-fractional partial differential equations with homogeneous boundary conditions proposed by M. Ilic, F. Liu, I. Turner and V. Anh[21]. This method interprets the following fractional differential equation as the matrix representation. Firstly, let us consider the simplest homogeneous diffusion equation with Dirichlet boundary conditions given by

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= \kappa \frac{\partial^2 \phi}{\partial x^2}, \qquad 0 < x < 1, \\ \phi(0,t) &= 0, \qquad \phi(1,y) = 0, \\ \phi(x,0) &= g(x). \end{aligned}$$

By introducing finite difference approximation to the space derivative, we obtain

$$\begin{aligned} \frac{d\phi_i}{dt} &= \frac{\kappa}{h^2}(\phi_{i+1} - 2\phi_i + \phi_{i-1}),\ i = 1, 2, \ldots, N-1 \\ \phi_0 &= 0, \qquad \phi_N = 0 \\ \phi_i(0) &= g(x_i) \end{aligned}$$

where $\phi_i(t) = \phi(x_i, t)$, h is the space step size defined as $h = 1/N$. The above equation can be approximated by the following system of ordinary differential equations as

$$\frac{d\Phi}{dt} = -\eta A \Phi$$

where $\eta = \kappa/h^2$ and

$$\Phi = \begin{bmatrix} \phi_1 \\ \vdots \\ \phi_{N-1} \end{bmatrix}, \quad A = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}.$$

The matrix A is a symmetric positive definite matrix. Therefore, eigenvalues of A are positive and eigenvectors of A are orthogonal. Initially, we have

$$\Phi(0) = [g(h), g(2h), \ldots, g((N-1)h)]^T.$$

In their paper, it is written that this mean if the operator $T = -\frac{\partial^2}{\partial x^2}$ has a matrix representation $m(T)$, the diffusion equation becomes

$$\frac{dm(\phi)}{dt} = -\kappa m(T)m(\phi)$$

where $m(\phi)$ is a vector representation of ϕ. In other words, A/h^2 is an approximate matrix representation of T. Therefore, their paper states that the following fractional partial differential equations with Dirichlet boundary conditions

$$\frac{\partial \phi}{\partial t} = -\kappa(-\triangle)^{\frac{q}{2}}\phi \tag{3.4}$$

can be approximated by

$$\frac{\partial \Phi}{\partial t} = -\overline{\eta} A^{\frac{q}{2}}\Phi$$

where

$$(-\triangle)^{\frac{q}{2}} = \frac{1}{2\cos\left(\frac{\pi q}{2}\right)}\left[{}_a^{\mathrm{R}}D_x^q +{}_x^{\mathrm{R}} D_b^q\right],$$

and $\overline{\eta} = \kappa/h^q$. Then, how can we develop this transform? Their paper firstly treats the spectral representation. Let H be the real Hilbert space $\mathbf{L}(0, L)$ with the inner product as

$$< \phi_1, \phi_2 >= \int_0^L \phi_1(x)\phi_2(x)dx.$$

Then, let us consider the operator $T : \mathtt{H} \to H$ defined by $T\phi = -\frac{d^2\phi}{dx^2}$ on

$$\mathtt{H} = \left\{\phi \in H; \phi' \text{ is absolutely continuous}, \phi', \phi'' \in \mathbf{L}(0, L), \mathbf{B}(\phi) = 0\right\},$$

where $\mathbf{B}(\phi)$ denotes boundary conditions. Their paper mentions that it is known that T is a closed, self-adjoint operator whose eigenfunctions $\{\phi_n\}_{n=1}^{\infty}$ become an orthogonal basis for H. Thus, $T\phi_n = \lambda_n\phi_n$, $n = 1, 2, \ldots$. For any $\phi \in H$, it holds

$$\phi = \sum_{n=1}^{\infty} c_n\phi_n, c_n =< \phi, \phi_n >,$$

$$T\phi = \sum_{n=1}^{\infty} \lambda_n c_n \phi_n.$$

Lastly, it is written that if ψ is a continuous function on $\mathbb{R}$, then we have

$$\psi(T)\phi = \sum_{n=1}^{\infty} \psi(\lambda_n)c_n\phi_n,$$

provided $\sum_{n=1}^{\infty} |\phi(\lambda_n)c_n| < \infty$. The present author considers that the explanation about T is not enough and their paper should contain the proof of this content, especially where the function ψ takes both the operator T and a real number λ_n. However, their paper solves Eq.(3.4) by putting $\psi(t) = t^{\frac{q}{2}}$, and shows this is the reason that Eq.(3.4) can be transformed as

$$\frac{\partial \Phi}{\partial t} = -\overline{\eta} A^{\frac{q}{2}}\Phi.$$

Then, next the present author introduces how we compute the above equation in their paper.

Since the matrix A is a symmetric positive definite matrix, the matrix A can be decomposed by using an orthogonal matrix P as

$$A = P\Lambda P^T$$

where Λ is the diagonal matrix whose entries are the eigenvalues λ_n, $n = 1, 2, \ldots, N-1$ of A. Then, the solution of Eq.(3.4) is given by

$$\Phi(t) = P\exp(-\overline{\eta}\Lambda^{\frac{q}{2}}t)P^T\Phi(0),$$

where $\exp(-\overline{\eta}\Lambda^{\frac{q}{2}}t)$ is the diagonal matrix whose entries are $\exp(-\overline{\eta}\lambda_1^{\frac{q}{2}}t)$, $\exp(-\overline{\eta}\lambda_2^{\frac{q}{2}}t)$, $\ldots$, $\exp(-\overline{\eta}\lambda_{N-1}^{\frac{q}{2}}t)$. To use this method, we have to compute the decomposition of the matrix or the $q/2$-th power of the matrix. Additionally, this method can be applied only to the equations which have zero Dirichlet boundary conditions, because the matrix A has a different form. However, this method analytically calculate the time derivative by using exponential function, so the error of this method seems to be smaller than other methods. In a later chapter, the present author makes experiments with this matrix transform method for the comparison.

3.4 Existing numerical computational methods for fractional ordinary differential equations

3.4.1 Explicit method

In this section, the present author discusses the related works about existing numerical computational methods for fractional ordinary differential equations. Especially, in this subsection, the present author introduces the predictor-corrector method proposed in the paper titled ”A predictor-corrector approach for the numerical solution of fractional differential equations” proposed by K. Diethelm, N.J. Ford, A.D. Freed as one of the explicit methods[13]. This method is the most popular explicit method to solve fractional ordinary differential equations[66, 5], since Euler methods or Runge-Kutta methods which is popular methods to solve integer order ordinary differential equations cannot be applied. Fractional differentiation is not local phenomena, and has the property that it includes the past information like integral. Therefore, this property makes it difficult to apply Euler methods or Runge-Kutta methods to fractional differential equations. However, by applying fractional integrals, fractional ordinary differential equations can be converted to fractional integral equations. The predictor-corrector method is rather alike the numerical methods for integral equations than for differential equations. Then, the present author introduces the predictor-corrector methods and how to be developed.

Here, let us consider the following fractional ordinary differential equations as

$$ {}_0^{\mathrm{C}}D_x^q y(x) = f(x, y(x)) \tag{3.5}$$

for $0 < q < 2$ and $0 < x < T$ with initial conditions as

$$y^{(k)}(0) = y_0^{(k)},\ k = 0, 1, \ldots, \lceil q \rceil - 1.$$

Note that the fractional differential operator in Eq.(3.5) is Caputo definition. The reason why we do not use Riemann-Liouville definition is written in their paper. Let us consider the equation with Riemann-Louville definition as

$$ {}_0^{\mathrm{R}}D_x^q y(x) = f(x, y(x)).$$

The solution of this equation contains the values of fractional derivatives as initial conditions. This means we have to deal with the fractional derivatives which does not have a concrete physical meaning and which we cannot observe in physical phenomena as initial conditions in applications. However, Eq.(3.5) can be solved with the initial conditions $y(0), y'(0), \ldots$. This property fits to consider about applications. Yet, how to solve the fractional ordinary differential equations with Riemann-Liouville definition is not written, and it is not verified that initial conditions can be represented with fractional derivatives. Therefore, in later section, the present author shows how to solve equations and confirm the initial conditions are expressed with fractional derivatives.

Returning to the story, their paper proposes the numerical method for Eq.(3.5). The solution of Eq.(3.5) is written as

$$y(x) = \sum_{k=0}^{\lceil q \rceil - 1} y_0^{(k)} \frac{x^k}{k!} + \frac{1}{\Gamma(q)} \int_0^x (x-t)^{q-1} f(t, y(t)) dt.$$

Here, the present author notes that for the time step grid t_j as $t_j = jh$, $j = 0, 1, \ldots, n+1$, to solve the above equation means to compute $y(t_{n+1})$ under the assumption that we already know the values of $y(t_j)$, $j = 0, 1, \ldots, n$. Or, to solve the equation equals to compute $y(t_j)$, $j = 0, 1, \ldots, n+1$ under the initial conditions. In this section, the present author introduces the explicit method, so the values of $y(t_j)$ are computed step by step. Then, they firstly consider how to approximate integral in the solution. They apply trapezoidal quadrature with equally distance nodes $t_j = jh$, $j = 0, 1, \ldots, n+1$ as

$$\int_0^{t_{n+1}} (t_{n+1} - z)^{q-1} g(z) dz \simeq \int_0^{t_{n+1}} (t_{n+1} - z)^{q-1} \tilde{g}(z) dz.$$

The function $\tilde{g}$ is the piecewise linear interpolate for g with nodes t_j, and we have

$$\int_0^{t_{n+1}} (t_{n+1} - z)^{q-1} \tilde{g}(z) dz = \frac{h^q}{q(q+1)} \sum_{j=0}^{n+1} a_{j,n+1} g(t_j), \tag{3.6}$$

where

$$a_{j,n+1} = \begin{cases} n^{q+1} - (n-q)(n+1)^q, & j = 0 \\ (n-j+2)^{q+1} - 2(n-j+1)^{q+1} + (n-j)^{q+1}, & 1 \leq j \leq n \\ 1, & j = n+1 \end{cases}$$

How to compute coefficients $a_{j,n+1}$ is written in their paper[16]. The present author also introduces the detail of how coefficients are derived. Let the function ϕ_j be as

$$\phi_j(u) = \begin{cases} (u - t_{j-1})/(t_j - t_{j-1}), & t_{j-1} < u < t_j \\ (t_{j+1} - u)/(t_{j+1} - t_j), & t_j < u < t_{j+1} \\ 0, & \text{otherwise} \end{cases}$$

Then, the coefficients $a_{j,n+1}$ are given by

$$a_{j,n+1} = \int_{t_0}^{t_{n+1}} (t_{n+1} - u)^{q-1} \phi_j(u) du.$$

The key point of this method is not to approximate the kernel of integral $(x-u)^{q-1}$ with trapezoidal rule. This method applies trapezoidal rule only to the function.

As a result, the solution is expressed by using coefficients $a_{j,n+1}$ as

$$\begin{aligned} y_h(t_{n+1}) &= \sum_{k=0}^{\lceil q\rceil-1} y_0^{(k)}\frac{x^k}{k!} + \frac{h^q}{\Gamma(q+2)} f(t_{n+1}, y^P(t_{n+1})) \\ &\quad + \frac{h^q}{\Gamma(q+2)} \sum_{j=0}^{n} a_{j,n+1} f(t_j, y(t_j)). \end{aligned}$$

In the above formula, we assume that we already know the values y at t_j, $j = 0, 1, 2, \ldots, n$ and assume that we do not know the value $y_h(t_{n+1})$. Therefore, we put the $y^P(t_{n+1})$ as a temporary value. Then, the remaining problem is to compute $y^P(t_{n+1})$. By applying rectangle rule to integral, we have

$$\int_0^{t_{n+1}} (t_{n+1} - z)^{q-1} g(z) dz \simeq \sum_{j=0}^{n} b_{j,n+1} g(t_j) \tag{3.7}$$

where

$$b_{j,n+1} = \int_{t_j}^{t_{j+1}} (t_{n+1} - u)^{q-1} du = \frac{h^q}{q}((n+1-j)^q - (n-j)^q).$$

By using above formula, we compute $y^P(t_{n+1})$ as

$$y^P(t_{n+1}) = \sum_{k=0}^{\lceil q\rceil-1} y_0^{(k)}\frac{x^k}{k!} + \frac{1}{\Gamma(q)} \sum_{j=0}^{n} b_{j,n+1} f(t_j, y(t_j)). \tag{3.8}$$

This algorithm is based on Adams-Bashforth-Moulton method, and they call this algorithm fractional Adams-Bashforth-Moulton method. They mention that the stability of the predictor-corrector method is at least as good as Adams-Bashforth-Moulton method, but there is no proof or analysis of this conjecture. About the accuracy, it is written as

$$\max_{j=0,1,\ldots,N} |y(t_j) - y_h(t_j)| = O(h^p)$$

where

$$p = \min(2, 1+q)$$

where ${}_0^{\mathrm{C}}D_t^q y(t) \in C^2[0,T]$, $q > 0$ and $h = T/N$. The detailed analysis of the accuracy is shown by K. Diethelm, N.J. Ford and A.D. Freed[14].

Firstly, they analyze the accuracy of quadrature rule which is used in predictor-corrector method. They show the analysis results for quadrature rule (3.7) in the following theorem,

Theorem 3.4.1 ([14]) *(a)Let $z \in C^1[0,T]$. Then,*

$$\left| \int_0^{t_{n+1}} (t_{n+1} - t)^{q-1} z(t) dt - \sum_{j=0}^{k} b_{j,n+1} z(t_j) \right| \le \frac{1}{q} ||z'||_\infty t_{n+1}^q h.$$

(b)Let $z(t) = t^p$ for some $p \int (0,1)$. Then,

$$\left| \int_0^{t_{n+1}} (t_{n+1} - t)^{q-1} z(t) dt - \sum_{j=0}^{k} b_{j,n+1} z(t_j) \right| \le C_{p,q} t_{n+1}^{q+p-1} h$$

where $C_{p,q}$ is a constant that depends only q and p.

This theorem means that the quadrature rule (3.7) is the first order accuracy if the value of t_{n+1} is independent to h. However, their paper does not refer the case of accuracy decaying. This means if the value n is independent to h, the accuracy becomes less than $O(h)$ in the case of (b). Actually, for example, the accuracy order becomes $O(h^{0.2})$ for $q = 0.1$, $p = 0.1$ and $n = 0$. Next, they analyze the quadrature rule (3.6) in a similar way in the form of theorem.

Theorem 3.4.2 ([14]) *(a)If $z \in C^2[0,T]$ then there is a constant C_q^{Tr} depending only on q such that*

$$\left| \int_0^{t_{n+1}} (t_{n+1}-t)^{q-1} z(t)dt - \sum_{j=0}^{k} a_{j,n+1} z(t_j) \right| \leq C_p^{Tr} ||z''||_\infty t_{n+1}^q h^2.$$

(b)Let $z \in C^1[0,T]$ and assume that z' fulfils a Lipschitz condition of order μ for some $\mu \in (0,1)$. Then, there exist some positive constants $B_{q,\mu}^{Tr}$ (depending only on q and μ) and $M(z,\mu)$ (depending only on z and μ) such that

$$\left| \int_0^{t_{n+1}} (t_{n+1}-t)^{q-1} z(t)dt - \sum_{j=0}^{k} a_{j,n+1} z(t_j) \right| \leq B_{q,\mu}^{Tr} M(z,\mu) t_{n+1}^q h^{1+\mu}.$$

(c)Let $z(t) = t^p$ for some $p \in (0,2)$ and $\theta = \min(2, p+1)$. Then,

$$\left| \int_0^{t_{n+1}} (t_{n+1}-t)^{q-1} z(t)dt - \sum_{j=0}^{k} a_{j,n+1} z(t_j) \right| \leq C_{q,p}^{Tr} t_{n+1}^{q+p-\theta} h^\theta.$$

In this theorem, their paper also does not refer the case which the value of n is independent to N or h, the accuracy decreases. Lastly, they show the accuracy of the predictor-corrector method by using two theorems in the following Lemma.

Lemma 3.4.3 ([14]) *Assume that the solution y of the fractional ordinary differential equations is such that*

$$\left| \int_0^{t_{n+1}} (t_{n+1}-t)^{q-1} \, {}_0^{\mathrm{C}}D_t^q y(t)dt - \sum_{j=0}^{k} b_{j,n+1} \, {}_0^{\mathrm{C}}D_t^q y(t_j) \right| \leq C_1 t_{n+1}^{\gamma_1} h^{\delta_1}$$

and

$$\left| \int_0^{t_{n+1}} (t_{n+1}-t)^{q-1} \, {}_0^{\mathrm{C}}D_t^q y(t)dt - \sum_{j=0}^{k} a_{j,n+1} \, {}_0^{\mathrm{C}}D_t^q y(t_j) \right| \leq C_2 t_{n+1}^{\gamma_2} h^{\delta_2}$$

with some $\gamma_1, \gamma_2 \geq 0$ and $\delta_1, \delta_2 > 0$. Then, we have

$$\max_{0 \leq j \leq N} |y(t_j) - y_j| = O(h^\theta)$$

where $\theta = \min\{\delta_1 + q, \delta_2\}$ and y_j is a numerical solution by the predictor corrector-method at t_j.

This theorem means that the accuracy depends on the form of y, ${}_0^{\mathrm{C}}D_t^q y$ and f. K. Diethelm, N.J. Ford and A.D. Freed analyze how the accuracy depends on the form of functions. As mentioned above, under the assumption ${}_0^{\mathrm{C}}D_t^q y(t) \in C^2[0,T]$, it holds $\max_{0 \leq j \leq N} |y(t_j) - y_j| = O(h^p)$ for $p = \min(2, 1+q)$. They also show the accuracy with another assumption in the following theorem.

Theorem 3.4.4 ([14]) *Let $0 < q < 1$ and assume that $y \in C^2[0, T]$. Then, for $1 \leq j \leq N$ we have*

$$|y(t_j) - y_j| \leq C t_j^{q-1} \cdot \begin{cases} h^{1+q} & \text{if } 0 < q < 1/2 \\ h^{2-q} & \text{if } 1/2 \leq q < 1 \end{cases}$$

where C is a constant independent of j and h.

This theorem refers to the accuracy decaying for $j = 1$. For $0 < q < 1/2$, the accuracy become $O(h^{2q})$ at the worst. Therefore, to improve the accuracy, they propose to apply Richardson extrapolation.

In this subsection, the present author introduces the predictor-corrector method as the explicit numerical method. This method has at most second accuracy, but the accuracy may decrease depending on the form of y, ${}_0^{\mathrm{C}}D_t^q y$ and f. The stability analysis has never been done, so in later chapter, the present author makes experiments about the stability, in addition to the accuracy, for the comparison to the present author's proposed new numerical methods.

3.4.2 Implicit method

Collocation method using Jacobi polynomials

In this subsection, the present author introduces the implicit numerical method for fractional ordinary differential equations proposed by S. Beheshti, H. Khosravian-Arab and I. Zare[4]. This method is based on the Jacobi polynomials, and utilizes the common points between Jacobi polynomials and fractional differentiation. By assuming that the solution is composed of the combination of Jacobi polynomials which are orthogonal polynomials, the accuracy of solutions depends on the number of combinations. Therefore, the accuracy is not written with order representation or big-O notation like the predictor corrector method. In addition, there is no reference to the stability of this method in their paper, but the stability seems to be high because of the implicit method. The present author firstly introduces the theorem which is used in the proposed method, and introduces the detail of this proposed implicit method in the next place. The definitions and properties of Jacobi polynomial are written in Section 2.7.

S. Beheshti, H. Khosravian-Arab and I. Zare show the relationship between Jacobi polynomials and fractional calculus in the following theorem.

Theorem 3.4.5 ([4]) *For $q > 0$ and $0 < x < L$, it holds*

$${}_0^{\mathrm{C}}D_x^q \left\{ x^q P_i^{(0,q)}\left(\frac{2x}{L} - 1\right) \right\} = g_i P_i^{(q,0)}\left(\frac{2x}{L} - 1\right)$$

where $g_i = \Gamma(i + q + 1)/\Gamma(i + 1)$, $i = 0, \ldots, n$.

Note that the Jacobi polynomial $P_i^{(0,q)}$ changes not to $P_i^{(0,q)}$ but to $P_i^{(q,0)}$. Next, the present author shows the proposed method in their paper. This method targets the following fractional ordinary differential equations as

$$\begin{aligned} &{}_0^{\mathrm{C}}D_x^q y(x) = f(x, y(x)), \ 0 < x < L \\ &y(0) = a \\ &y'(0) = b, \ q > 1 \end{aligned}$$

where the fractional calculus order is $0 < q < 2$. Then, we approximate $y(x)$ by using unknown coefficients c_i as

$$\tilde{y}_n(x) = a + b^* x + \sum_{i=0}^{n} c_i x^q P_i^{(0,q)}\left(\frac{2x}{L} - 1\right),$$

where

$$b^* = \begin{cases} 0, & 0 < q \le 1 \\ b, & 1 < q < 2. \end{cases}$$

From Theorem (3.4.5), we can approximate ${}_0^{\mathrm{C}}D_x^q y(x)$ as

$${}_0^{\mathrm{C}}D_x^q \tilde{y}_n(x) = \sum_{i=}^{n} c_i g_i P_i^{(q,0)}\left(\frac{2x}{L} - 1\right).$$

Then, fractional ordinary differential equations are represented as

$$\sum_{i=}^{n} c_i g_i P_i^{(q,0)}\left(\frac{2x}{L} - 1\right) = f\left(x, a + b^* x + \sum_{i=0}^{n} c_i x^q P_i^{(0,q)}\left(\frac{2x}{L} - 1\right)\right).$$

By multiplying both sides of the above equations by $P_k^{(q,0)}(2x/L - 1)(1 - x/L)^q$ and integrating them in the interval $[0, L]$, we have

$$\begin{aligned} &\sum_{i=}^{n} c_i g_i \int_0^L P_i^{(q,0)}\left(\frac{2x}{L} - 1\right) P_k^{(q,0)}\left(\frac{2x}{L} - 1\right)\left(1 - \frac{x}{L}\right)^q dx \\ = &\int_0^L f\left(x, = a + b^* x + \sum_{i=0}^{n} c_i x^q P_i^{(0,q)}\left(\frac{2x}{L} - 1\right)\right) P_k^{(q,0)}\left(\frac{2x}{L} - 1\right)\left(1 - \frac{x}{L}\right)^q dx. \end{aligned}$$

By changing variables for $x = L(u + 1)/2$, using orthogonality and applying Gauss-Jacobi quadrature, we have

$$\begin{aligned} &\frac{2^{q+1}}{2k + q + 1} g_k c_k \\ = &\sum_{j=0}^{n} \omega_j^{(q,0)} f\left(\hat{\xi}_j^{(q,0)}, a + b^* \hat{\xi}_j^{(q,0)} + \sum_{i=0}^{n} c_i (\hat{\xi}_j^{(q,0)})^q P_i^{(0,q)}(\xi_j^{(q,0)})\right) P_k^{(q,0)}(\xi_j^{(q,0)}) \\ &k = 0, 1, \ldots, n \end{aligned}$$

where $\hat{\xi}_j^{(q,0)} = L(\xi_j^{(q,0)} + 1)/2$. Note that the above equations in their paper has a misprint which is corrected in the above expression, so refer to this thesis's expression. The above equations have a form of a system of non-linear equations. Therefore, we can solve about c_i by using Newton's method. There is no remark in their paper that the number of nodes of Gauss-Jacobi quadrature is the same to number of Jacobi-polynomials which the solution contains. The present author considers that the number of nodes of Gauss-Jacobi quadrature can be increased if the error of quadrature is big. However, the experiments in their paper are done with the same number.

Lastly, the experimental results in their paper are introduced. Let $f(x, y)$ be $f(x, y) = x/10 - y(x)$, then the exact solution is

$$y(x) = \frac{x}{10}\left(1 - E_{\alpha,2}(-x^\alpha)\right) + y(0) E_{\alpha,1}(-x^\alpha)$$

where the function $E_{a,b}(t)$ is a Mittag-Leffler function given by

$$E_{a,b}(t) = \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(ak + b)}, \quad a, b > 0.$$

In addition, initial conditions are $y(0) = 1, y'(0) = 0$. For fractional calculus order $\alpha = 0.25, 1.5$ and $L = 6.4$, the results are shown in Tab. 3.2 and Tab. 3.3. These results indicate that the proposed numerical method in their paper actually calculates the numerical results with high accuracy. In a later chapter, the present author makes experiments of the proposed method with the comparison to this method which is introduced in this subsection.

x	$n = 10$	$n = 100$
0.8	-2.77D-4	-1.83D-6
1.6	8.89D-4	2.36D-6
2.4	-6.48D-4	1.12D-7
3.2	4.35D-4	-7.88D-7
4.0	-1.71D-4	-1.37D-6
4.8	1.33D-4	3.35D-7
5.6	-5.58D-4	2.10D-6
6.4	-3.50D-3	-2.36D-5

Table 3.2: Errors of the present method at different x with $q = 0.25$

x	$n = 10$	$n = 50$
0.8	-2.46D-5	-8.10D-9
1.6	8.24D-6	-5.63D-9
2.4	-1.19D-5	-7.88D-10
3.2	1.50D-5	1.59D-9
4.0	-1.81D-5	1.80D-9
4.8	2.08D-5	-4.26D-10
5.6	3.39D-6	2.10D-9
6.4	1.43D-4	1.83D-8

Table 3.3: Errors of the present method at different x with $q = 1.5$

3.4.3 Collocation method using double exponential transform method

In addition to implicit method using Lagrange polynomials, the present author introduces the method using double exponential transform method. A method using double exponential transform method for fractional ordinary differential equations is ever proposed[48]. However, this method assumes only linear differential equations. This method is also a collocation method, and assumes that the solution is given by

$$y_N(t) = y_0 + \sum_{i=-N}^{M} c_i \frac{\sin(\pi(\phi^{-1}(t)/h - i))}{\pi(\phi^{-1}(t)/h - i)} + c_{M+1}\omega(t), \ t_0 \le t \le L \tag{3.9}$$

where $\omega(t)$ is defined by

$$\omega(t) = \frac{t - t_0}{L - t_0}$$

and the function ϕ is defined by

$$\phi(x) = \exp\left(\frac{\pi}{2}\sinh(x)\right).$$

The sampling points s_k are defined by

$$s_k = \begin{cases} \phi(kh), & k = -N, -(N-1), \ldots, M, \\ L, & k = M+1. \end{cases}$$

Then, we have $y_N(s_k) = y_0 + c_k$ for $k = -N, -(N-1), \ldots, M, M+1$. The solution function is composed of sinc functions. Sinc functions are defined by

$$\mathrm{sinc}(x) = \frac{\sin(x)}{x}.$$

This function takes 1 at $x = 0$ as $sinc(0) = 1$. Here, a definition is introduced from the paper[48].

Definition 3.4.6 ([48]) *Let α and β be positive constants with $\alpha, \beta \le 1$. Let f be a function which is analytical in a simply-connected bounded domain $\mathbb{D}$ including the interval (t_0, L), and it holds*

$$\begin{aligned} |f(z) - f(t_0)| &\le K|z - t_0|^\alpha \\ |f(L) - f(z)| &\le K|L - z|^\beta \end{aligned}$$

where there exists some positive integer K. Let $\mathbb{M}_{\alpha,\beta}(\mathbb{D})$ be the set of such functions f. In addition, let d be a positive integer, and define $\mathbb{D}_d$ by

$$\mathbb{D}_d = \{\zeta \in \mathbb{C} : |\mathrm{Im}\zeta| < d\}.$$

From this definition, this method assume that the solution function must be analytical, and $f(t_0) = 0, f(L) = 0$. Actually, the summation of the function (3.9) takes 0 for $t = t_0, L$. In other words, this method does not assume that the solution function takes infinity in the closed interval $[t_0, L]$. However, if the solution function satisfies the above definition, the accuracy of this method is represented with

$$\max_{t_0 \le t \le L} |y(t) - y_N(t)| \le C \log^2(N+1) \exp(-\pi d N / \log(2dN/q))$$

according to the paper[48]. Here, let us obtain the non-linear system of equations by using double exponential transform. By applying changing variable to fractional ordinary differential equations as $u = (t_0 + vt)/(1+v)$, we have

$$y(t) - y_0 = \frac{(t-t_0)^q}{\Gamma(q)} \int_0^\infty (1+v)^{-1-q} f\left(\frac{t_0 + vt}{1+v}, y\right) dv.$$

By applying double exponential transform as $v = \phi(x) = \exp\left(\frac{\pi}{2}\sinh(x)\right)$, we have

$$\begin{aligned} & y(t) - y_0 \\ = \ & \frac{(t-t_0)^q}{\Gamma(q)} \int_{-\infty}^{\infty} (1+\phi(x))^{-1-q} f\left(\frac{t_0 + \phi(x)t}{1+\phi(x)}, y\right) \\ & \cdot \phi(x) \frac{\pi}{2} \cosh(x) dx. \end{aligned} \tag{3.10}$$

From the paper[48], let the value of M and h be

$$\begin{aligned} h &= \frac{\log(2dN/q)}{N} \\ M &= N + \lceil \frac{\log(q)}{h} \rceil. \end{aligned}$$

Applying trapezoidal rule, we obtain

$$\begin{aligned} & c_k - y_0 \\ = \ & \frac{(s_k - t_0)^q h}{\Gamma(q)} \sum_{j=-N+1}^{M-1} (1+\phi(jh))^{-1-q} f\left(\frac{t_0 + \phi(jh)s_k}{1+\phi(jh)}, y_N\right) \phi(jh) \frac{\pi}{2} \cosh(jh) \\ & + \frac{(s_k - t_0)^q h}{2\Gamma(q)} (1+\phi(-Nh))^{-1-q} f\left(\frac{t_0 + \phi(-Nh)s_k}{1+\phi(-Nh)}, y_N\right) \phi(-Nh) \frac{\pi}{2} \cosh(-Nh) \\ & + \frac{(s_k - t_0)^q h}{2\Gamma(q)} (1+\phi(Mh))^{-1-q} f\left(\frac{t_0 + \phi(Mh)s_k}{1+\phi(Mh)}, y_N\right) \phi(Mh) \frac{\pi}{2} \cosh(Mh) \end{aligned}$$

where $k = -N, \ldots, M+1$. By solving this non-linear system of equations, the coefficients c_k are obtained.

Generally, the function $v = \tanh(\pi \sinh(x)/2)$ is used for double exponential transformation. However, for the computation of fractional integral, that transform tends to make the cancellation of significant digits. To solve this difficulty, the present author employs the transform as $v = \exp\left(\frac{\pi}{2}\sinh(x)\right)$ in the experiments of Section 7.4.3. Note that double exponential transform methods are likely to cause other computational errors. Hence, we have to make a code attentively.

Chapter 4

Finite difference formulae for fractional calculus

4.1 Existing high accuracy finite difference formulae

Before the discussion of the proposed numerical methods for fractional differential equations, the author presents the existing high accuracy finite difference formulae proposed in the author's master thesis[57]. The proposed numerical methods in this thesis are based on those finite difference formulae, and the high accuracy of the proposed methods is produced from the high accuracy of those formulae. Therefore, the author briefly introduces how those formulae are obtained, and makes some experiments to confirm the accuracy. Let the fractional calculus order q be an arbitrary real number, a be a constant and a function f be infinitely many times continuously differentiable. Then, the first order accuracy finite difference formula is given by

$$ {}_a^{\mathrm{R}}D_x^q f(x) = \frac{h^q}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-jh) + O\left(\frac{1}{N}\right) \tag{4.1} $$

where h is $h = (x-a)/N$. This formula is the same to the formula proposed by K.B. Oldham[49]. However, the author proves that the accuracy of the formula (4.1) is actually first order accuracy. The second order accuracy formula is given by

$$ \begin{aligned} & {}_a^{\mathrm{R}}D_x^q f(x) \\ = \; & \frac{h^q}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} \left[f(x-jh) + \frac{qh}{2} f'(x-jh) \right] \\ & + \frac{h^{-q}}{\Gamma(-q)} \frac{1+q}{2} f(a) N^{-1-q} + O\left(\frac{1}{N^2}\right). \end{aligned} \tag{4.2} $$

This second accuracy formula (4.2) is used in the proposed finite difference methods and explicit methods for fractional partial and ordinary differential equations to get high accuracy. The third order accuracy formula and fourth order accuracy formula are given by

$$
\begin{aligned}
& {}^{\mathrm{R}}_{a}D^q_x f(x) \\
= \; & \frac{h^q}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} \left[f(x-jh) + \frac{qh}{2} f'(x-jh) + \frac{(3q^2-q)h^2}{24} f''(x-jh) \right] \\
& + \frac{h^{-q}}{\Gamma(-q)} \frac{1+q}{2} f(a) N^{-1-q} + \frac{h^{-q}}{\Gamma(-q)} \frac{(1+q)(2+q)(1+3q)}{24} f(a) N^{-2-q} \\
& + \frac{h^{1-q}}{\Gamma(-q)} \frac{(1+q)(2+3q)}{48} f'(a) N^{-1-q} + O\left(\frac{1}{N^3}\right)
\end{aligned}
\tag{4.3}
$$

and

$$
\begin{aligned}
& {}^{\mathrm{R}}_{a}D^q_x f(x) \\
= \; & \frac{h^q}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} \left[f(x-jh) + \frac{qh}{2} f'(x-jh) \right. \\
& \left. + \frac{(3q^2-q)h^2}{24} f''(x-jh) + \frac{(q^3-q^2)h^3}{48} f'''(x-jh) \right] \\
& + \frac{h^{-q}}{\Gamma(-q)} \frac{1+q}{2} f(a) N^{-1-q} + \frac{h^{-q}}{\Gamma(-q)} \frac{(1+q)(2+q)(1+3q)}{24} f(a) N^{-2-q} \\
& + \frac{h^{1-q}}{\Gamma(-q)} \frac{(1+q)(2+3q)}{48} f'(a) N^{-1-q} + \frac{h^{-q}}{\Gamma(-q)} \frac{q(1+q)^2(2+q)(3+q)}{48} f(a) N^{-3-q} \\
& - \frac{h^{1-q}}{\Gamma(-q)} \frac{(1+q)^2(2+q)}{24} f'(a) N^{-2-q} - \frac{h^{2-q}}{\Gamma(-q)} \frac{q(1+q)^2}{48} f''(a) N^{-1-q} \\
& + O\left(\frac{1}{N^4}\right).
\end{aligned}
\tag{4.4}
$$

Note that all formulae have the accuracy not for $h \to 0$ but for $N \to \infty$. This means that for $N = 1$ and $h \to 0$, all formulae do not guarantee their accuracy. Those formulae are approximation of Riemann-Liouville fractional differential for $q > 0$ and fractional integral for $q < 0$. Next, the author shows how to obtain those formulae.

Let us assume that fractional calculus order q is $q < 0$. This means that we firstly consider the case of fractional integral. Then, fractional integral is defined as

$$
{}_aD^q_x f(x) = \frac{1}{\Gamma(-q)} \int_a^x \frac{f(t)}{(x-t)^{1+q}} dt.
$$

By dividing the integral into N parts and applying changing variables for $u = x - t$, we have

$$
= \lim_{\epsilon \to 0} \frac{1}{\Gamma(-q)} \int_0^h \frac{f(x-u)}{u^{1+q}} du + \frac{1}{\Gamma(-q)} \sum_{j=1}^{N-1} \int_{jh}^{(j+1)h} \frac{f(x-u)}{u^{1+q}} du.
$$

By applying changing variables for $u = jh - t$ and Taylor expansion to function

$g(y) = f(y)/(x-y)^{1+q}$, and we have

$$
\begin{aligned}
&= \lim_{\epsilon\to 0} \frac{1}{\Gamma(-q)} \int_{-h}^{0} g(x-h+t-\epsilon)dt + \frac{1}{\Gamma(-q)} \sum_{j=1}^{N-1} \int_{-h}^{0} g(x-jh+t)dt \\
&= \frac{1}{\Gamma(-q)} \sum_{j=0}^{N-1} \sum_{n=0}^{\infty} g^{(n)}(x-jh)(-1)^n \frac{h^{n+1}}{(n+1)!} \\
&= \frac{1}{\Gamma(-q)} \sum_{j=0}^{N-1} \left[f(x-jh) \frac{h^{-q}}{j^q} \sum_{n=1}^{\infty} \frac{\prod_{k=1}^{n}(k-1+q)}{qj^n n!} (-1)^{n+1} \right. \\
&\quad - f'(x-jh) \frac{h^{1-q}}{j^q} \sum_{n=1}^{\infty} \frac{\prod_{k=1}^{n}(k-1+q)}{q} \frac{n}{j^n (n+1)!} (-1)^{n+1} \\
&\quad + f''(x-jh) \frac{h^{2-q}}{j^q} \sum_{n=2}^{\infty} \frac{\prod_{k=2}^{n}(k-2+q)}{q} \frac{n(n-1)}{2j^{n-1}(n+1)!} (-1)^{n+1} \\
&\quad \left. - f'''(x-jh) \frac{h^{3-q}}{j^q} \sum_{n=3}^{\infty} \frac{\prod_{k=3}^{n}(k-3+q)}{q} \frac{n(n-1)(n-2)}{6j^{n-2}(n+1)!} (-1)^{n+1} \right] + O\left(\frac{1}{N^4}\right).
\end{aligned}
$$

Here, by using the Lemma 5.5 in the thesis[57], we can also prove that each term has a unique order as

$$
\begin{aligned}
& \frac{1}{\Gamma(-q)} \sum_{j=0}^{N-1} f^{(m)}(x-jh) \frac{h^{m-q}}{j^q} \sum_{n=1}^{\infty} \frac{\prod_{k=m}^{n}(k-m+q)}{q} \frac{\prod_{l=1}^{m}(n+1-l)}{m! j^{n-m+1}(n+1)!} (-1)^{n+1} \\
&= O\left(\frac{1}{N^m}\right).
\end{aligned}
$$

Then, infinite sums of each term can be folded by applying Taylor expansion. For example, define $\xi(x)$ as

$$
\xi_1(x) = \frac{-1}{(1+x-b)^q}
$$

where $x-b = 1/j$. By using this function, the infinite sum in the first term can be represented as

$$
\begin{aligned}
& f(x-j) \frac{h^{-q}}{qj^q} \left\{ \frac{q}{j} - \frac{q(1+q)}{j^2 2!} + \frac{q(1+q)(2+q)}{j^3 3!} - \dots \right\} \\
&= f(x-j) \frac{h^{-q}}{qj^q} \left\{ \xi_1'(b)(x-b) + \frac{\xi_1''(b)(x-b)^2}{2!} + \frac{\xi_1'''(b)(x-b)^3}{3!} + \dots \right\} \\
&= f(x-j) \frac{h^{-q}}{qj^q} \{ \xi_1(x) - \xi_1(b) \} \\
&= f(x-j) \frac{h^{-q}}{qj^q} \left\{ \frac{-1}{(1+1/j)^q} + 1 \right\} \\
&= f(x-j) \frac{h^{-q}}{q} \{ -(1+j)^{-q} + j^{-q} \}
\end{aligned}
$$

The infinite sum in the second term can be folded by using two functions $\xi_1(x)$ and $\xi_2(x)$ where

$$
\xi_2(x) = \frac{-1}{(1+x-b)^{q-1}}.
$$

Then, the infinite sum in the second term can be folded as

$$
\begin{aligned}
& -f'(x-jh)\frac{h^{1-q}}{j^q}\left\{\frac{1}{j2!}-\frac{2(1+q)}{j^2 3!}+\frac{3(1+q)(2+q)}{j^3 4!}-\dots\right\} \\
= & -f'(x-jh)\frac{h^{1-q}}{j^q}\left\{\left(\frac{1}{1}-\frac{1}{2}\right)\frac{1}{j}-\left(\frac{1}{2!}-\frac{1}{3!}\right)\frac{(1+q)}{j^2}+\left(\frac{1}{3!}-\frac{1}{4!}\right)\frac{(1+q)(2+q)}{j^3}-\dots\right\} \\
= & -f'(x-jh)\frac{h^{1-q}}{j^q}\left\{\frac{1}{1}\frac{1}{j}-\frac{1}{2!}\frac{(1+q)}{j^2}+\frac{1}{3!}\frac{(1+q)(2+q)}{j^3}-\dots\right\} \\
& -f'(x-jh)\frac{h^{1-q}}{j^{q-1}}\left\{-\frac{1}{2}\frac{1}{j^2}+\frac{1}{3!}\frac{(1+q)}{j^3}-\frac{1}{4!}\frac{(1+q)(2+q)}{j^4}-\dots\right\}.
\end{aligned}
$$

Here, by substituting with $\xi_1(x)$ and $\xi_2(x)$, we have

$$
\begin{aligned}
= & -f'(x-jh)\frac{h^{1-q}}{qj^q}\left\{\xi_1'(b)(x-b)+\frac{\xi_1''(b)(x-b)^2}{2!}+\frac{\xi_1'''(b)(x-b)^3}{3!}+\dots\right\} \\
& -f'(x-jh)\frac{h^{1-q}}{(q-1)qj^{q-1}}\left\{\frac{\xi_2''(b)(x-b)^2}{2!}+\frac{\xi_2'''(b)(x-b)^3}{3!}+\frac{\xi_4''''(b)(x-b)^4}{4!}+\dots\right\} \\
= & -f'(x-jh)\frac{h^{1-q}}{qj^q}\left\{\xi_1(x)-\xi_1(b)\right\} \\
& -f'(x-jh)\frac{h^{1-q}}{(q-1)qj^{q-1}}\left\{\xi_2(x)-\xi_2(b)-\xi_2'(b)(x-b)\right\} \\
= & -f'(x-jh)\frac{h^{1-q}}{qj^q}\left\{\frac{-1}{(1+1/j)^q}+1\right\} \\
& -f'(x-jh)\frac{h^{1-q}}{(q-1)qj^{q-1}}\left\{\frac{-1}{(1+1/j)^{q-1}}+1-\frac{q-1}{j}\right\} \\
= & -f'(x-jh)\frac{h^{1-q}}{q}\left\{-(1+j)^{-q}+j^{-q}\right\} \\
& -f'(x-jh)\frac{h^{1-q}}{(q-1)q}\left\{-(1+j)^{1-q}+j^{1-q}-(q-1)j^{-q}\right\}
\end{aligned}
$$

In a similar way, we can fold the infinite sums. Then, fractional integral can be approximated as

$$
\begin{aligned}
& {}_aD_x^q f(x) \\
= & \; h^{-q}\sum_{j=0}^{N-1}\left[f(x-jh)\frac{(j+1)^{-q}-j^{-q}}{\Gamma(1-q)}\right]+O\left(\frac{1}{N}\right),
\end{aligned}
\tag{4.5}
$$

$$
\begin{aligned}
& {}_aD_x^q f(x) \\
= & \; h^{-q}\sum_{j=0}^{N-1}\left[f(x-jh)\frac{(j+1)^{-q}-j^{-q}}{\Gamma(1-q)}\right. \\
& \left. +hf'(x-jh)\left\{\frac{-(j+1)^{-q}}{\Gamma(1-q)}+\frac{(j+1)^{1-q}}{\Gamma(2-q)}-\frac{j^{1-q}}{\Gamma(2-q)}\right\}\right] \\
& +O\left(\frac{1}{N^2}\right),
\end{aligned}
\tag{4.6}
$$

$$
\begin{aligned}
&{}_aD_x^q f(x) \\
= \; & h^{-q}\sum_{j=0}^{N-1}\Bigg[f(x-jh)\frac{(j+1)^{-q}-j^{-q}}{\Gamma(1-q)} \\
&+hf'(x-jh)\left\{\frac{-(j+1)^{-q}}{\Gamma(1-q)}+\frac{(j+1)^{1-q}}{\Gamma(2-q)}-\frac{j^{1-q}}{\Gamma(2-q)}\right\} \\
&+h^2f''(x-jh)\left\{\frac{(j+1)^{-q}}{2!\Gamma(1-q)}-\frac{(j+1)^{1-q}}{\Gamma(2-q)}+\frac{(j+1)^{2-q}}{\Gamma(3-q)}-\frac{j^{2-q}}{\Gamma(3-q)}\right\} \\
&+O\left(\frac{1}{N^3}\right),
\end{aligned} \tag{4.7}
$$

$$
\begin{aligned}
&{}_aD_x^q f(x) \\
= \; & h^{-q}\sum_{j=0}^{N-1}\Bigg[f(x-jh)\frac{(j+1)^{-q}-j^{-q}}{\Gamma(1-q)} \\
&+hf'(x-jh)\left\{\frac{-(j+1)^{-q}}{\Gamma(1-q)}+\frac{(j+1)^{1-q}}{\Gamma(2-q)}-\frac{j^{1-q}}{\Gamma(2-q)}\right\} \\
&+h^2f''(x-jh)\left\{\frac{(j+1)^{-q}}{2!\Gamma(1-q)}-\frac{(j+1)^{1-q}}{\Gamma(2-q)}+\frac{(j+1)^{2-q}}{\Gamma(3-q)}-\frac{j^{2-q}}{\Gamma(3-q)}\right\} \\
&+h^3f'''(x-jh)\Bigg\{-\frac{(j+1)^{-q}}{3!\Gamma(1-q)}+\frac{(j+1)^{1-q}}{2!\Gamma(2-q)}-\frac{(j+1)^{2-q}}{\Gamma(3-q)} \\
&+\frac{(j+1)^{3-q}}{\Gamma(4-q)}-\frac{j^{3-q}}{\Gamma(4-q)}\Bigg\}\Bigg]+O\left(\frac{1}{N^4}\right).
\end{aligned} \tag{4.8}
$$

The above formula (4.8) is essential to calculate fractional integral numerically. In fact, a part of formula (4.8) is used in the predictor-corrector method proposed by K. Diethelm, N.J. Ford, A.D. Freed[13]. The first term in the formula (4.8) can be transformed to the first order accuracy method (3.8) which is used in the predictor-corrector method. By changing counting order, we have

$$
\begin{aligned}
&h^{-q}\sum_{j=0}^{N-1}f(x-jh)\frac{(j+1)^{-q}-j^{-q}}{\Gamma(1-q)} \\
= \; & h^{-q}\sum_{j=0}^{N-1}f(a+h+jh)\frac{(N-j)^{-q}-(N-1-j)^{-q}}{\Gamma(1-q)}.
\end{aligned}
$$

By applying Taylor expansion, we have

$$
= h^{-q}\sum_{j=0}^{N-1}f(a+jh)\frac{(N-j)^{-q}-(N-1-j)^{-q}}{\Gamma(1-q)}+O\left(\frac{1}{N}\right).
$$

By converting constants as $-q := q$, $N-1 := n$, $a := t_0$, $x := t_n$, $h := (t_n-t_0)/n$, the above formula equals to the first order accuracy formula (3.8) in the predictor-corrector method. In a similar way, the second order accuracy formula (3.6) in the predictor-corrector method is also developed from the formula (4.8). In addition, the third order accuracy formula and higher order accuracy formulae also can be constructed.

The formula (4.8) can compute fractional integral accurately, but cannot compute fractional differential. Actually, for $j=0$ and $q>0$, that formula diverges. To avoid this divergence and to change that formula for the computation of fractional differential, we compare it to a ratio of gamma functions. The detail is written in Lemma 5.8 in the thesis[57]. The author introduces that lemma.

Lemma 4.1.1 *If function f is infinitely many times continuously differentiable and analytical on x, it holds*

$$\left|\frac{h^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1} f(x-jh)\left\{-\frac{(j+1)^{-q}}{q}+\frac{j^{-q}}{q}-\frac{\Gamma(j-q)}{\Gamma(j+1)}\right\}\right| = O\left(\frac{1}{N}\right)$$

This lemma means that the formula (4.8) can be converted into a ratio of gamma functions. By applying this lemma, we obtain the fourth order accuracy formula (4.4). When we develop this formula, we assume that fractional calculus order q is negative. However, this formula also can compute fractional differential in the meaning of Riemann-Liouville definition. This fact can be verified by applying integer order differential to both sides. For example, the first order accuracy formula is given by

$$\begin{aligned}
&\left[\frac{d}{dx}\right] {}_aD_x^q f(x)\\
= \; & {}_aD_x^{1+q} f(x)\\
= \; & \left[\frac{d}{dx}\right]\frac{h^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-jh)\\
= \; & \frac{-q}{N}\frac{h^{-q-1}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-jh)\\
& +\frac{h^{-q}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}\frac{N-j}{N} f'(x-jh).
\end{aligned}$$

By applying Taylor expansion to $f'(x-jh)$, we have

$$\begin{aligned}
= \; & \frac{h^{-q-1}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}\left[\frac{-q}{N} f(x-jh)\right.\\
& \left. + \frac{N-j}{N}\left\{f(x-jh)-f(x-(j+1)h)+\frac{h^2}{2}f''(x-jh)+O\left(\frac{1}{N^3}\right)\right\}\right]
\end{aligned}$$

Here, the terms about $h^2 f''(x-jh)/2$ and $O(1/N^3)$ are the first order $O(1/N)$ as

$$\frac{h^{-q-1}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}\frac{N-j}{N}\left\{\frac{h^2}{2}f''(x-jh)+O\left(\frac{1}{N^3}\right)\right\} = O\left(\frac{1}{N}\right)$$

Therefore, we have

$$\begin{aligned}
= \; & \frac{h^{-q-1}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-q)}{\Gamma(j+1)}\left[\frac{N-j-q}{N}f(x-jh)-\frac{N-j}{N}f(x-(j+1)h)\right]+O\left(\frac{1}{N}\right)\\
= \; & \frac{h^{-q-1}}{\Gamma(-q)}\sum_{j=0}^{N-1} f(x-jh)\left[\frac{N-j-q}{N}\frac{\Gamma(j-q)}{\Gamma(j+1)}-\frac{N-j+1}{N}\frac{\Gamma(j-1-q)}{\Gamma(j)}\right]\\
& -\frac{h^{-1-q}}{\Gamma(-q)}\frac{\Gamma(N-1-q)}{\Gamma(N)}\frac{f(a)}{N}+O\left(\frac{1}{N}\right)\\
= \; & \frac{h^{-q-1}}{\Gamma(-q)}\sum_{j=0}^{N-1}\frac{\Gamma(j-1-q)}{\Gamma(j+1)}f(x-jh)\left\{\frac{q+q^2}{N}+(-1-q)\right\}+O\left(\frac{1}{N}\right)\\
= \; & \frac{h^{-q-1}}{\Gamma(-q-1)}\sum_{j=0}^{N-1}\frac{\Gamma(j-1-q)}{\Gamma(j+1)}f(x-jh)+O\left(\frac{1}{N}\right).
\end{aligned}$$

By repeating this operation, we have arbitrary degree fractional differential. In a similar way, it is verified that the formula (4.2), the formula (4.3) and the formula (4.4) are respectively second order accuracy, third order accuracy and fourth order accuracy for fractional differential.

4.2 Numerical experiments

In this section, let us check the accuracy of formulae which are proposed in the thesis[57]. The experiments are done with the following five formulae.

$$ {}_{a}^{\mathrm{R1}}D_x^q f(x) = \frac{h^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} f(x-jh) \tag{4.9} $$

$$ \begin{aligned} & {}_{a}^{\mathrm{R2}}D_x^q f(x) \\ = & \frac{h^{-q}}{\Gamma(-q)} \sum_{j=0}^{N-1} \frac{\Gamma(j-q)}{\Gamma(j+1)} \left[f(x-jh) + \frac{q}{2}\{f(x-jh) - f(x-(j+1)h)\} \right] \\ & + \frac{h^{-q}}{\Gamma(-q)} \frac{1+q}{2} f(a) N^{-1-q} \end{aligned} \tag{4.10} $$

$$ {}_{a}^{1}D_x^q f(x) = h^{-q} \sum_{j=0}^{N-1} f(x-(j+1)h) \frac{(j+1)^{-q} - j^{-q}}{\Gamma(1-q)} \tag{4.11} $$

$$ \begin{aligned} {}_{a}^{2}D_x^q f(x) = & h^{-q} \sum_{j=0}^{N-1} \left[f(x-jh) \left\{ \frac{-j^{-q}}{\Gamma(1-q)} + \frac{(j+1)^{1-q} - j^{1-q}}{\Gamma(2-q)} \right\} \right. \\ & \left. - f(x-(j+1)h) \left\{ \frac{-(j+1)^{-q}}{\Gamma(1-q)} + \frac{(j+1)^{1-q} - j^{1-q}}{\Gamma(2-q)} \right\} \right] \end{aligned} \tag{4.12} $$

$$ \begin{aligned} & {}_{a}^{3}D_x^q f(x) \\ = & h^{-q} \sum_{j=0}^{N-2} \left[f(x-jh) \frac{(j+1)^{-q} - j^{-q}}{\Gamma(1-q)} \right. \\ & + \frac{3f(x-jh) - 4f(x-(j+1)h) + f(x-(j+2)h)}{2} \\ & \cdot \left\{ \frac{-(j+1)^{-q}}{\Gamma(1-q)} + \frac{(j+1)^{1-q} - j^{1-q}}{\Gamma(2-q)} \right\} \\ & + \{f(x-jh) - 2f(x-(j+1)h) + f(x-(j+2)h)\} \left\{ \frac{(j+1)^{-q}}{2!\Gamma(1-q)} \right. \\ & \left. \left. - \frac{(j+1)^{1-q}}{\Gamma(2-q)} + \frac{(j+1)^{2-q} - j^{2-q}}{\Gamma(3-q)} \right\} \right] \\ & + h^{-q} \left[f(a+h) \frac{N^{-q} - (N-1)^{-q}}{\Gamma(1-q)} \right. \\ & + \left\{ 3f(a+h) - 4f(a+\frac{h}{2}) + f(a) \right\} \left\{ \frac{-N^{-q}}{\Gamma(1-q)} + \frac{N^{1-q} - (N-1)^{1-q}}{\Gamma(2-q)} \right\} \\ & + \left\{ 2f(a+h) - 4f(a+\frac{h}{2}) + 2f(a) \right\} \left\{ \frac{N^{-q}}{2!\Gamma(1-q)} \right. \\ & \left. \left. - \frac{N^{1-q}}{\Gamma(2-q)} + \frac{N^{2-q} - (N-1)^{2-q}}{\Gamma(3-q)} \right\} \right] \end{aligned} \tag{4.13} $$

The formula (4.9) is the first order accuracy, and has the form which is eliminated the limitation from Grunwald-Letnikov definition. Therefore, this formula is sometimes called Grunwald-Letnikov formula. The formula (4.10) is the second order accuracy formula, and is given by applying Taylor expansion to $f'(x-jh)$ in the formula (4.2). Before the introduction of this second order accuracy formulae in the thesis[57], the second order accuracy formula which can compute not only fractional integral but fractional differential has never found. By some transformation to the formula (4.10), the author's proposed finite difference methods will be developed. The formula (4.11) is first order accuracy formula, and given by applying Taylor expansion to the formula (4.5). This formula is equivalent to the formula (3.8) which is used in the predictor-corrector method. The formula (4.12) is the second order accuracy, and is given by applying Taylor expansion to $f'(x-jh)$ in the formula (4.6). This formula is equivalent to the formula (3.6) in the predictor-corrector method. From this, we can see that the formulae (4.5) and (4.6) are the general form of the formulae which is used in the predictor-corrector method. The last formula (4.13) is a third order accuracy formula, and is obtained by applying Taylor expansion as

$$\begin{aligned}
hf'(x-jh) &= \frac{3f(x-jh)-4f(x-(j+1)h)+f(x-(j+2)h)}{2} + O\left(\frac{1}{N^3}\right), \\
& \quad j=0,1,\ldots,N-2 \\
h^2f''(x-jh) &= \{f(x-jh)-2f(x-(j+1)h)+f(x-(j+2)h)\} + O\left(\frac{1}{N^3}\right), \\
& \quad j=0,1,\ldots,N-2 \\
hf'(a+h) &= \{3f(a+h)-4f(a+\frac{h}{2})+f(a)\} + O\left(\frac{1}{N^3}\right), \\
h^2f''(a+h) &= \{2f(a+h)-4f(a+\frac{h}{2})+2f(a)\} + O\left(\frac{1}{N^3}\right).
\end{aligned}$$

This formula will be used in the author's proposed numerical methods for fractional ordinary differential equations. The formulae (4.11), (4.12) and (4.13) can compute only fractional integral and the fractional calculus order q must be $q < 0$.

The first experiments deal with the following function

$$f(x) = 1 - x + x^2 - x^3 + x^4$$

where $a = 0$. The analytical result is given by

$${}_0D_x^q f(x) = \frac{x^{-q}}{\Gamma(1-q)} - \frac{x^{1-q}}{\Gamma(2-q)} + \frac{2x^{2-q}}{\Gamma(3-q)} - \frac{6x^{3-q}}{\Gamma(4-q)} + \frac{24x^{4-q}}{\Gamma(5-q)}.$$

The experiments are done with various q and N.

Figure (4.1) shows the errors of each numerical method for $q = 0.3$ at $x = 2$ with the function f. The formula (4.9) and the formula (4.10) calculate with the first and second order accuracy respectively. Figure (4.2) also shows the errors for $q = 1.3$ at $x = 2$ with the function f. The results indicate each numerical methods calculate with the expected accuracy. Figure (4.3) and Figure (4.4) are the results of errors for $q = -0.3$ and $q = -1.3$ respectively at $x = 2$ with the function f. All numerical methods calculate with the expected accuracy also in integrals.

The second experiments deal with the following function

$$g(x) = 1 - x^{0.2} + x^{0.4} - x^{0.6} + x^{0.8} - x$$

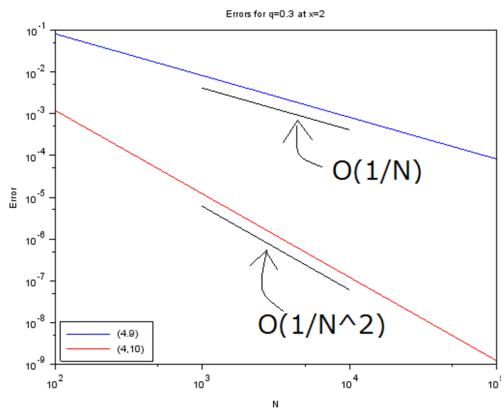


Figure 4.1: Errors for $q = 0.3$ at $x = 2$

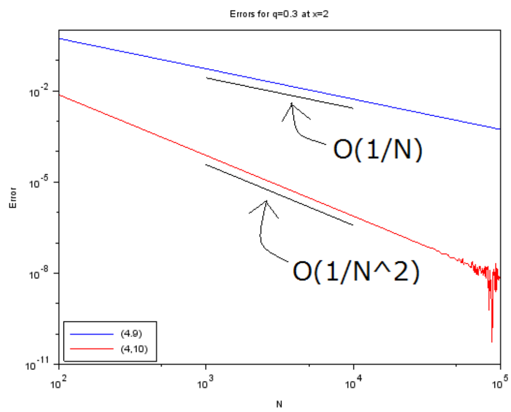


Figure 4.2: Errors for $q = 1.3$ at $x = 2$

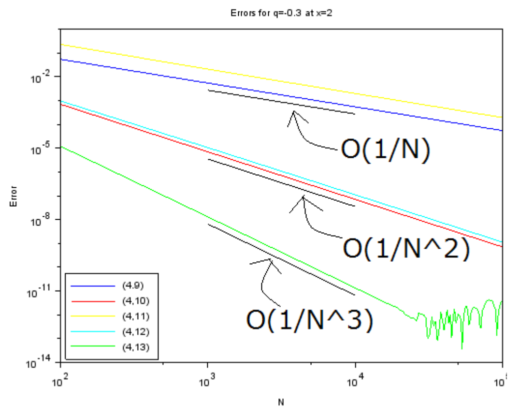


Figure 4.3: Errors for $q = -0.3$ at $x = 2$

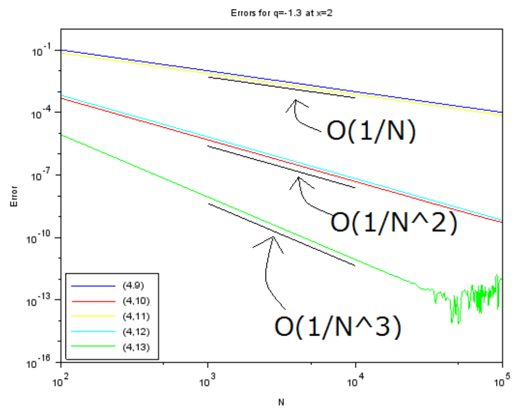


Figure 4.4: Errors for $q = -1.3$ at $x = 2$

where $a = 0$. This function is not differentiable at $x = 0$. The analytical result is given by

$$\begin{aligned} {}_0D_x^q g(x) &= \frac{x^{-q}}{\Gamma(1-q)} - \frac{\Gamma(1.2)x^{0.2-q}}{\Gamma(1.2-q)} + \frac{\Gamma(1.4)x^{0.4-q}}{\Gamma(1.4-q)} \\ &\quad - \frac{\Gamma(1.6)x^{0.6-q}}{\Gamma(1.6-q)} + \frac{\Gamma(1.8)x^{0.8-q}}{\Gamma(1.8-q)} - \frac{x^{1-q}}{\Gamma(2-q)}. \end{aligned}$$

The experiments are done with various q and N.

Figure 4.5 shows the errors produced by the formulae 4.9 and 4.10 for $q = 0.3$ at $x = 2$ with the function g. The results indicate that the errors of the formula 4.9 is the first order accuracy, and the errors of the formula 4.10 is 1.2 order accuracy. This means that the accuracy order of the formula 4.10 decays from the second order to 1.2 order. The reason is the function g is not differentiable at $x = a = 0$. If we numerically differentiate the function which is not smooth at $x = a$, the accuracy of numerical methods may decay and the expected accuracy order may be not obtained. Figure 4.6 also shows the results of accuracy decaying for $q = 1.3$ with the function g. The results in Figure 4.7 and Figure 4.8 show that the accuracy decaying is also caused for fractional integral. This phenomenon also happens for the formulae 4.10 and 4.13. However, this phenomenon is also

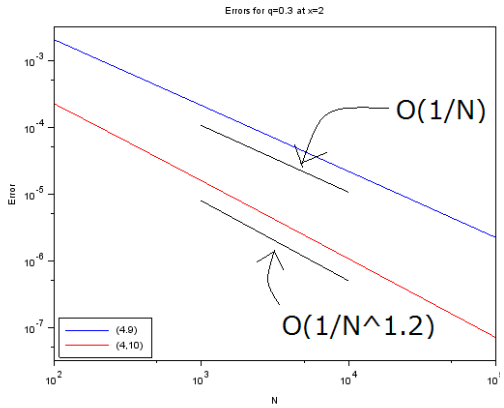


Figure 4.5: Errors for $q = 0.3$ at $x = 2$

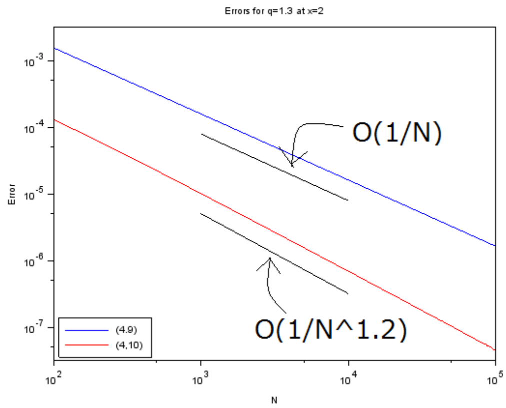


Figure 4.6: Errors for $q = 1.3$ at $x = 2$

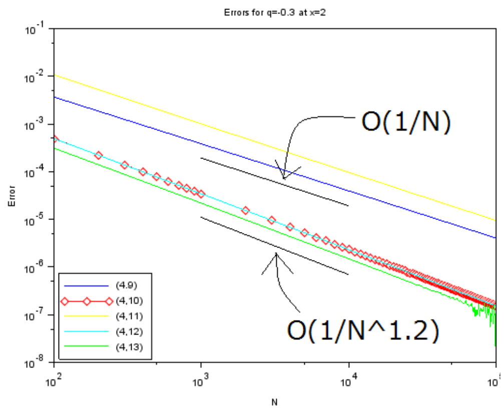


Figure 4.7: Errors for $q = 0.3$ at $x = 2$

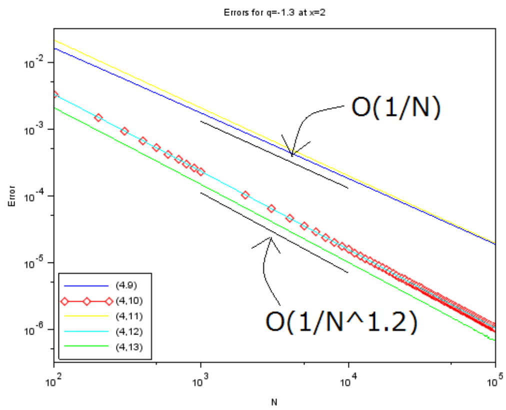


Figure 4.8: Errors for $q = 1.3$ at $x = 2$

common to integer order integral. Figure (4.9) shows the errors of trapezoidal rule at $x = 2$ with the function g. This means this result is for $q = 1$. The expected accuracy order of trapezodal rule is the second order, but the results have only 1.2 order. From this experiment, we see that this accuracy decaying happens not only in fractional calculus but in integer order calculus. Then, how much does the accuracy decay? Experiments indicate that the accuracy order decrease to $1 + p$ order if the differentiated function $f(x)$ is $f(x) = t^p$ for non-integer p. K. Diethelm, K. Ford and N.J. Freed also point out that the accuracy order of the formula (4.12) decrease from 2 to $1+p$ for the differentiated function $f(x) = t^p$[14]. However, there is not any detail of the proof which how much the accuracy decays. Generally, it seems to be difficult to prove how much the accuracy decays. For example, let us consider to integrate the function $z(x) = x^p$

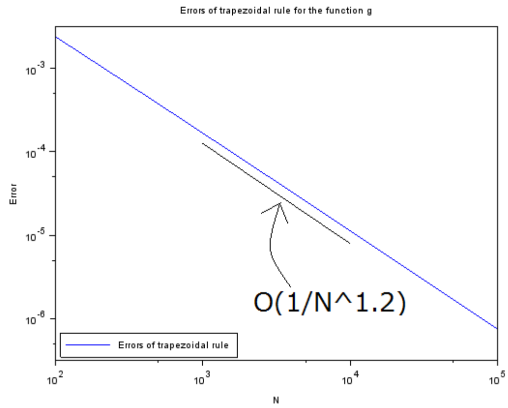


Figure 4.9: Errors of trapezoidal rule at $x = 2$

from 0 to 1 by using trapezoidal rule. Then, for non-integer $0 < p < 1$, we have

$$
\begin{aligned}
& \int_0^1 x^p dx - \frac{h}{2} \sum_{j=0}^{N-1} (jh)^p + ((j+1)h)^p \\
= \quad & \frac{1}{1+p} + \frac{h}{2}(Nh)^p - h \sum_{j=1}^{N} (jh)^p \\
= \quad & \frac{1}{1+p} + \frac{1}{2N} - \left(\frac{1}{N}\right)^{1+p} \sum_{j=1}^{N} j^p \\
= \quad & \left(\frac{1}{N}\right)^{1+p} \left[\frac{N^{1+p}}{1+p} + \frac{N^p}{2} - \sum_{j=1}^{N} j^p \right] \\
= \quad & \left(\frac{1}{N}\right)^{1+p} \sum_{j=1}^{N} \frac{j^{1+p} - (j-1)^{1+p}}{1+p} + \frac{j^p - (j-1)^p}{2} - j^p \\
= \quad & \left(\frac{1}{N}\right)^{1+p} \sum_{j=1}^{N} \left(\frac{1}{3!} - \frac{1}{2 \cdot 2!}\right) \frac{p(p-1)}{j^{2-p}} - \left(\frac{1}{4!} - \frac{1}{2 \cdot 3!}\right) \frac{p(p-1)(p-2)}{j^{3-p}} \cdots .
\end{aligned}
$$

Here, the infinite summations $\sum_{j=1}^{\infty} j^{p-k}$, $k = 2, 3, \ldots$ are Riemann zeta functions, and converge to constants. Therefore, the above expression has the order $O(1/N^{1+p})$ for $N \to \infty$. However, this accuracy decaying is not significant in integer order calculus, because integer order calculus tends to assume smooth functions and differentiated and integrated functions are also smooth. In contrast, fractional calculus gives the singularity to functions, and we have to assume the non-smooth functions as $f(x) = t^p$.

Chapter 5

Fractional partial differential equations

5.1 Space-fractional partial differential equations

5.1.1 Our proposed finite difference method for fractional partial differential equations

In this section, the author discusses the finite difference methods for space-fractional differential equations. As the author introduced in Chapter 2, space-fractional differential equations express a diffusion process whose particles have an infinite variance. Therefore, to solve these equations, we can simulate such a diffusion process and predict physical phenomenon which is controlled by the process which is not represented with integer order calculus. The finite difference method is one of the numerical solving methods for fractional partial differential equations, and is popular method because of easiness of coding. However, to use that method, we have to care about not only accuracy but stability. If we use unstable methods, the error is amplified and the solution diverges. Although the stability is a significant factor, we cannot make stable methods simply by substituting difference formulae. In addition, there are two kinds of finite difference methods in general, explicit methods and implicit methods. Explicit methods mean that we can compute the solutions without solving equations, and we can calculate the solutions with easy arithmetic operations. In contrast, implicit methods mean that we have to solve equations for each time step. Therefore, if the size of problem is very large, it takes longer time to solve by using implicit methods than explicit methods in the same time steps. This property sometimes does not fit some applications. However, there is also property that implicit methods are generally more stable than explicit methods. Hence, this thesis propose both explicit and implicit finite difference methods.

In this thesis, the author treats the following one dimensional space-fractional partial differential equation as

$$\frac{\partial u(x,t)}{\partial t} = \frac{C}{2}\left[{}^{\mathrm{R}}_{L}D^{q}_{x}u(x,t) + {}^{\mathrm{R}}_{x}D^{q}_{R}u(x,t)\right], \tag{5.1}$$

and the following two dimensional space-fractional partial differential equation as

$$\begin{aligned} &\frac{\partial u(x,y,t)}{\partial t} \\ = \;& \frac{C}{2}\left[{}^{\mathrm{R}}_{LX}D^{q}_{x}u(x,y,t)\right. \\ &\left. + {}^{\mathrm{R}}_{x}D^{q}_{RX}u(x,y,t) + {}^{\mathrm{R}}_{LY}D^{q}_{y}u(x,y,t) + {}^{\mathrm{R}}_{y}D^{q}_{RY}u(x,y,t)\right]. \end{aligned} \tag{5.2}$$

Space-fractional partial differential equations express diffusion phenomena whose particles follow random walk with heavy tailed distribution. The derivation of

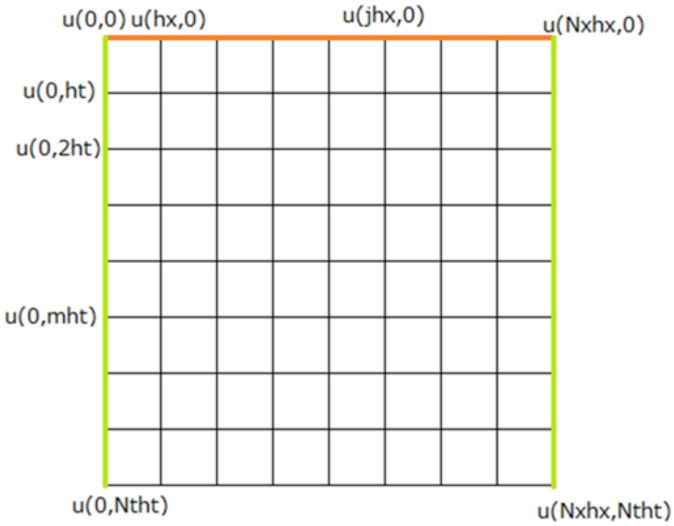


Figure 5.1: Grids

fractional partial differential equations are written in Chapter 2. From the derivation, it is obvious that the range of the fractional order q is limited as $0 < q < 2$ and the constant C is defined as $C < 0$ for $0 < q < 1$ and $C > 0$ for $1 < q < 2$. Sometimes equations have the force term f like

$$\frac{\partial u(x,t)}{\partial t} = \frac{C}{2}\left[{}_{L}^{\mathrm{R}}D_x^q u(x,t) + {}_{x}^{\mathrm{R}}D_R^q u(x,t)\right] + f(x,t).$$

There are many kinds of boudary conditions for partial differential equations, but this thesis treats only Dirichlet boundary conditions. Dirichlet boundary conditions are defined as the solution function takes a constant at boundaries like $u(L,t) = a$, $u(R,t) = b$.

Finite difference methods calculate numerical solutions at each grid. In this thesis, we assume the grid in Figure 5.1. This grid is for one dimensional partial differential equations, but partial differential equations on two dimensional space will be discussed as well. Red line denotes the initial condition and green lines denote the boundary conditions. Let N_x and N_y be the grid number for space with x axis and y axis respectively, and let N_t be the grid number for time. In addition, let h_x be the grid size for space as $(R-L)/N_x$, and let h_t be the grid size for time as T/N_t where T is a constant. Let U_j^m be an approximate solution to $u(jh_x, mh_t)$. For two dimensional equations, Let $U_{j,k}^m$ be an approximate solution to $u(jh_x, kh_y, mh_t)$. Let f_j^m and $f_{j,k}^m$ be the approximation of the force term $f(jh_x, mh_t)$ for one-dimensional problem and $f(jh_x, kh_y, mh_t)$ for two-dimensional problem respectively.

The existing finite difference methods, which is explained in Chapter 3, have been proposed by M.M. Meerschaert and C. Tadjeran[40]. The existing explicit scheme (3.2) is given by

$$\begin{aligned} &\frac{U_j^{m+1} - U_j^m}{h_t} \\ = \; &\frac{1}{h_x^q}\frac{C}{2}\left[\sum_{i=0}^{j+1}\frac{\Gamma(i-q)}{\Gamma(-q)\Gamma(i+1)}U_{j-i+1}^m + \sum_{i=0}^{N_x-j+1}\frac{\Gamma(i-q)}{\Gamma(-q)\Gamma(i+1)}U_{j+i-1}^m\right] \\ &+ f_j^m \end{aligned} \tag{5.3}$$

where $1 < q < 2$. The stability condition is $h_t \le h_x^q/(Aq)$. The existing implicit scheme (3.1) is given by

$$\begin{aligned}
&\frac{U_j^{m+1} - U_j^m}{h_t} \\
= \; & \frac{1}{h_x^q}\frac{C}{2}\left[\sum_{i=0}^{j+1} \frac{\Gamma(i-q)}{\Gamma(-q)\Gamma(i+1)} U_{j-i+1}^{m+1} + \sum_{i=0}^{N_x-j+1} \frac{\Gamma(i-q)}{\Gamma(-q)\Gamma(i+1)} U_{j+i-1}^{m+1}\right] \\
&+ f_j^{m+1}. \qquad (5.4)
\end{aligned}$$

where $1 < q < 2$. This scheme is unconditionally stable. The accuracy of both scheme is $O(h_t) + O(h_x)$. This means that the accuracy is the first order for time and space, and depends on both the time and the space step sizes. In contrast, all the author's proposed schemes have the accuracy order $O(h_t) + O(h_x^2)$. The accuracy about time step can be improved with existing methods in the same way of finite difference methods for integer order differential equations. Our proposed explicit method for one dimensional equation is given by

$$\begin{aligned}
&\frac{U_j^{m+1} - U_j^m}{h_t} \\
= \; & \frac{C}{2}\left[\frac{h_x^{-q}}{\Gamma(-q)} \sum_{i=0}^{j-1} \frac{\Gamma(i-q)}{\Gamma(i+1)} \left\{\frac{4s+q}{4} U_{j+1-i}^m + (1-2s) U_{j-i}^m + \frac{4s-q}{4} U_{j-1-i}^m\right\}\right. \\
&+ \frac{h_x^{-q}}{\Gamma(-q)} \sum_{i=0}^{N_x-j-1} \frac{\Gamma(i-q)}{\Gamma(i+1)} \left\{\frac{4s+q}{4} U_{j-1+i}^m + (1-2s) U_{j+i}^m + \frac{4s-q}{4} U_{j+1+i}^m\right\} \\
&+ \frac{h_x^{-q}}{\Gamma(-q)} \frac{\Gamma(j-q)}{\Gamma(j+1)} \frac{4s+q}{4} U_1^m + \frac{h_x^{-q}}{\Gamma(-q)} \frac{\Gamma(N_x-j-q)}{\Gamma(N_x-j+1)} \frac{4s+q}{4} U_{N_x-1}^m \\
&+ h_x^{-q}\left\{\frac{j^{-q}}{\Gamma(1-q)} - \frac{\Gamma(j-q)}{\Gamma(1-q)\Gamma(j)} - \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)} \frac{4s+q}{4}\right\} U_0^m \\
&\left.+ h_x^{-q}\left\{\frac{(N_x-j)^{-q}}{\Gamma(1-q)} - \frac{\Gamma(N_x-j-q)}{\Gamma(1-q)\Gamma(N_x-j)} - \frac{\Gamma(N_x-j-q)}{\Gamma(-q)\Gamma(N_x-j+1)} \frac{4s+q}{4}\right\} U_{N_x}^m\right] \\
&+ f_j^m \qquad (5.5)
\end{aligned}$$

for $j = 1, 2, \ldots, N_x - 1$. As a significant property, this scheme has a parameter s, and the stability of the scheme depends on the value of s. This scheme can be represented by using matrices as $\vec{U}^{m+1} = (E + A)\vec{U}^m + \vec{f}^m$ where $\vec{U}^m = (U_0^m, U_1^m, \ldots, U_{N_x}^m)^T$ and $\vec{f}^m = (f_0^m, f_1^m, \ldots, f_{N_x}^m)^T$ and the matrix E is an identity matrix. The entries $a_{i,j}$ of the matrix A are defined as

$$A = \begin{pmatrix}
0 & 0 & 0 & \cdots & 0 & 0 \\
a_{1,0} & a_{1,1} & a_{1,2} & \cdots & a_{1,N_x-1} & a_{1,N_x} \\
a_{2,0} & a_{2,1} & a_{2,2} & \cdots & a_{2,N_x-1} & a_{2,N_x} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
a_{N_x-1,0} & a_{N_x-1,1} & a_{N_x-1,2} & \cdots & a_{N_x-1,N_x-1} & a_{N_x-1,N_x} \\
0 & 0 & 0 & \cdots & 0 & 0
\end{pmatrix}.$$

Here, the entries $a_{i,j}$ for $i = 1, 2, \ldots, N_x - 1$, $j = 1, 2, \ldots, N_x - 1$ are symmetric and given by

$$
\begin{aligned}
a_{n,n} &= \frac{Cr}{2}\left[2g_0(1-2s)+2g_1\frac{4s+q}{4}\right] \\
a_{n,n+1} &= a_{n+1,n} = \frac{Cr}{2}\left[g_0\frac{4s+q}{4}+g_0\frac{4s-q}{4}+g_1(1-2s)+g_2\frac{4s+q}{4}\right] \\
a_{n,n+2} &= a_{n+2,n} = \frac{Cr}{2}\left[g_1\frac{4s-q}{4}+g_2(1-2s)+g_3\frac{4s+q}{4}\right] \\
a_{n,n+3} &= a_{n+3,n} = \frac{Cr}{2}\left[g_2\frac{4s-q}{4}+g_3(1-2s)+g_4\frac{4s+q}{4}\right] \\
&\vdots \\
a_{n,n+k} &= a_{n+k,n} = \frac{Cr}{2}\left[g_{k-1}\frac{4s-q}{4}+g_k(1-2s)+g_{k+1}\frac{4s+q}{4}\right] \\
&\vdots
\end{aligned}
$$

for $n = 1, 2, \ldots, N_x - 1$ where $r = h_t/h_x^q$ and $g_k = \Gamma(k-q)/(\Gamma(-q)\Gamma(k+1))$. The author's proposed implicit method for one dimensional equation is given by

$$
\begin{aligned}
&\frac{U_j^m - U_j^{m-1}}{h_t} \\
= \ & \frac{C}{2}\left[\frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j+1-i}^m+(1-2s)U_{j-i}^m+\frac{4s-q}{4}U_{j-1-i}^m\right\}\right. \\
&+\frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{N_x-j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j-1+i}^m+(1-2s)U_{j+i}^m+\frac{4s-q}{4}U_{j+1+i}^m\right\} \\
&+\frac{h_x^{-q}}{\Gamma(-q)}\frac{\Gamma(j-q)}{\Gamma(j+1)}\frac{4s+q}{4}U_1^m+\frac{h_x^{-q}}{\Gamma(-q)}\frac{\Gamma(N_x-j-q)}{\Gamma(N_x-j+1)}\frac{4s+q}{4}U_{N_x-1}^m \\
&+h_x^{-q}\left\{\frac{j^{-q}}{\Gamma(1-q)}-\frac{\Gamma(j-q)}{\Gamma(1-q)\Gamma(j)}-\frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\frac{4s+q}{4}\right\}U_0^m \\
&\left.+h_x^{-q}\left\{\frac{(N_x-j)^{-q}}{\Gamma(1-q)}-\frac{\Gamma(N_x-j-q)}{\Gamma(1-q)\Gamma(N_x-j)}-\frac{\Gamma(N_x-j-q)}{\Gamma(-q)\Gamma(N_x-j+1)}\frac{4s+q}{4}\right\}U_{N_x}^m\right] \\
&+f_j^m \qquad (5.6)
\end{aligned}
$$

for $j = 1, 2, \ldots, N_x - 1$. The matrix representation of the scheme (5.6) is expressed as $(E-A)\vec{U}^m = \vec{U}^{m-1} + \vec{f}^m$. The entries of the matrix A are the same to that of the explicit scheme (5.5). For two dimensional fractional partial equations (5.2), the author proposes the following explicit scheme

$$
\begin{aligned}
&\frac{U_{j,k}^{m+1}-U_{j,k}^{m}}{h_t}\\
= \quad & \frac{C}{2}\left[\frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j+1-i,k}^{m}+(1-2s)U_{j-i,k}^{m}+\frac{4s-q}{4}U_{j-1-i,k}^{m}\right\}\right.\\
&+\frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{N_x-j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j-1+i,k}^{m}+(1-2s)U_{j+i,k}^{m}+\frac{4s-q}{4}U_{j+1+i,k}^{m}\right\}\\
&+\frac{h_y^{-q}}{\Gamma(-q)}\sum_{i=0}^{j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j,k+1-i}^{m}+(1-2s)U_{j,k-i}^{m}+\frac{4s-q}{4}U_{j,k-1-i}^{m}\right\}\\
&+\frac{h_y^{-q}}{\Gamma(-q)}\sum_{i=0}^{N_y-j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j,k-1+i}^{m}+(1-2s)U_{j,k+i}^{m}+\frac{4s-q}{4}U_{j,k+1+i}^{m}\right\}\\
&+\frac{h_x^{-q}}{\Gamma(-q)}\frac{\Gamma(j-q)}{\Gamma(j+1)}\frac{4s+q}{4}U_{1,k}^{m}+\frac{h_x^{-q}}{\Gamma(-q)}\frac{\Gamma(N_x-j-q)}{\Gamma(N_x-j+1)}\frac{4s+q}{4}U_{N_x-1,k}^{m}\\
&+h_x^{-q}\left\{\frac{j^{-q}}{\Gamma(1-q)}-\frac{\Gamma(j-q)}{\Gamma(1-q)\Gamma(j)}-\frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\frac{4s+q}{4}\right\}U_{0,k}^{m}\\
&+h_x^{-q}\left\{\frac{(N_x-j)^{-q}}{\Gamma(1-q)}-\frac{\Gamma(N_x-j-q)}{\Gamma(1-q)\Gamma(N_x-j)}-\frac{\Gamma(N_x-j-q)}{\Gamma(-q)\Gamma(N_x-j+1)}\frac{4s+q}{4}\right\}U_{N_x,k}^{m}\\
&+\frac{h_y^{-q}}{\Gamma(-q)}\frac{\Gamma(k-q)}{\Gamma(k+1)}\frac{4s+q}{4}U_{j,1}^{m}+\frac{h_y^{-q}}{\Gamma(-q)}\frac{\Gamma(N_y-k-q)}{\Gamma(N_y-k+1)}\frac{4s+q}{4}U_{j,N_y-1}^{m}\\
&+h_y^{-q}\left\{\frac{k^{-q}}{\Gamma(1-q)}-\frac{\Gamma(k-q)}{\Gamma(1-q)\Gamma(k)}-\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k+1)}\frac{4s+q}{4}\right\}U_{j,0}^{m}\\
&\left.+h_y^{-q}\left\{\frac{(N_y-k)^{-q}}{\Gamma(1-q)}-\frac{\Gamma(N_y-k-q)}{\Gamma(1-q)\Gamma(N_y-k)}-\frac{\Gamma(N_y-k-q)}{\Gamma(-q)\Gamma(N_y-k+1)}\frac{4s+q}{4}\right\}U_{j,N_y}^{m}\right]\\
&+f_j^m
\end{aligned}
\tag{5.7}
$$

This scheme also can be represented with the matrix representation as $\hat{U}^{m+1}=(E+A)\hat{U}^m+\hat{f}^m$ for

$$\hat{U}^m=(U_{0,0}^m,U_{1,0}^m,U_{2,0}^m,\dots,U_{N_x,0}^m,U_{0,1}^m,U_{1,1}^m,\dots,U_{N_x,1}^m,U_{0,2}^m,\dots)^T$$

and $\hat{f}^m=(f_{0,0}^m,f_{1,0}^m,\dots)$. The matrix A is constructed with submatrices $\hat{A}_{i,j}$ as

$$
A=\begin{pmatrix}
0 & 0 & 0 & \dots & 0 & 0\\
\hat{A}_{1,0} & \hat{A}_{1,1} & \hat{A}_{1,2} & \dots & \hat{A}_{1,N_y-1} & \hat{A}_{1,N_y}\\
\hat{A}_{2,0} & \hat{A}_{2,1} & \hat{A}_{2,2} & \dots & \hat{A}_{2,N_y-1} & \hat{A}_{2,N_y}\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
\hat{A}_{N_y-1,0} & \hat{A}_{N_y-1,1} & \hat{A}_{N_y-1,2} & \dots & \hat{A}_{N_y-1,N_y-1} & \hat{A}_{N_y-1,N_y}\\
0 & 0 & 0 & \dots & 0 & 0
\end{pmatrix}.
$$

Then, the non-diagonal submatrices $\hat{A}_{i,j}$ for $i \neq j$ are diagonal matrices as

$$
\begin{aligned}
\hat{A}_{n,n+1} &= \hat{A}_{n+1,n} = \frac{Cr_y}{2}\left[g_0\frac{4s+q}{4} + g_0\frac{4s-q}{4} + g_1(1-2s) + g_2\frac{4s+q}{4}\right]\cdot E \\
\hat{A}_{n,n+2} &= \hat{A}_{n+2,n} = \frac{Cr_y}{2}\left[g_1\frac{4s-q}{4} + g_2(1-2s) + g_3\frac{4s+q}{4}\right]\cdot E \\
\hat{A}_{n,n+3} &= \hat{A}_{n+3,n} = \frac{Cr_y}{2}\left[g_2\frac{4s-q}{4} + g_3(1-2s) + g_4\frac{4s+q}{4}\right]\cdot E \\
&\vdots \\
\hat{A}_{n,n+k} &= \hat{A}_{n+k,n} = \frac{Cr_y}{2}\left[g_{k-1}\frac{4s-q}{4} + g_k(1-2s) + g_{k+1}\frac{4s+q}{4}\right]\cdot E \\
&\vdots
\end{aligned}
$$

where $r_y = h_t/h_y^q$, $n = 1, 2, \ldots, N_y - 1$. The entries $a_{i,j}$ of the diagonal submatrices $\hat{A}$ is defined as

$$
\begin{aligned}
a_{n,n} &= \frac{Cr_x}{2}\left[2g_0(1-2s) + 2g_1\frac{4s+q}{4}\right] + \frac{Cr_y}{2}\left[2g_0(1-2s) + 2g_1\frac{4s+q}{4}\right] \\
a_{n,n+1} &= a_{n+1,n} = \frac{Cr_x}{2}\left[g_0\frac{4s+q}{4} + g_0\frac{4s-q}{4} + g_1(1-2s) + g_2\frac{4s+q}{4}\right] \\
a_{n,n+2} &= a_{n+2.n} = \frac{Cr_x}{2}\left[g_1\frac{4s-q}{4} + g_2(1-2s) + g_3\frac{4s+q}{4}\right] \\
a_{n,n+3} &= a_{n+3.n} = \frac{Cr_x}{2}\left[g_2\frac{4s-q}{4} + g_3(1-2s) + g_4\frac{4s+q}{4}\right] \\
&\vdots \\
a_{n,n+k} &= a_{n+k.n} = \frac{Cr_x}{2}\left[g_{k-1}\frac{4s-q}{4} + g_k(1-2s) + g_{k+1}\frac{4s+q}{4}\right] \\
&\vdots
\end{aligned}
$$

where $r_x = h_t/h_x^q$, where $n = 1, 2, \cdots, N_x - 1$. The implicit scheme for two dimensional equations is also constructed in a similar way as

$$
(E - A)\hat{U}^m = \hat{U}^{m-1} + \hat{f}^m. \tag{5.8}
$$

The characteristic of the author's proposed schemes is the existence of the parameter s. The stability of the author's proposed schemes depends on the parameter q and s. This means that the parameter s should be chosen depending on the fractional calculus order q. The relation between the stability and the parameter s will be discussed in the next subsection.

All these schemes which the author proposes are made with the second order accuracy formula (4.2). However, the most important problem is how to introduce the second order accuracy formula (4.2) to schemes. In any form, the scheme which uses the formula (4.2) is the second order accuracy for space grid size. This means that one can create a formula of second order accuracy in space dimension by using the formula (4.2). For example, the following implicit scheme also has the accuracy order $O(h_t) + O(h_x)$,

$$
\begin{aligned}
& \frac{U_j^m - U_j^{m-1}}{h_t} \\
= \; & \frac{C}{2}\left[\frac{h_x^{-q}}{\Gamma(-q)} \sum_{i=0}^{j-1} \frac{\Gamma(i-q)}{\Gamma(i+1)} \left\{\frac{2-q}{2} U_{j-i}^m + \frac{q}{2} U_{j+1-i}^m\right\}\right. \\
& + \frac{h_x^{-q}}{\Gamma(-q)} \sum_{i=0}^{N_x-j-1} \frac{\Gamma(i-q)}{\Gamma(i+1)} \left\{\frac{2-q}{2} U_{j+i}^m + \frac{q}{2} U_{j-1+i}^m\right\} \\
& + \frac{h_x^{-q}}{\Gamma(-q)} \frac{1+q}{2} \frac{\Gamma(j-1-q)}{\Gamma(j)} U_0^m \\
& \left. + \frac{h_x^{-q}}{\Gamma(-q)} \frac{1+q}{2} \frac{\Gamma(N_x-j-1-q)}{\Gamma(N_x-j)} U_{N_x}^m \right] \\
& + f_j^m.
\end{aligned} \tag{5.9}
$$

This scheme utilizes the following second order accuracy formula, which is transformed from the formula (4.2) by using Taylor expansion,

$$
\begin{aligned}
& {}_L^{\mathrm{R}}D_x^q u(x) \\
\simeq \; & \frac{h_x^{-q}}{\Gamma(-q)} \sum_{i=0}^{N-1} \frac{\Gamma(i-q)}{\Gamma(i+1)} \left\{\frac{2-q}{2} u(x - i h_x) + \frac{q}{2} u(x-(i-1)h_x)\right\} \\
& + \frac{h_x^{-q}}{\Gamma(-q)} \frac{1+q}{2} \frac{\Gamma(N-1-q)}{\Gamma(N)} u(L).
\end{aligned} \tag{5.10}
$$

This formula is also second order accuracy, but we should not use the scheme (5.9) because of the instability. This scheme is not stable for $1 < q < 2$, and the errors are amplified in the computations. This problem about the stability is also shown in the related work[40]. In that paper, M.M. Meerschaert and C. Tadjeran introduce an example scheme which has the accuracy $O(h_t) + O(h_x)$ and is not stable. Therefore, we cannot simply apply the high accuracy difference formulae to the high accuracy finite difference methods. Then, how can we construct high accuracy finite difference methods? There are three points for the author's scheme constructing. One is to embed a freedom of schemes by introducing the parameter. To be stable, the author's proposed schemes include the parameter s, and are derived from the following second order accuracy formula

$$
\begin{aligned}
& {}_L^{\mathrm{R}}D_x^q u(x) \\
\simeq \; & \frac{h_x^{-q}}{\Gamma(-q)} \sum_{i=0}^{N-1} \frac{\Gamma(i-q)}{\Gamma(i+1)} \left\{\frac{4s+q}{4} u(x-(i-1)h_x)\right. \\
& \left. + (1-2s) u(x - i h_x) + \frac{4s-q}{4} u(x-(i+1)h_x)\right\} \\
& + \frac{h_x^{-q}}{\Gamma(-q)} \frac{\Gamma(N-q)}{\Gamma(N+1)} \frac{4s+q}{4} u(L+h_x) \\
& + h_x^{-q}\left\{\frac{N^{-q}}{\Gamma(1-q)} - \frac{\Gamma(N-q)}{\Gamma(1-q)\Gamma(N)}\right. \\
& \left. - \frac{\Gamma(N-q)}{\Gamma(-q)\Gamma(N+1)} \frac{4s+q}{4}\right\} u(L).
\end{aligned} \tag{5.11}
$$

Depending on the value of q, the schemes become stable by changing the value of s.

Second point for the author's scheme construction is a symmetric Toeplitz matrix. Let us consider the matrix A in the matrix representation of the scheme (5.5). The submatrix including entries $a_{i,j}$ for $1 \le i, j \le N_x - 1$ is a symmetric Toeplitz matrix. For example, the following scheme is less stable than scheme (5.5),

$$\begin{aligned}
&\frac{U_j^{m+1} - U_j^m}{h_t} \\
= \quad & \frac{C}{2}\left[\frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j+1-i}^m + (1-2s)U_{j-i}^m + \frac{4s-q}{4}U_{j-1-i}^m\right\}\right. \\
& + \frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{N_x-j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}U_{j-1+i}^m + (1-2s)U_{j+i}^m + \frac{4s-q}{4}U_{j+1+i}^m\right\} \\
& + h_x^{-q}\left\{\frac{j^{-q}}{\Gamma(1-q)} - \frac{\Gamma(j-q)}{\Gamma(1-q)\Gamma(j)}\right\}U_0^m \\
& \left. + h_x^{-q}\left\{\frac{(N_x-j)^{-q}}{\Gamma(1-q)} - \frac{\Gamma(N_x-j-q)}{\Gamma(1-q)\Gamma(N_x-j)}\right\}U_{N_x}^m\right] \\
& + f_j^m.
\end{aligned}$$

The entries $a_{i,j}$ of the matrix representation of the above scheme is not a symmetric Toeplitz matrix for $1 \le i, j \le N_x - 1$ because of first and $N_x - 1$-th column, for example, $a_{2,1} \ne a_{1,2}$. The matrix representations of the author's schemes include the symmetric Toeplitz matrix around $a_{N_{x/2},N_{x/2}}$. By constructing formulas in such a way, the author succeeded to define stable formulae. The author has discovered this feature in the results of trial and error and has noticed that the matrix representation of the existing scheme (3.2) also has a symmetric Toeplitz matrix. This means that the author forms schemes to have a symmetric Toeplitz scheme in the results of analyzing stability. Generally, it is not easy to prove that the symmetric Toeplitz matrix is the most appropriate to be stable. This is a heuristic, and there is no proof that a stable formula must have such a structure. However, it is a fact that this feature significantly improves the stability.

Third point for the author's scheme construction is to approximate the fractional differentiation with a few nodes. This means the author's scheme can compute solutions with a few number of N in the formula (5.11). For example, to calculate U_1^m in the scheme (5.5), we have to approximate the left derivative ${}_L^{\mathrm{R}}D_x^q u(x)$ at $L + h_x$ with $N = 1$ as

$$\begin{aligned}
& {}_L^{\mathrm{R}}D_x^q u(L+h_x) \\
\simeq \quad & \frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{0}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}u(L+h_x-(i-1)h_x)\right. \\
& \left. + (1-2s)u(L+h_x-ih_x) + \frac{4s-q}{4}u(L+h_x-(i+1)h_x)\right\} \\
& + \frac{h_x^{-q}}{\Gamma(-q)}\frac{\Gamma(1-q)}{\Gamma(2)}\frac{4s+q}{4}u(L+h_x) \\
& + h_x^{-q}\left\{\frac{1}{\Gamma(1-q)} - \frac{\Gamma(1-q)}{\Gamma(1-q)\Gamma(1)} - \frac{\Gamma(1-q)}{\Gamma(-q)\Gamma(2)}\frac{4s+q}{4}\right\}u(L).
\end{aligned}$$

The finite difference formulae calculate with the expected accuracy with $N \to \infty$, but we have to calculate even with $N = 1$. This limitation also increases the error. For example, let us consider to calculate fractional differentiation of the constant function $u(x) = c$ at h_x with the formula (5.10) for $N = 1$. Then, the error is given by

$$\begin{aligned}
& \left| {}_0^{\mathrm{R}}D_x^q c - h_x^{-q}\left\{\frac{2-q}{2}c + \frac{q}{2}c\right\}\right| \\
= & \left|\frac{\Gamma(1)}{\Gamma(1-q)}ch_x^{-q} - \frac{2-q}{2}ch_x^{-q} - \frac{q}{2}ch_x^{-q}\right| \\
= & O(h_x^{-q}).
\end{aligned}$$

This means that the formula (5.10) produces the error of $O(h_x^{-q})$ for $N = 1$. Because $q > 0$ in finite difference methods, the error will diverge for $h_x \to 0$. To avoid this accuracy decaying, the formula (5.11) has a little ingenuity. This formula has a more complicate expression than the formula (5.10), but this formula has a feature of error cancelling. In a similar way, let us consider the error for the constant function $u(x) = c$ at $x = jh_x$. Then, we have

$$\begin{aligned}
& \left| {}_0^{\mathrm{R}}D_x^q c - \frac{h_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)}\left\{\frac{4s+q}{4}c + (1-2s)c + \frac{4s-q}{4}c\right\}\right. \\
& -\frac{h_x^{-q}}{\Gamma(-q)}\frac{\Gamma(j-q)}{\Gamma(j+1)}\frac{4s+q}{4}c \\
& \left. -h_x^{-q}\left\{\frac{j^{-q}}{\Gamma(1-q)} - \frac{\Gamma(j-q)}{\Gamma(1-q)\Gamma(j)} - \frac{\Gamma(j-q)}{\Gamma(-q)\Gamma(j+1)}\frac{4s+q}{4}\right\}c\right| \\
= & \left|\frac{c(jh_x)^{-q}}{\Gamma(1-q)} - \frac{ch_x^{-q}}{\Gamma(-q)}\sum_{i=0}^{j-1}\frac{\Gamma(i-q)}{\Gamma(i+1)} - \frac{ch_x^{-q}}{\Gamma(1-q)}\left\{j^{-q} - \frac{\Gamma(j-q)}{\Gamma(j)}\right\}\right| \\
= & 0.
\end{aligned}$$

Therefore, the author's scheme calculates the constant function without errors. This means that we can assume non-zero Dirichlet boundary conditions. Other existing finite difference methods do not have a feature of this error cancelling, so we cannot assume non-zero Dirichlet boundary conditions when we use them. Not only the better accuracy, this feature of our proposed finite difference methods is also good point comparing to existing methods.

5.1.2 Stability analysis of the author's proposed finite difference methods

In this subsection, let us analyze the stability of the author's proposed finite difference methods. In the beginning, let us review the concept of stability. Figures 5.2 and 5.3 show examples of being stable and not being stable, respectively. The errors, which are derived from rounding errors and so on, are amplified over time and the numerical solution does not converge if the scheme is unstable. The idea of the stability is independent of the accuracy, so we have to analyze the stability differently from the accuracy of schemes. Generally, there are two well-known methods to analyze the stability of finite difference methods. One is Von Neumann stability analysis, and the other is the matrix method which is the method to analyze the eigenvalues. In this thesis, the author analyzes the stability by using the matrix methods because of the reason as explained below.

Von Neumann stability analysis to the author's proposed scheme

Firstly, let us consider to apply Von Neumann stability analysis to the scheme (5.5). Let U_j^m be $U_j^m = \kappa^m \exp(i\xi jh_x)$ where κ is an amplifier factor and ξ is

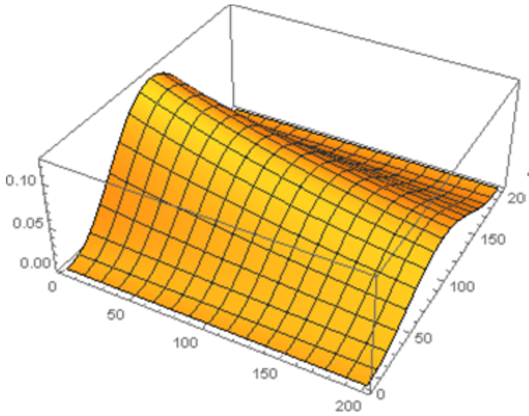


Figure 5.2: Example of stable scheme

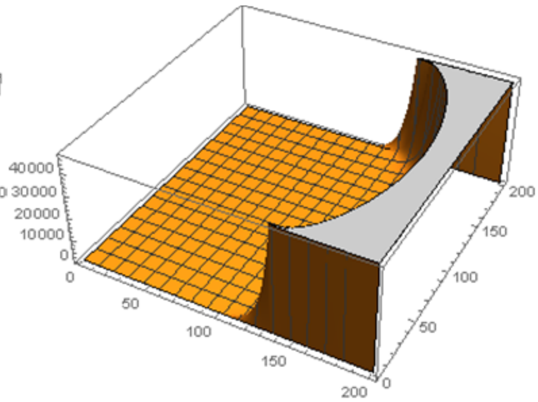


Figure 5.3: Example of unstable scheme

a wave number. By substituting to the explicit scheme (5.5), for $g_n = \Gamma(n-q)/(\Gamma(-q)\Gamma(n+1))$ we have

$$
\begin{aligned}
&\kappa \\
= \;& 1+\frac{Cr}{2}\Bigg[\sum_{n=0}^{j-1} g_n\left\{\frac{4s+q}{4}\exp(i\xi(1-n)h_x)+(1-2s)\exp(-i\xi n h_x)\right. \\
&\left.+\frac{4s-q}{4}\exp(i\xi(-1-n)h_x)\right\} \\
&+\sum_{n=0}^{N_x-j-1} g_n\left\{\frac{4s+q}{4}\exp(i\xi(n-1)h_x)+(1-2s)\exp(i\xi n h_x)\right. \\
&\left.+\frac{4s-q}{4}\exp(i\xi(1+n)h_x)\right\} \\
&+g_j\frac{4s+q}{4}\exp(i\xi(1-j)h_x)+g_{N_x-j}\frac{4s+q}{4}\exp(i\xi(N_x-j-1)h_x) \\
&+\left\{\frac{j^{-q}}{\Gamma(1-q)}-\frac{\Gamma(j-q)}{\Gamma(1-q)\Gamma(j)}-g_j\frac{4s+q}{4}\right\}\exp(-i\xi j h_x) \\
&+\left\{\frac{(N_x-j)^{-q}}{\Gamma(1-q)}-\frac{\Gamma(N_x-j-q)}{\Gamma(1-q)\Gamma(N_x-j)}-g_{N_x-j}\frac{4s+q}{4}\right\}\exp(i\xi(N_x-j)h_x)\Bigg].
\end{aligned}
$$

For $j < N_x/2$, we have

$$
\begin{aligned}
= \;& 1+\frac{Cr}{2}\Bigg[\sum_{n=0}^{j-1} g_n\left\{\frac{4s+q}{2}\cos(\xi(n-1)h_x)+2(1-2s)\cos(\xi n h_x)+\frac{4s-q}{2}\cos(\xi(n+1)h_x)\right\} \\
&+\sum_{n=j}^{N_x-j-1} g_n\left\{\frac{4s+q}{4}\exp(i\xi(n-1)h_x)+(1-2s)\exp(i\xi n h_x)\right. \\
&\left.+\frac{4s-q}{4}\exp(i\xi(1+n)h_x)\right\} \\
&+g_j\frac{4s+q}{4}\exp(i\xi(1-j)h_x)+g_{N_x-j}\frac{4s+q}{4}\exp(i\xi(N_x-j-1)h_x) \\
&+\left\{\frac{j^{-q}}{\Gamma(1-q)}-\frac{\Gamma(j-q)}{\Gamma(1-q)\Gamma(j)}-g_j\frac{4s+q}{4}\right\}\exp(-i\xi j h_x) \\
&+\left\{\frac{(N_x-j)^{-q}}{\Gamma(1-q)}-\frac{\Gamma(N_x-j-q)}{\Gamma(1-q)\Gamma(N_x-j)}-g_{N_x-j}\frac{4s+q}{4}\right\}\exp(i\xi(N_x-j)h_x)\Bigg].
\end{aligned}
$$

As shown in Section 3.2, E. Sousa makes Von Neumann stability analysis under the assumption $j, N_x \to \infty$[54]. However, the significant feature of all finite difference methods for fractional partial differential equations is that schemes has the different form depending on the value j and N_x. This means that we have to consider the case that the value of j is a finite number, for example, the right side derivative is approximated with one node and the left side derivative is approximated with $N_x - 1$ nodes for $j = 1$. By applying von Neumann stability analysis, we cannot analyze with considering this feature. Therefore, the author analyze the stability by using the matrix method.

Stability analysis in the matrix method to the author's proposed explicit methods

The matrix method is the method to analyze the eigenvalues of the matrix representation of a scheme. Let us analyze the stability of the scheme (5.5) for $1 < q < 2$ by using the matrix method. In the matrix representation, this scheme is expressed as $\vec{U}^{m+1} = (E + A)\vec{U}^m + \vec{f}^m$. If an arbitrary eigenvalue λ of the matrix $(E+A)$ satisfies $|\lambda| \leq -1$, this scheme is stable. To estimate the eigenvalues, we use Gerschgorin's theorem. From Gerschgorin's theorem, the eigenvalues derived from the first row and the last row are 1 as $|\lambda - 1| \leq \sum_{j \neq 0} |a_{0,j}| = 0$. The eigenvalue bound derived from the i-th column satsifies the following expression as

$$|\lambda - (1 + a_{i,i})| \leq \sum_{j \neq i} |a_{j,i}|\,, \ i = 1, 2, \ldots, N_x - 1.$$

Note that we treat not rows but columns different to the first and the last rows. By eliminating the absolute values, we have

$$\begin{aligned} & -\sum_{j \neq i} |a_{j,i}| \leq \lambda - (1 + a_{i,i}) \leq \sum_{j \neq i} |a_{j,i}| \\ \Rightarrow \quad & -\sum_{j \neq i} |a_{j,i}| + (1 + a_{i,i}) \leq \lambda \leq \sum_{j \neq i} |a_{j,i}| + (1 + a_{i,i}) \end{aligned}$$

Therefore, the stability condition is represented with two expressions as

$$\begin{aligned} -\sum_{j \neq i} |a_{j,i}| + (1 + a_{i,i}) \quad &\geq \quad -1, \\ \sum_{j \neq i} |a_{j,i}| + (1 + a_{i,i}) \quad &\leq \quad 1. \end{aligned}$$

Let us assume that the diagonal entries $a_{i,i}$ are negative or equal to 0 as $a_{i,i} \leq 0$ and the non-diagonal entries $a_{j,i}$ for $j \neq i$ are positive or equal to 0 as $a_{j,i} \geq 0$ except some entries $a_{l,i}$ as $a_{l,i} > 0$. Then, we have the following lemma.

Lemma 5.1.1 *All diagonal entries are negative or equal to* 0 *if the parameter* s *satisfies the following expression as*

$$s \geq \frac{2 - q}{4}. \tag{5.12}$$

Proof
The condition that the diagonal entries are negative or equal to 0 is given by

$$\begin{aligned} & a_{i,i} \leq 0 \\ \Rightarrow\quad & \frac{Cr}{2}\left[2g_0(1-2s)+2g_1\frac{4s+q}{4}\right] \leq 0 \\ \Rightarrow\quad & s \geq \frac{2-q}{4}. \end{aligned}$$

□

From this assumption, the stability condition can be represented as

$$-\sum_{j=1}^{N_x-1} a_{j,i} + 2a_{i,i} + 2\sum_{l} a_{l,i} \geq -2, \tag{5.13}$$

and

$$\sum_{j=1}^{N_x-1} a_{j,i} - 2\sum_{l} a_{l,i} \leq 0. \tag{5.14}$$

The summation $\sum_{j=1}^{N_x-1} a_{j,i}$ is given by

$$\begin{aligned} & \sum_{j=1}^{N_x-1} a_{j,i} \\ = \quad & \frac{Cr}{2}\left[\frac{4s+q}{4}\sum_{n=0}^{i} g_n + (1-2s)\sum_{n=0}^{i-1} g_n + \frac{4s-q}{4}\sum_{n=0}^{i-2} g_n \right. \\ & \left. + \frac{4s+q}{4}\sum_{n=0}^{N_x-i} g_n + (1-2s)\sum_{n=0}^{N_x-i-1} g_n + \frac{4s-q}{4}\sum_{n=0}^{N_x-i-2} g_n \right] \\ = \quad & \frac{Cr}{2}\left[-\frac{4s+q}{4q}\frac{\Gamma(i+1-q)}{\Gamma(-q)\Gamma(i+1)} - \frac{(1-2s)}{q}\frac{\Gamma(i-q)}{\Gamma(-q)\Gamma(i)} \right. \\ & -\frac{4s-q}{4q}\frac{\Gamma(i-1-q)}{\Gamma(-q)\Gamma(i-1)} - \frac{4s+q}{4q}\frac{\Gamma(N_x-i+1-q)}{\Gamma(-q)\Gamma(N_x-i+1)} \\ & \left. -\frac{(1-2s)}{q}\frac{\Gamma(N_x-i-q)}{\Gamma(-q)\Gamma(N_x-i)} - \frac{4s-q}{4q}\frac{\Gamma(N_x-i-1-q)}{\Gamma(-q)\Gamma(N_x-i-1)} \right] \end{aligned}$$

where $2 \leq i \leq N_x - 2$ and g_n is $g_n = \Gamma(n-q)/(\Gamma(-q)\Gamma(n+1))$. For $i = 1, N_x - 1$, the summation is given by

$$\begin{aligned} & \sum_{j=1}^{N_x-1} a_{j,i} \\ = \quad & \frac{Cr}{2}\left[\frac{4s+q}{4}g_1 + (1-2s)g_0 \right. \\ & \left. -\frac{4s+q}{4q}\frac{\Gamma(N_x-q)}{\Gamma(-q)\Gamma(N_x)} - \frac{(1-2s)}{q}\frac{\Gamma(N_x-1-q)}{\Gamma(-q)\Gamma(N_x-1)} - \frac{4s-q}{4q}\frac{\Gamma(N_x-2-q)}{\Gamma(-q)\Gamma(N_x-2)}\right]. \end{aligned}$$

If the value of i increases proportional to N_x, for example, $i = N_x/2$, this summation converges to 0 for $N_x \to \infty$. Then, Exp. (5.14) can be written as

$$-2\sum_{l} a_{l,i} \leq 0.$$

Since we assume that the entries $a_{l,i} < 0$, it is shown that there never exists negative non-diagonal entries $a_{l,i}$. Next, let us show the conditions that all non-diagonal entries are positive or equal to 0. Here, we have the following lemma.

Lemma 5.1.2 *All non-diagonal entries are positive or equal to* 0 *if the parameter* s *satisfies the following three expressions as*

$$s \geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \tag{5.15}$$

$$s \leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \tag{5.16}$$

$$s \geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4}. \tag{5.17}$$

Proof
The condition that the entry $a_{i,i+1}$ is positive or equal to 0 is given by

$$\begin{aligned} & a_{i,i+1} \geq 0 \\ \Rightarrow \quad & 2g_0 s + g_1(1-2s) + g_2\frac{4s+q}{4} \geq 0 \\ \Rightarrow \quad & s \geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}. \end{aligned}$$

The condition that the entry $a_{i,i+2}$ is positive or equal to 0 is given by

$$\begin{aligned} & a_{i,i+2} \geq 0 \\ \Rightarrow \quad & g_1\frac{4s-q}{4} + g_2(1-2s) + g_3\frac{4s+q}{4} \geq 0 \\ \Rightarrow \quad & s \leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}. \end{aligned}$$

The condition that the entry $a_{i,i+k}$, $k \geq 3$ is positive or equal to 0 is given by

$$\begin{aligned} & a_{i,i+k} \geq 0 \\ \Rightarrow \quad & g_{k-1}\frac{4s-q}{4} + g_k(1-2s) + g_{k+1}\frac{4s+q}{4} \geq 0 \\ \Rightarrow \quad & s \geq \frac{qg_{k-1} - 4g_k - qg_{k+1}}{4g_{k-1} - 8g_k + 4g_{k+1}}. \end{aligned}$$

Then, we have the expressions (5.15) and (5.16). Next, let $f_k(q)$ be

$$f_k(q) = \frac{qg_{k-1} - 4g_k - qg_{k+1}}{4g_{k-1} - 8g_k + 4g_{k+1}},$$

and we prove $f_k(q) > f_{k+1}(q)$ for $k \geq 3$. The coefficients g_k has relations to next coefficients as $g_{k-1} = kg_k/(k-1-q)$ and $g_{k+1} = (k-q)g_k/(k+1)$. Then, it holds

$$\begin{aligned} & f_k(q) \\ = \quad & \frac{\frac{qk}{k-1-q}g_k - 4g_k - \frac{q(k-q)}{k+1}g_k}{\frac{4k}{k-1-q}g_k - 8g_k + \frac{4(k-q)}{k+1}g_k} \\ = \quad & \frac{-4k^2 + q(6+2q)k + (4-q^2)(1+q)}{(4q+8)(1+q)}. \end{aligned}$$

Then, we have

$$\begin{aligned} & f_k(q) - f_{k+1}(q) \\ = \quad & \frac{8k+4-q(6+2q)}{(4q+8)(1+q)} > 0 \end{aligned}$$

for $1 < q < 2$ and $k \geq 3$. Therefore, we have the third condition (5.17).

□

Under the assumption that all diagonal entries are negative or equal to 0 and non-diagonal entries are positive or equal to 0, we discuss the conditions that the parameter s satisfies the expression (5.14). Then, we have the following lemma

Lemma 5.1.3 *The conditions to hold the stability condition (5.14) are that the parameter s satisfies the following three expressions as*

$$s \geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \tag{5.18}$$

$$s \leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \tag{5.19}$$

$$s \geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4}. \tag{5.20}$$

Proof
In addition, for $i = 1$, $N_x \to \infty$, the stability condition (5.14) is given by

$$\begin{aligned} & \sum_{j=1}^{N_x-1} a_{j,1} \leq 0 \\ \Rightarrow \quad & \frac{Cr}{2}\left[\frac{4s+q}{4}g_1 + (1-2s)g_0\right] \leq 0 \\ \Rightarrow \quad & s \geq -\frac{qg_1 + 4g_0}{4(g_1 - 2g_0)} = \frac{2-q}{4} \end{aligned}$$

For $i = k$, $k = 2$, $N_x \to \infty$, the stability condition (5.14) is given by

$$\begin{aligned} & \sum_{j=1}^{N_x-1} a_{j,k} \leq 0 \\ \Rightarrow \quad & \frac{Cr}{2}\left[-\frac{4s+q}{4q}\frac{\Gamma(3-q)}{\Gamma(-q)\Gamma(3)} - \frac{(1-2s)}{q}\frac{\Gamma(2-q)}{\Gamma(-q)\Gamma(2)} - \frac{4s-q}{4q}\frac{\Gamma(1-q)}{\Gamma(-q)\Gamma(1)}\right] \leq 0 \\ \Rightarrow \quad & s \leq \frac{qh_1 - 4h_2 - qh_3}{4h_1 - 8h_2 + 4h_3} \end{aligned}$$

where h_k is $h_k = \Gamma(k-q)/(\Gamma(-q)\Gamma(k))$. For $i = k$, $k = 3, 4, \ldots$, $N_x \to \infty$, the stability condition (5.14) is given by

$$\begin{aligned} & \sum_{j=1}^{N_x-1} a_{j,k} \leq 0 \\ \Rightarrow \quad & \frac{Cr}{2}\left[-\frac{4s+q}{4q}\frac{\Gamma(k+1-q)}{\Gamma(-q)\Gamma(k+1)} - \frac{(1-2s)}{q}\frac{\Gamma(k-q)}{\Gamma(-q)\Gamma(k)} - \frac{4s-q}{4q}\frac{\Gamma(k-1-q)}{\Gamma(-q)\Gamma(k-1)}\right] \leq 0 \\ \Rightarrow \quad & s \geq \frac{qh_{k-1} - 4h_k - qh_{k+1}}{4h_{k-1} - 8h_k + 4h_{k+1}}. \end{aligned}$$

Here, in a similar discussion in the above proof, it holds that

$$\frac{qh_{k-1} - 4h_k - qh_{k+1}}{4h_{k-1} - 8h_k + 4h_{k+1}} > \frac{qh_k - 4h_{k+1} - qh_{k+2}}{4h_k - 8h_{k+1} + 4h_{k+2}}$$

for $k = 3, 4, \ldots$. By comparing the above expressions to expressions (5.12), (5.15), (5.16) and (5.17), we have the following results as

$$\begin{aligned} s &\geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2} \geq \frac{2-q}{4}, \\ s &\leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3} \leq \frac{qh_1 - 4h_2 - qh_3}{4h_1 - 8h_2 + 4h_3}, \\ s &\geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4} \geq \frac{qh_2 - 4h_3 - qh_4}{4h_2 - 8h_3 + 4h_4} \end{aligned}$$

for $1 < q < 2$. Therefore, we have the above lemma.

□

Next, we consider the condition (5.13). Under the assumption that all non-diagonal entries are positive or equal to 0, we have the following lemma.

Lemma 5.1.4 *The conditions to hold the stability condition (5.13) are that the step size h_t satsfies the following expression as*

$$h_t \leq \frac{4h_x^q}{C((8+4q)s + q^2 - 4)}. \tag{5.21}$$

Proof

$$-\sum_{j=1}^{N_x - 1} a_{j,i} + 2a_{i,i} \geq -2.$$

From the above discussion and the condition (5.14), it holds $\sum_{j=1}^{N_x-1} a_{j,i} \leq 0$ if the parameter s satisfies the conditions in Lemma 5.1.3. Therefore, we have

$$\begin{aligned} &-\sum_{j=1}^{N_x - 1} a_{j,i} + 2a_{i,i} \geq 2a_{i,i} \geq -2 \\ \Rightarrow\ &\frac{Cr}{2}\left[2g_0(1-2s) + 2g_1\frac{4s+q}{4}\right] \geq -1 \end{aligned}$$

The diagonal entries are negative, so the stability condition is given by

$$\begin{aligned} \Rightarrow\ & Cr \leq \frac{4}{(8+4q)s + q^2 - 4} \\ \Rightarrow\ & h_t \leq \frac{4h_x^q}{C((8+4q)s + q^2 - 4)}. \end{aligned}$$

□

From the expression (5.21), we can take larger time step size h_t by taking smaller s for $s > 0$. Let us summarize the lemmas 5.1.1, 5.1.2, 5.1.3 and 5.1.4.

Theorem 5.1.5 *The scheme (5.5) for $1 < q < 2$ is stable if the following inequalities are satisfied.*

$$\begin{aligned} s &\geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \\ s &\leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \\ s &\geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4}, \\ h_t &\leq \frac{4h_x^q}{C((8+4q)s + q^2 - 4)}. \end{aligned}$$

Figure 5.4 shows the range in which the parameter s must exist. As is seen in this figure, the parameter s is always positive. These stability conditions are

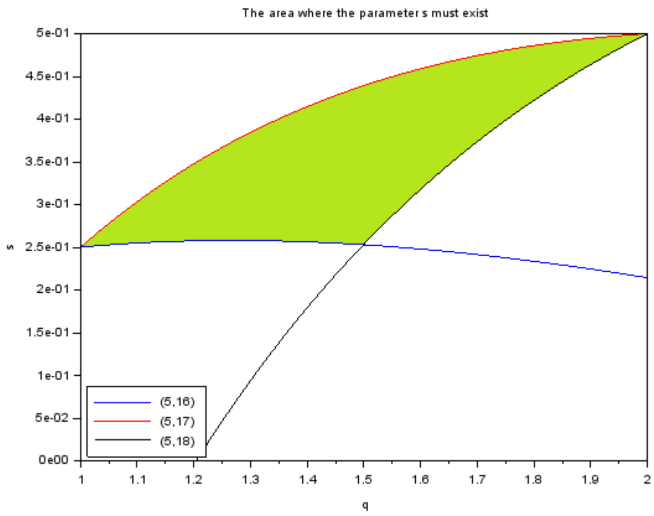


Figure 5.4: The area where the parameter s must exist

sufficient conditions and not necessary and sufficient conditions. This means that the scheme may be stable if we break these inequalities a little. In a similar way, we have the following theorem about stability conditions of the scheme (5.7) for explicit two dimensional fractional partial differential equations.

Theorem 5.1.6 *The scheme (5.7) is stable for $1 < q < 2$, $h = h_x = h_y$ and $N = N_x = N_y$ if the following inequalities hold.*

$$\begin{aligned} s &\geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \\ s &\leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \\ s &\geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4}, \\ h_t &\leq \frac{2h^q}{C((8+4q)s + q^2 - 4)}. \end{aligned}$$

Proof
In the matrix representation, the scheme (5.7) can be expressed as $\vec{U}^{m+1} =$

$(E+A)\vec{U}^m + \vec{f}^m$. Then, for $h = h_x = h_y$ and $r = r_x = r_y$, the diagonal entries $b_{i,i}$ of the matrix B are given by

$$b_{i,i} = \frac{Cr}{2}\left[4g_0(1-2s) + 2g_1\frac{4s+q}{4}\right].$$

In addition, the following summation about a column is given by

$$\sum_{j=1}^{N-1} b_{i,j} = \begin{cases} Cr\left[-\frac{4s+q}{4q}\frac{\Gamma(i+1-q)}{\Gamma(-q)\Gamma(i+1)} - \frac{(1-2s)}{q}\frac{\Gamma(i-q)}{\Gamma(-q)\Gamma(i)} - \frac{4s-q}{4q}\frac{\Gamma(i-1-q)}{\Gamma(-q)\Gamma(i-1)}\right. \\ \left.-\frac{4s+q}{4q}\frac{\Gamma(N-i+1-q)}{\Gamma(-q)\Gamma(N-i+1)} - \frac{(1-2s)}{q}\frac{\Gamma(N-i-q)}{\Gamma(-q)\Gamma(N-i)} - \frac{4s-q}{4q}\frac{\Gamma(N-i-1-q)}{\Gamma(-q)\Gamma(N-i-1)}\right], \\ \quad 2 \le i \le N-2, \\ Cr\left[\frac{4s+q}{4}g_1 + (1-2s)g_0\right. \\ \left.-\frac{4s+q}{4q}\frac{\Gamma(N-q)}{\Gamma(-q)\Gamma(N)} - \frac{(1-2s)}{q}\frac{\Gamma(N-1-q)}{\Gamma(-q)\Gamma(N-1)} - \frac{4s-q}{4q}\frac{\Gamma(N-2-q)}{\Gamma(-q)\Gamma(N-2)}\right], \\ \quad i = 1, N-1. \end{cases}$$

Therefore, with the same discussion, the conditions that the parameter s must satisfy are the same to the conditions in Lemma 5.1.3. Then, the condition (5.13) is given by

$$\begin{aligned} & -\sum_{j=1}^{N_x-1} b_{j,i} + 2b_{i,i} \ge 2b_{i,i} \ge -2 \\ \Rightarrow \quad & \frac{Cr}{2}\left[4g_0(1-2s) + 4g_1\frac{4s+q}{4}\right] \ge -1. \end{aligned}$$

This establishes the above theorem.

□

From the two theorems 5.1.5 and 5.1.6, we have the stability conditions of the author's proposed schemes (5.5) and (5.7). Next, let us compare these stability conditions to those of existing methods. The author's proposed methods have better accuracy than existing methods, but the author's proposed methods are not effective if the stability conditions of the author's proposed methods are more strict than that of existing methods. The author's proposed explicit scheme (5.5) has the following stability condition about h_x and h_t,

$$h_t \le \frac{h_x^q}{C}\frac{4}{((8+4q)s + q^2 - 4)}.$$

In this expression, we have to take a smaller step size of h_t for larger s from $s = (2-q)/4$. This means we can take any step size of h_t if the parameter s is $s = (2-q)/4$. Therefore, we take $s = (qg_1 - 4g_2 - qg_3)/(4g_1 - 8g_2 + 4g_3)$ as its largest possible value during satisfying the stability conditions about s. Next, let us compare it with two kinds of the stability conditions of existing methods proposed by M.M. Meerschaert and C. Tadjeran as

$$h_t \le \frac{h_x^q}{C}\frac{1}{q},$$

and proposed by E. Sousa as

$$h_t \le \frac{h_x^q}{C}2^{1-q}.$$

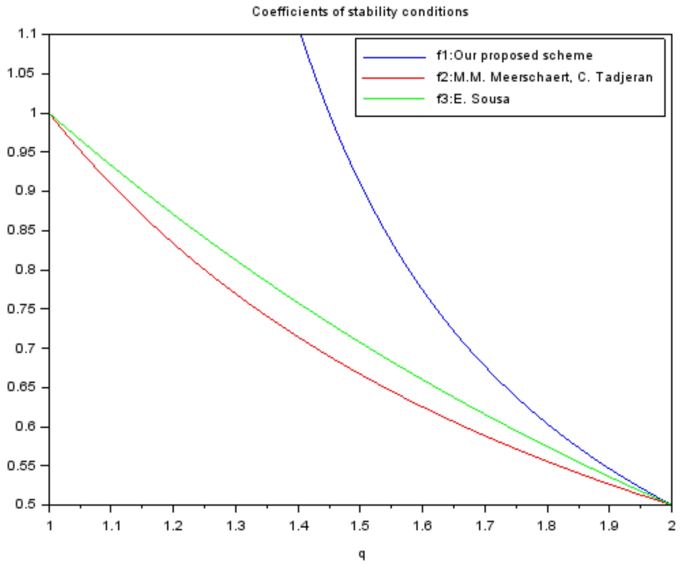


Figure 5.5: Comparison of the stability conditions to the existing methods

Figure 5.5 shows the results of comparing the coefficients of three stability conditions as

$$\begin{aligned} f_1(q) &= \frac{4}{((8+4q)s+q^2-4)}, \\ f_2(q) &= \frac{1}{q}, \\ f_3(q) &= 2^{1-q}, \end{aligned}$$

where

$$s = (qg_1 - 4g_2 - qg_3)/(4g_1 - 8g_2 + 4g_3).$$

From Figure 5.5, we have

$$h_t \leq \frac{h_x^q}{C} \frac{4}{((8+4q)s+q^2-4)} \leq \frac{h_x^q}{C} 2^{1-q} \leq \frac{h_x^q}{C} \frac{1}{q}$$

for $1 < q < 2$. The author's proposed method can take much larger step size of h_t than existing methods for $1 < q < 2$. In addition, we have the following theorem about the stability condition.

Theorem 5.1.7 *There exists a parameter s for arbitrary q with $1 < q < 2$, and the author's proposed explicit scheme (5.5) and (5.7) can take the largest step size of h_t for*

$$s = \max_q \left\{ \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4} \right\}.$$

Stability analysis by the matrix method to the author's proposed implicit methods

Next to the explicit methods as discussed above, let us analyze the stability of our proposed implicit methods. The way of stability analysis for implicit methods is similar to that for explicit methods. The matrix representation of our proposed implicit method (5.6) is given by $(E-A)\vec{U}^m = \vec{U}^{m-1} + \vec{f}^m$. In a similar way to explicit methods, the scheme is stable if each eigenvalue λ of the matrix $(E-A)$ satisfies $|\lambda| \geq 1$ where the eigenvalue of the matrix $(E-A)^{-1}$ is represented as $1/\lambda$. By Gerschgorin's theorem, the scheme is stable if one of the following two inequality holds.

$$-a_{i,i} + \sum_{j \neq i} |a_{j,i}| \leq -2, \tag{5.22}$$

or

$$-a_{i,i} - \sum_{j \neq i} |a_{j,i}| \geq 0. \tag{5.23}$$

If we assume that all diagonal entries are negative or equal to 0, then the stability condition (5.22) never holds. As mentioned in Lemma 5.1.1, the condition that the all diagonal entries are negative or equal to 0 is

$$s \geq \frac{2-q}{4}.$$

In addition, we assume that non-diagonal entries are positive or equal to 0 as $a_{j,i}$, $j \neq i$ except some entries $a_{l,i}$ as $a_{l,i} < 0$. Then, we have

$$-\sum_{j=1}^{N_x-1} a_{j,i} + 2\sum_{l} a_{l,i} \geq 0.$$

The summation in the above expression converges to 0 for $N_x \to \infty$ if the value of j increases proportional to the value of N_x. Then, we have

$$+2\sum_{l} a_{l,i} \geq 0.$$

Since we assume $a_{l,i} < 0$, it is shown that there never exists negative non-diagonal entries, and all non-diagonal must be positive or equal to 0. The conditions for positive non-diagonal entries are represented in Lemma (5.1.2). Thus, we have the following theorem.

Theorem 5.1.8 *The scheme (5.6) is stable for $1 < q < 2$ if all the following inequalities hold.*

$$\begin{aligned}
s &\geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \\
s &\leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \\
s &\geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4}.
\end{aligned}$$

In contrast to the explicit method, the implicit method does not have the stability condition about h_x and h_t. This indicates we can take arbitrary step sizes of h_x and h_t by using the implicit methods. In a similar way, the stability conditions about the scheme (5.8) are also shown in the next theorem.

Theorem 5.1.9 *The scheme (5.8) is stable for* $1 < q < 2$ *if all the following inequalities hold.*

$$\begin{aligned} s &\geq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \\ s &\leq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \\ s &\geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4}. \end{aligned}$$

By the above stability analysis, it is shown that the stability conditions for the author's proposed explicit methods are less restrictive in choosing h_x than that for existing methods as long as we take the appropriate parameter s. In addition, the author's proposed implicit methods do not impose any conditions on step sizes h_x and h_t like existing methods as long as we take the appropriate parameter s. Therefore, it is indicated that we can improve not only the accuracy but also the stability conditions by using the author's proposed methods.

5.1.3 Stability analysis to the author's proposed schemes for $0 < q < 1$

In the above discussion, we assume that the fractional calculus order q is $1 < q < 2$. The way to analyze the stability for $0 < q < 1$ is almost the same to that for $1 < q < 2$, and we apply the matrix method. Let us analyze the stability of the scheme (5.5) for $0 < q < 1$. In a similar way to the case of $1 < q < 2$, the stability conditions are represented as

$$-\sum_{j \neq i} |a_{j,i}| + (1 + a_{i,i}) \geq -1,$$

and

$$\sum_{j \neq i} |a_{j,i}| + (1 + a_{i,i}) \leq 1.$$

Here, we assume that all diagonal entries are negative or equal to 0 and all non-diagonal entries are positive or equal to 0 in the same way to $1 < q < 2$. Then, we have the following lemma about this assumption.

Lemma 5.1.10 *All diagonal entries are negative or equal to* 0 *and all non-diagonal entries are positive or equal to* 0 *if the following inequalities hold.*

$$\begin{aligned} s &\leq \frac{2-q}{4} \\ s &\leq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2} \\ s &\geq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3} \end{aligned}$$

Proof
The condition that any diagonal entry $a_{i,i}$ for $i = 1, 2, \dots, N_x - 1$ is negative or equal to 0 for $0 < q < 1$ is given by

$$\begin{aligned} & a_{i,i} \leq 0, \ \ i = 1, 2, \dots, N_x - 1 \\ \Rightarrow \ \ & s \leq \frac{2-q}{4}. \end{aligned}$$

The conditions that any non-diagonal entries $a_{j,i}$ for $i = 1, 2, \ldots, N_x - 1,\ j \neq i$ are positive or equal to 0 for $0 < q < 1$ are given by

$$\begin{aligned} & a_{i+1,i} \geq 0 \\ \Rightarrow \quad & s \leq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2} \end{aligned}$$

and

$$\begin{aligned} & a_{i+k,i} \geq 0 \\ \Rightarrow \quad & s \geq \frac{qg_{k-1} - 4g_k - qg_{k+1}}{4g_{k-1} - 8g_k + 4g_{k+1}},\ k \geq 2, \end{aligned}$$

from the symmetry property as $a_{i+k,i} = a_{i-k,i}$. Note that we have the following relation in the above expression

$$s \geq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3} \geq \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4} \geq \ldots$$

Therefore, we have the above lemma.

$\square$

From the above assumption, the stability conditions can be represented with two expressions as

$$2a_{i,i} - \sum_{j=1}^{N_x-1} a_{j,i} \quad \geq \quad -2, \tag{5.24}$$

and

$$\sum_{j=1}^{N_x-1} a_{j,i} \quad \leq \quad 0. \tag{5.25}$$

Firstly, we discuss the conditions that the entries $a_{i,j}$ satisfy the inequality (5.25) with the following lemma.

Lemma 5.1.11 *The parameter s must satisfy the following conditions so that the stability condition (5.25) holds for $0 < q < 1$.*

$$s \leq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \tag{5.26}$$

$$s \geq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}. \tag{5.27}$$

Proof
The conditions that the summation $\sum_{j=1}^{N_x-1} a_{j,i}$ is negative or equal to 0 are given by

$$\begin{aligned} & \sum_{j=1}^{N_x-1} a_{j,1} \leq 0 \\ \Rightarrow \quad & s \leq \frac{2-q}{4} \end{aligned}$$

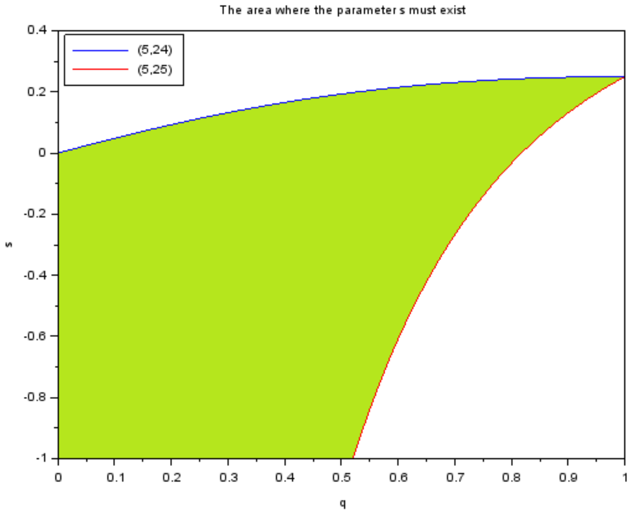


Figure 5.6: The area where the parameter s must exist

and

$$\sum_{j=1}^{N_x-1} a_{j,k} \leq 0$$
$$\Rightarrow \quad s \geq \frac{qh_{k-1} - 4h_k - qh_{k+1}}{4h_{k-1} - 8h_k + 4h_{k+1}}, \quad k \geq 2$$

for $0 < q < 1$. Note that it holds the following relation in the above expressions

$$s \geq \frac{qh_1 - 4h_2 - qh_3}{4h_1 - 8h_2 + 4h_3} \geq \frac{qh_2 - 4h_3 - qh_4}{4h_2 - 8h_3 + 4h_4} \geq \dots$$

By summarizing the conditions, we have the above lemma.

□

Figure 5.6 shows the range of parameter s, depending on the value q, given by Lemma 5.1.11. In contrast to the case for $1 < q < 2$, the parameter s can take a negative number. Next, we discuss the condition that the step size h_t satisfy the inequality (5.24) in the following lemma.

Lemma 5.1.12 *The parameter h_t must satisfy the following conditions so that the stability condition (5.24) holds for $0 < q < 1$.*

$$h_t \leq \frac{h_x^q}{C} \frac{4}{(8+4q)s + q^2 - 4}. \tag{5.28}$$

Proof
Under the assumption that the summation $\sum_{j=1}^{N_x-1} a_{j,i}$ is negative or equal to 0, the stability condition (5.24) is represented as

$$2a_{i,i} - \sum_{j=1}^{N_x-1} a_{j,i} \geq 2a_{i,i} \geq -2$$
$$\Rightarrow \quad h_t \leq \frac{h_x^q}{C} \frac{4}{(8+4q)s + q^2 - 4}.$$

Therefore, we have the above lemma.

$\square$

By summarizing Lemmas 5.1.10, 5.1.11 and 5.1.12, we have the following theorem about the stability of the scheme (5.5) for $0 < q < 1$.

Theorem 5.1.13 *The scheme (5.5) is stable for* $0 < q < 1$ *if the followings are satisfied.*

$$\begin{aligned} s &\leq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \\ s &\geq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \\ h_t &\leq \frac{h_x^q}{C} \frac{4}{(8+4q)s + q^2 - 4}. \end{aligned}$$

In this theorem, we can take larger step size of h_t when the denominator of right hand side is smaller. In the range that the parameter s can take, the denominator become the smallest for $s = (-4g_1 - qg_2)/(8g_0 - 8g_1 + 4g_2)$. Therefore, we should put the parameter s as

$$s = \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}$$

when we use the scheme (5.5). In a similar way, we obtain the stability conditions of the scheme (5.7).

Theorem 5.1.14 *The scheme (5.7) is stable for* $0 < q < 1$, $h = h_x = h_y$ *and* $N = N_x = N_y$ *if the followings are satisfied.*

$$\begin{aligned} s &\leq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \\ s &\geq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}, \\ h_t &\leq \frac{h^q}{C} \frac{2}{(8+4q)s + q^2 - 4}. \end{aligned}$$

Also for the implicit methods, we have the following results as theorem.

Theorem 5.1.15 *The scheme (5.6) and the scheme (5.8) are stable for* $0 < q < 1$ *if the followings are satisfied.*

$$\begin{aligned} s &\leq \frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \\ s &\geq \frac{qg_1 - 4g_2 - qg_3}{4g_1 - 8g_2 + 4g_3}. \end{aligned}$$

5.1.4 Accuracy order and accuracy decaying

The author introduces that all the author's proposed schemes are second order accuracy for space as $O(h_t) + O(h_x^2)$. In addition, the existing methods are also introduced as first order accuracy method with $O(h_t) + O(h_x)$. In some aspects, the accuracy order of the author's proposed schemes and existing schemes are not $O(h_t) + O(h_x^2)$ and $O(h_t) + O(h_x^2)$, and decays for two reasons. One reason is the smoothness of the function. In Chapter 4, the author shows that the accuracy of finite difference formulae depends on the form of the differentiated functions. For the function $f(x) = x^p$, $0 < p < 1$, the accuracy order of the formula (4.2) decays from second order accuracy to $O(1/N^{1+p})$. The reason of this accuracy decaying is the differentiated function is not differentiable at $x = 0$. The similar phenomenon happens for finite difference methods for fractional partial differential equations. For the function $u(x,t) = \exp(-t)(x-L)^p(R-x)^p$ with $0 < p < 1$, the accuracy of the author's proposed schemes and existing schemes decays from second and first order accuracy to $O(h^p)$. In the numerical computation of fractional derivative, the accuracy order decreases to $O(1/N^{1+p})$ for $f(x) = x^p$. On the other hand, the accuracy order decreases not to $O(h^{1+p})$ but $O(h^p)$ in finite difference methods. The reason of this difference is the number of sampling points when we can calculate fractional derivative. Let us consider to calculate the fractional derivative to the function $f(x) = x^{p+q}$ with $0 < p < 1$ where q is the fractional calculus order $q > 0$. By using the formula (4.9), we have the following result

$$
{}_{0}^{\mathrm{R}}D_x^q f(x) - {}_{0}^{\mathrm{R1}}D_x^q f(x) = O(h^p)
$$

for $x = jh$, $N = j$ and $h \to 0$ where j does not depend on h. This expression indicates x comes near to $x = 0$ for $h \to 0$. For the case of $j = 1$, the above expression is developed as

$$
\begin{aligned}
& {}_{0}^{\mathrm{R}}D_x^q f(h) - {}_{0}^{\mathrm{R1}}D_x^q f(h) \\
= \ & \frac{\Gamma(p+q+1)}{\Gamma(p+1)} h^p - h^{-q} \frac{\Gamma(-q)}{\Gamma(-q)\Gamma(1)} h^{p+q} \\
= \ & \left(\frac{\Gamma(p+q+1)}{\Gamma(p+1)} - 1 \right) h^p.
\end{aligned}
$$

For $h \to 0$, the variable $x = h$ comes near to $x = 0$. This phenomenon means that the numerical solution around an initial point has bad accuracy. Yet, the assumption of $x = jh$ may seem to be strange, but this computation is done in finite different methods for fractional partial differential equations. Actually, in the scheme (3.2), a similar situation occurs for $i = 1$. Right side derivative has to be calculated with $i + 2$ points which does not depend on h. This is the second reason, and the accuracy of the scheme (3.2) and (3.1) decreases from the expected accuracy because of these two reasons. If we use high accuracy formulae, the accuracy does not improve. The formula (4.10) is the second order accuracy, but we have the same result

$$
{}_{0}^{\mathrm{R}}D_x^q f(x) - {}_{0}^{\mathrm{R2}}D_x^q f(x) = O(h^p) \tag{5.29}
$$

for the function $f(x) = x^{p+q}$, $x = jh$, $N = j$ and $h \to 0$ where j does not depend on h. This situation can be seen, for example, in the scheme (5.5). Therefore, we cannot improve the accuracy if we apply high accuracy formulae to finite difference methods.

In integer order calculus, this phenomenon is seen. For the second derivative of $f(x) = x^{p+2}$, the error of analytical differential and numerical differential at $x = jh$ for $j \geq 2$ and the value of j does not depend on h is given by

$$
\begin{aligned}
& f''(jh) - \frac{f((j+1)h) - 2f(jh) + f((j-1)h)}{h^2} \\
= \ & (p+2)(p+1)(jh)^p - \frac{((j+1)h)^{p+2} - 2(jh)^{p+2} + ((j-1)h)^{p+2}}{h^2} \\
= \ & (p+2)(p+1)(jh)^p - \left\{ (j+1)^{p+2} - 2j^{p+2} + (j-1)^{p+2} \right\} h^p \\
= \ & -\frac{2(p+2)(p+1)p(p-1)}{4!} j^{p-2} h^p - \cdots \\
= \ & O(h^p), \ 0 < p < 1
\end{aligned} \tag{5.30}
$$

Thus, this accuracy decaying is the problem not only among fractional calculus but also among integer order calculus.

In the previous paragraph, the author shows two reasons that cause the accuracy decaying in finite difference methods. However, note that there is a difference between the above examples and schemes for differential equations. For the function $f(x) = x^{p+q}$, the accuracy of every difference formulae decreases to $O(h^p)$. On the other hand, the accuracy of every finite difference methods decreases $O(h^p)$ for the analytical solution $u(x,t) = \exp(-t)(x-L)^p(R-x)^p$. If the analytical solution converges at boundaries, the error of finite difference methods also converges. This difference can be explained as follows. For a function $f(x) = x^{p+q}$, fractional derivative of its function is given by ${}_0^{\mathrm{R}}D_x^q f(x) = x^p\Gamma(p+q+1)/\Gamma(p+1)$. This derivative has the order $O(x^p)$ around an initial point. Therefore, the accuracy decays to $O(h^p)$. In a similar way, both side fractional derivative to the function $u(x,t) = \exp(-t)(x-L)^p(R-x)^p$ is given by

$$\begin{aligned} & {}_L^{\mathrm{R}}D_x^q u(x,t) + {}_x^{\mathrm{R}}D_R^q u(x,t) \\ = \;& \frac{C}{2}\frac{\partial}{\partial t}u(x,t) \\ = \;& -\frac{C}{2}\exp(-t)(x-L)^p(R-x)^p. \end{aligned}$$

This expression has the order $O(x^p)$ around boundaries. Therefore, the accuracy decays to $O(h^p)$ around boundaries.

By the way, what happens if $p = 0$? It seems that the accuracy order is a constant $O(1)$. Actually, the accuracy order of existing methods is $O(1)$ for $p = 0$, and the solutions do not converge even if we take small step sizes. Yet, the author's proposed methods have the feature of error cancelling, and the solutions are not influenced if the analytical solution is not zero at boundaries. This improvement is significant to apply to actual problems.

As mentioned above, this accuracy decaying also happens in integer order finite difference methods. However, this problem is not common in integer order calculus because of two reasons. The first reason is the accuracy decaying does not happen if the function is polynomial function. In the expressions (5.30), the error is zero for $p = -2, -1, 0, 1$, and is $O(h^2)$ for a positive integer $p \geq 2$. However, the accuracy of the author's proposed formula (4.10) decays to first order accuracy even if the differentiated function is defined as $f(x) = x^{p+q}$ for $p = 1$ in under the conditions of the expression (5.29). In finite difference schemes, for the analytical function $u(x,t) = \exp(-t)(x-L)(R-x)$, the accuracy of the author's proposed second order accuracy schemes decays to first order accuracy $O(h_t) + O(h_x)$. In integer order calculus, the accuracy of numerical methods does not decay if the function is represented with polynomials. Therefore, we do not care about the error of the numerical derivative in the case of $x = jh$ and the value of j does not depend on h. Second reason is non-smooth function like $u(x) = \exp(-t)(x-L)^p(R-x)^p$, $0 < p < 1$ does not appear if we assume smooth function as the initial condition. In fractional calculus, fractional differentiation and integration give a singularity to the function. This means that the analytical solution of fractional partial differential equations may be a non-smooth function for the initial condition of a smooth function. In contrast to integer order calculus, we have to consider this accuracy decaying from these two reason when we use fractional calculus.

5.1.5 Experiments about space-fractional partial differential equations

Measurement of errors

When we measure the errors of finite difference methods, there is one mistake which we tend to make. The errors of finite difference methods are usually constructed from two components. One is the error derived from time derivative, and the other is the error derived from space derivative. The accuracy order of existing scheme (3.2) is first order accuracy to both derivatives as $O(h_t)+O(h_x)$. However, the result which the error decreases with first order accuracy does not mean the accuracy order of this scheme is first order accuracy. Because, if one error have the big coefficients comparing to the other error, the other error is hidden. For example, let the error about time derivative be $E_t = 1000h_t$, and let the error about space derivative be $E_x = h_x^{0.5}$. This case assumes that the accuracy decaying happens at space derivative. Then the accuracy order is namely $O(h_t)+O(h_x^{0.5})$, but we are likely to misunderstand the accuracy order as $O(h_t)+O(h_x)$. Because, the error is $1000*0.01+0.01^{0.5} = 10.1$ for $h_t = h_x = 0.01$ and the error is $1000*0.001+0.001^{0.5} \simeq 1.032$ for $h_t = h_x = 0.001$. By decreasing of the values of h_t and h_x with $0.01 \to 0.001$, the error also decrease $10.1 \to 1.032$. This error looks the first order accuracy because of the big coefficients for time derivative. This phenomenon also occurs when we use the author's proposed high accuracy schemes. The method to avoid this problem is to make step size h_t and h_x sufficiently small individually. This is effective to avoid the misunderstanding, but to make step size small amounts to increase the problem size. Another method to avoid the misunderstanding is to make the diffusion coefficient C large. By making the diffusion constant C large, the error of space derivative also becomes large and the error of time derivative becomes relatively small. In the experiments, the large diffusion coefficients appears for making clear the accuracy order.

Stability

The stability is the problem in the form of schemes, and does not depend on the analytical solution of equations. Therefore, we check the eigenvalues of the matrix in the matrix representation. Firstly, we experiment about stability condition of existing explicit scheme proposed by E. Sousa[54], M.M. Meerschaert and C. Tadjeran[40] as

$$\begin{aligned} h_t &\leq \frac{h_x^q}{C}2^{1-q} \\ h_t &\leq \frac{h_x^q}{C}\frac{1}{q}. \end{aligned}$$

Let h_x be $h_x = 1/40$, and let C be $C = 1$, and we experiment with various h_t and q. Figure 5.7 shows whether the existing explicit scheme is stable or not for each q and h_t. The sign 'o' denotes the scheme is stable at that point, and the sign 'x' denotes the scheme is not stable. The stability is confirmed by checking eigenvalues. The eigenvalues are numerically calculated by using Mathematica. The distinct result is at $q = 1.2$, $h_t = 0.01$. This point is stable with the stability condition proposed by E. Sousa, but not stable with the stability condition proposed by M.M. Meerschaert and C. Tadjeran. This result shows that the stability condition derived from Gerschgorin's theorem is not strict, and scheme may be stable if the stability condition is not satisfied.

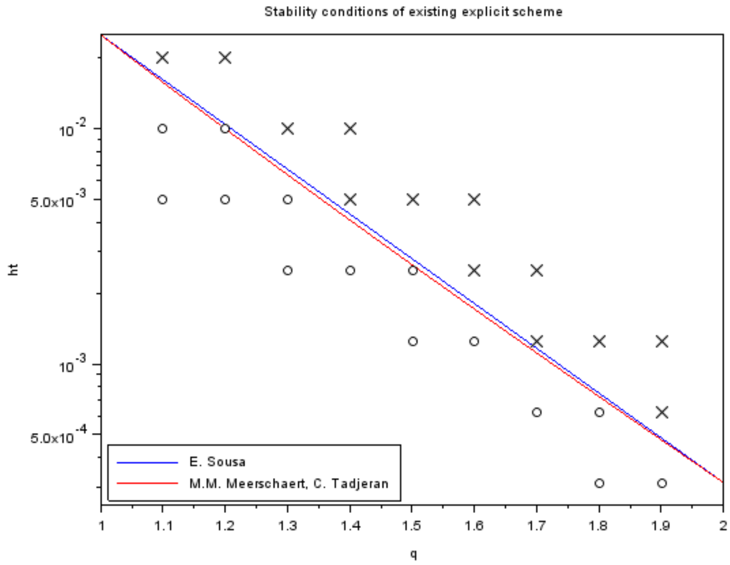


Figure 5.7: Stability conditions of existing explicit scheme

Next, let us verify the stability condition of the author's proposed implicit methods. Figure 5.8 shows whether the proposed implicit scheme (5.6) is stable or not for each q and s with $h_t = h_x = 0.025$. The sign 'o' denotes the scheme is stable at that point, and the sign 'x' denotes the scheme is not stable. Since the stability conditions are analyzed by using Gerschgorin's theorem, the author's proposed stability conditions are not strict. Table 5.1 shows the absolute maximum eigenvalues except eigenvalues derived from first and last row, which are always 1. From this table, it is expected that the stability condition is strict for small q, since the maximum eigenvalues are close to 1.

	q=1.1	q=1.2	q=1.3	q=1.4	q=1.5	q=1.6	q=1.7	q=1.8	q=1.9
s=0.5	0.9896	0.9771	0.9623	0.9452	0.9257	0.9039	0.8802	0.8550	0.8287
s=0.45	0.9896	0.9771	0.9624	0.9453	0.9257	0.9040	0.8803	0.8550	0.8287
s=0.4	0.9896	0.9772	0.9625	0.9454	0.9258	0.9041	0.8804	0.8551	0.8288
s=0.35	0.9897	0.9773	0.9626	0.9455	0.9260	0.9043	0.8805	0.8553	0.8289
s=0.3	0.9898	0.9774	0.9627	0.9457	0.9262	0.9045	0.8808	0.8556	0.8293
s=0.25	0.9990	0.9969	0.9925	0.9840	0.9683	0.9408	0.8957	0.8577	0.8310

Table 5.1: The maximum eigenvalues for scheme (5.6) with $1 < q < 2$

Figure 5.9 represents the stability of the scheme (5.6) for various q and s with $0 < q < 1$. In contrast to the case of $1 < q < 2$, the scheme is not at $s = 0.3$. However, for negative s, the stability condition is not strict. Table 5.2 shows the absolute maximum eigenvalues for $0 < q < 1$.

Lastly, we make experiments about the stability condition of the author's proposed explicit methods. The stability condition about h_t and h_x is represented as

$$h_t \leq \frac{h_x^q}{C} \frac{4}{((8+4q)s + q^2 - 4)}.$$

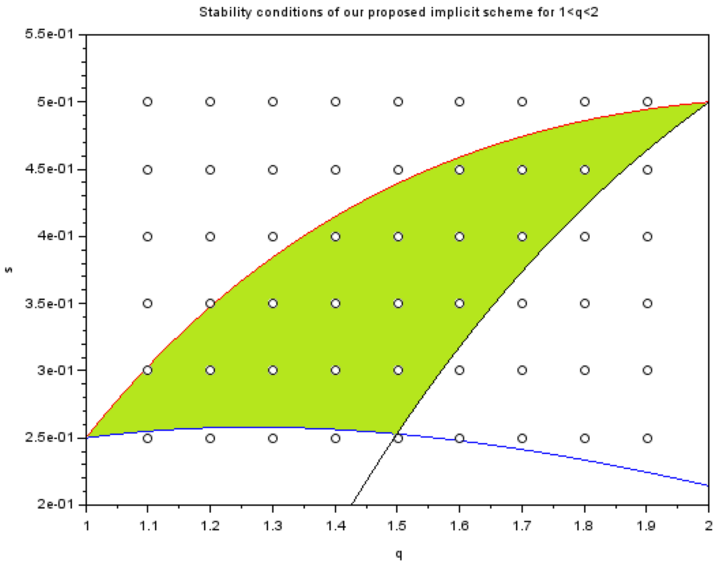


Figure 5.8: Stability conditions of the implicit scheme (5.6) for $1 < q < 2$

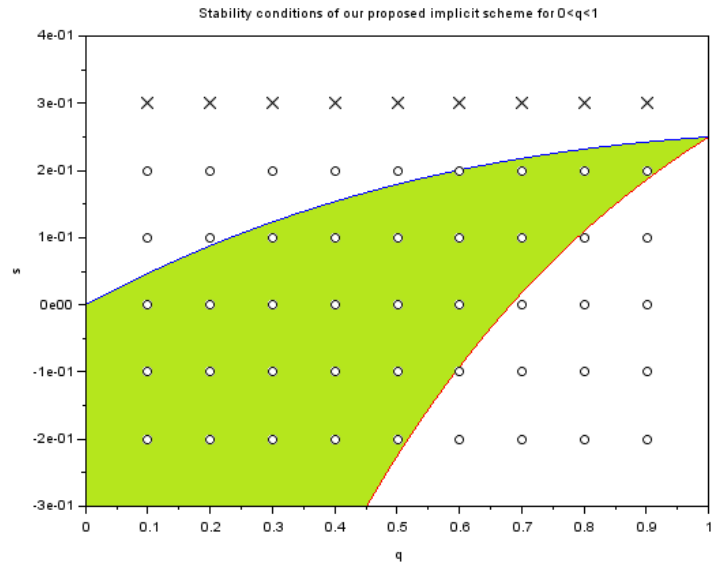


Figure 5.9: Stability conditions of the implicit scheme (5.6) for $0 < q < 1$

	q=0.1	q=0.2	q=0.3	q=0.4	q=0.5	q=0.6	q=0.7	q=0.8	q=0.9
s=0.3	1.0077	1.0121	1.0188	1.0295	1.0464	1.0739	1.1195	1.1985	1.3459
s=0.2	0.9923	0.9881	0.9816	0.9751	0.9763	0.9784	0.9815	0.9859	0.9919
s=0.1	0.9773	0.9745	0.9745	0.9750	0.9762	0.9782	0.9813	0.9857	0.9918
s=0	0.9749	0.9744	0.9744	0.9749	0.9761	0.9781	0.9812	0.9856	0.9917
s=-0.1	0.9748	0.9744	0.9743	0.9748	0.9760	0.9780	0.9811	0.9856	0.9917
s=-0.2	0.9748	0.9743	0.9743	0.9747	0.9759	0.9779	0.9810	0.9855	0.9916

Table 5.2: The maximum eigenvalues for scheme (5.6) with $0 < q < 1$

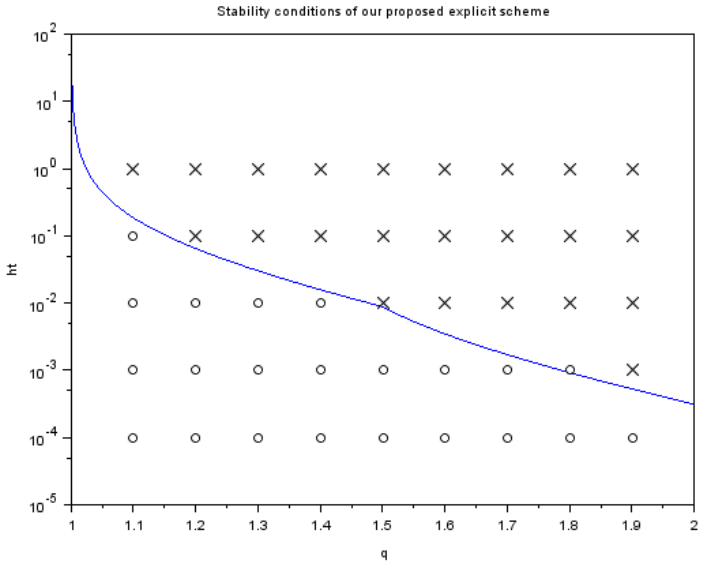


Figure 5.10: Stability conditions of the explicit scheme (5.5) for $1 < q < 2$

To maximize the step size of h_t, we take the parameter s for $1 < q < 2$ as

$$s = \max\left\{\frac{-4g_1 - qg_2}{8g_0 - 8g_1 + 4g_2}, \frac{qg_2 - 4g_3 - qg_4}{4g_2 - 8g_3 + 4g_4}\right\}.$$

Then, Figure 5.10 shows the stability conditions for each q and h_t with $1 < q < 2$, $C = 1$ and $h_x = 1/40$. This result indicates that the author's stability analysis express sufficient stability conditions, and if it is shown that the scheme is stable for $q = 1.8$ and $h_t = 0.001$, where the analyzed stability condition is not hold, but the scheme is actually stable.

Figure 5.11 shows the stability conditions for each q and h_t with $0 < q < 1$, $C = -1$ and $h_x = 1/40$. The stability condition of $0 < q < 1$ is less strict than that of $1 < q < 2$. Comparing to the case of $1 < q < 2$, the scheme is stable with wide step size of h_t.

Figure 5.12 shows the stability conditions of three methods, the author's proposed condition, the condition proposed by E. Sousa and the condition proposed by M.M. Meerschaert and C. Tadjeran for each q and h_t with $1 < q < 2$, $C = 1$ and $h_x = 1/40$. This graph represents that the stability condition of the author's proposed explicit scheme allows a larger step size h_t than that of existing scheme. This means that the author's proposed explicit scheme has a weak condition about step sizes comparing to other existing explicit method.

Accuracy

Next, we make experiments about the accuracy of the author's proposed schemes and existing methods. As existing methods, we compare not only finite difference method proposed by M.M. Meerschaert and C. Tadjeran[40], but also the matrix transform method proposed by M. Ilic, F. Liu, I. Turner and V. Anh[21]. The detail of the matrix transform method is explained in Chapter 3. All experiments are done with Mathematica. Firstly, we experiment for one dimensional fractional partial differential equations 5.1 with zero-Dirichlet boundary conditions. Let the

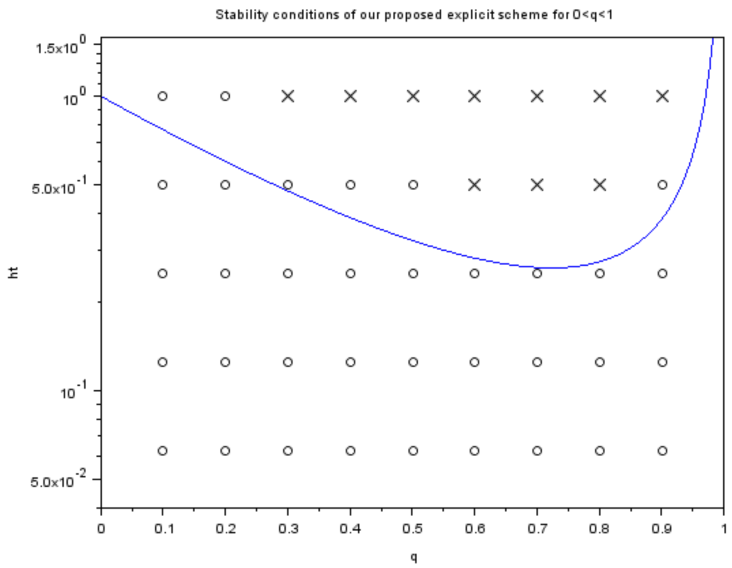


Figure 5.11: Stability conditions of the explicit scheme (5.5) for $0 < q < 1$

analytical solution $u(x,t)$ be

$$u(x,t) = 4\exp(-t)x^p(1-x)^p$$

where p is a constant to control the order of functions around boundaries. This means the order of the analytical solution is $O(x^p)$ for $x \to L$ and $x \to R$. Figure (5.13) is the graph of the analytical solution function for $p = 0.5$. Then, let the

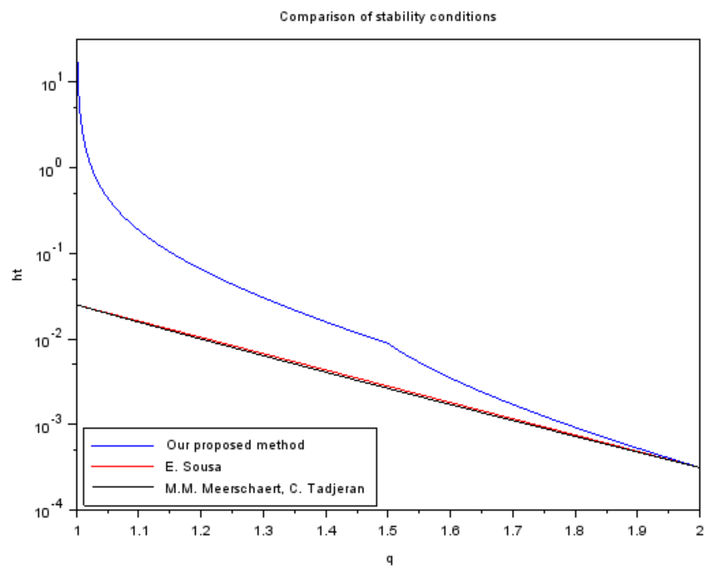


Figure 5.12: Comparison of stability conditions for $1 < q < 2$

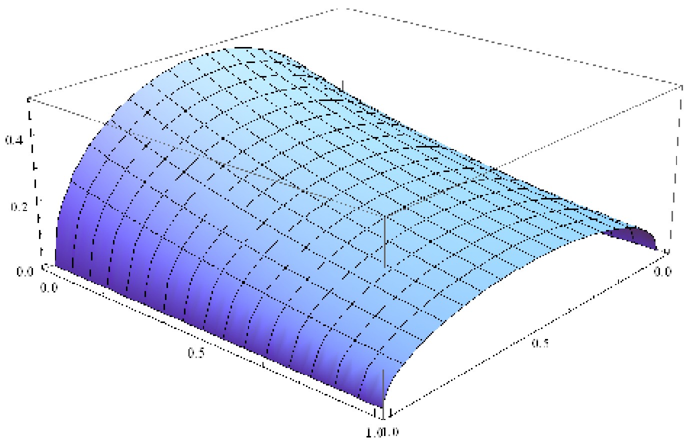


Figure 5.13: The analytical solution function for $p = 0.5$

force term $f(x,t)$ be

$$
\begin{aligned}
& f(x,t) \\
= \; & -\exp(-t)\left\{4x^p(1-x)^p\right. \\
& +2Cx^{p-q}\frac{\Gamma(p+1)}{\Gamma(p-q+1)}\,{}_2F_1\left[\begin{matrix}-p, p+1\\ p-q+1\end{matrix};x\right] \\
& \left.+2C(1-x)^{p-q}\frac{\Gamma(p+1)}{\Gamma(p-q+1)}\,{}_2F_1\left[\begin{matrix}-p, p+1\\ p-q+1\end{matrix};1-x\right]\right\}
\end{aligned}
$$

where the function ${}_2F_1$ is the hypergeometric series. The initial condition is given by $u(x,0) = x^p(1-x)^p$, and the boundary conditions are given by $u(0,t) = u(1,t) = 0$ as zero-Dirichlet boundary conditions. All experiments are done for $0 \le t \le 1$.

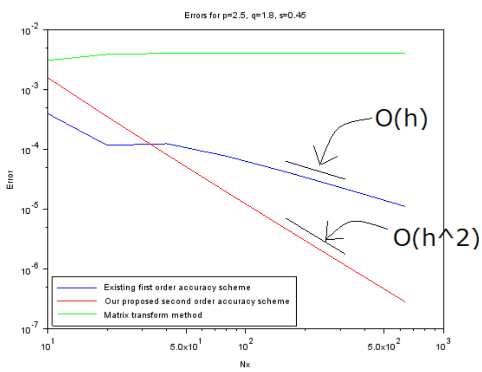


Figure 5.14: Errors of three numerical methods for $q = 1.8$, $p = 2.5$, $s = 0.4$

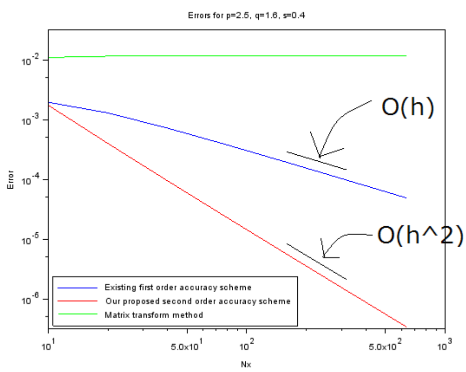


Figure 5.15: Errors of three numerical methods for $q = 1.6$, $p = 2.5$, $s = 0.4$

Figures 5.14, 5.15, 5.16 and 5.17 show the errors about three methods, existing implicit finite difference method (3.1) proposed by M.M. Meerschaert and C. Tadjeran in blue lines, the author's proposed implicit finite difference method in red lines and the matrix transform method proposed by M. Ilic, F. Liu, I. Turner and V. Anh in green lines for $q = 1.8, 1.6, 14, 1.2$ respectively. The conditions of three experiments Figures 5.14, 5.15, 5.16 and 5.17 are $p = 2.5$, $N_t = 1000$,

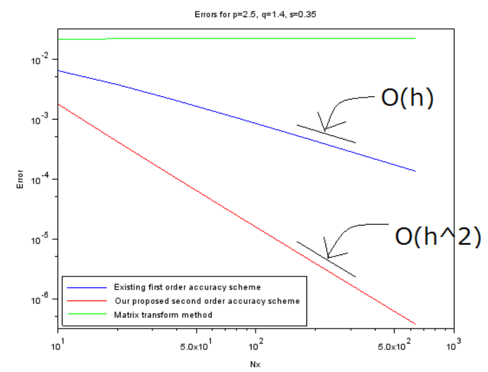


Figure 5.16: Errors of three numerical methods for $q = 1.4$, $p = 2.5$, $s = 0.35$

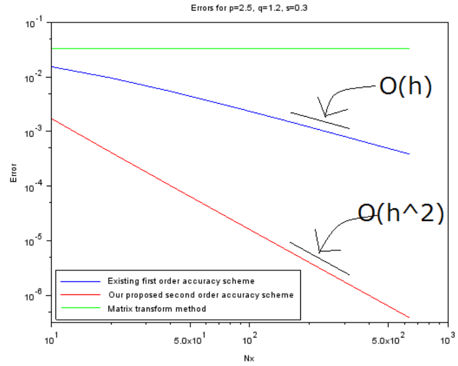


Figure 5.17: Errors of three numerical methods for $q = 1.2$, $p = 2.5$, $s = 0.3$

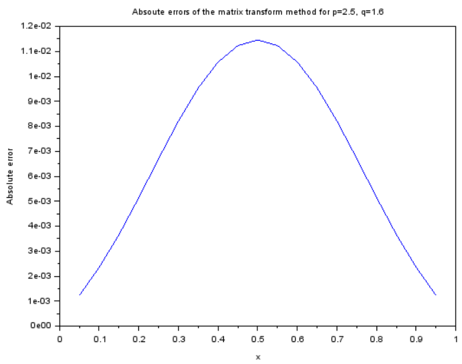


Figure 5.18: Absolute errors of the matrix transform method for $q = 1.6$, $p = 2.5$, $t = 1$

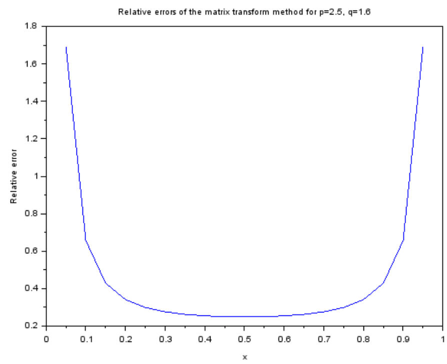


Figure 5.19: Relative errors of the matrix transform method for $q = 1.6$, $p = 2.5$, $t = 1$

$C = 100000$ and $s = 0.45, 0.4, 0.35, 0.3$. Figures 5.18 and 5.19 show the errors of the results of the matrix transform method at $t = 1$ for $q = 1.6$ and $N_x = 20$. It is shown that the results of existing method are actually first order accuracy and the results of the author's proposed method are second order accuracy in any fractional calculus order q. In addition, these results indicate the numerical solutions by the matrix transform method do not converge to the analytical solution. The matrix transform method is the method to approximate fractional derivative with a power of the matrix. From these results, it is shown that the author was not able to implement the matrix transform method so to obtain appropriate solutions. Therefore, from next experiments, we show the results by only existing finite difference methods proposed by M.M. Meerschaert and the author's proposed finite difference methods.

Figures 5.20, 5.21 5.22 and 5.23 are the results for respectively $q = 1.8, 1.6, 1.4, 1.2$ and $s = 0.45, 0.4, 0.35, 0.3$ with $p = 1.5$, $C = 100000$, $N_t = 1000$. These graphs indicate that existing first order accuracy methods numerically calculate actually with first order accuracy. On the other hand, the author's proposed second order accuracy scheme cannot calculate with second order accuracy. This is because the accuracy decaying happens. By the accuracy decaying, the accuracy order

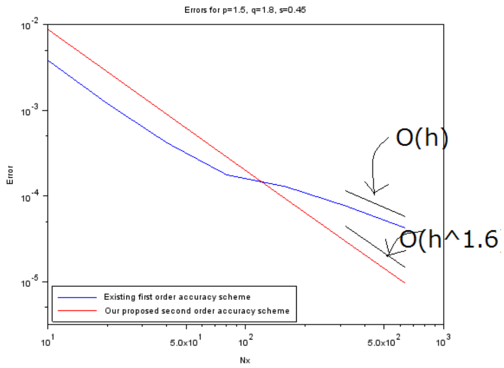


Figure 5.20: Errors of two numerical methods for $q = 1.8$, $p = 1.5$, $s = 0.45$

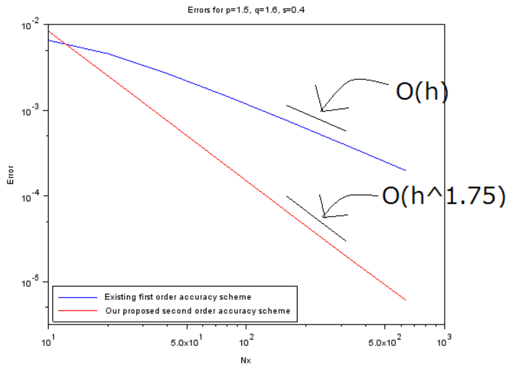


Figure 5.21: Errors of two numerical methods for $q = 1.6$, $p = 1.5$, $s = 0.4$

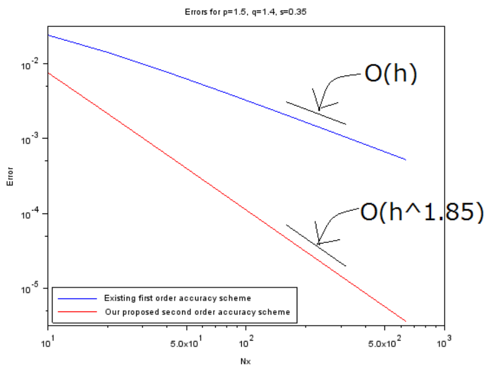


Figure 5.22: Errors of two numerical methods for $q = 1.4$, $p = 1.5$, $s = 0.35$

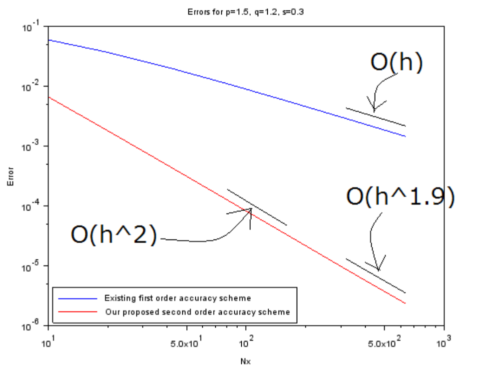


Figure 5.23: Errors of two numerical methods for $q = 1.2$, $p = 1.5$, $s = 0.3$

around boundaries decreases from $O(h_x^2)$ to $O(h_x^{1.5})$. However, the accuracy order $O(h_x^2)$ and $O(h_x^{1.5})$ are near, and it is difficult to obtain that difference well. Therefore, the author's proposed scheme calculate not with second order accuracy but with a little higher accuracy than $O(h_x^{1.5})$.

Figures 5.24, 5.25, 5.26 and 5.27 show the results for respectively $q = 1.8, 1.6, 1.4, 1.2$ and $s = 0.45, 0.4, 0.35, 0.3$ with $p = 0.5$, $C = 100000$ and $N_t = 1000$. These graphs indicate that the numerical solutions are influenced by the form of the analytical solution, and the accuracy decays to $O(h_x^p)$. This accuracy decaying occurs both to the existing first order accuracy scheme and the author's proposed second order accuracy scheme. In addition, not depending on the fractional calculus order q, the accuracy decays to $O(h_x^p)$.

Figures 5.28, 5.29 and 5.30 show the errors of the author's proposed explicit scheme with $C = 1$, $N_t = 5000$, $q = 1.8, 1.6, 1.4, 1.2$, $s = 0.45, 0.4, 0.35, 0.3$ for $p = 2.5, 1.5, 0.5$ respectively. The time step size h_t is $h_t = 1/5000$, and this satisfies the stability conditions of the author's proposed explicit scheme. These results show that the numerical solutions are stable, but the expected accuracy orders cannot be obtained. The reason is that the number of space grids is at most $N_x = 80$ in these experiments and so small that errors cannot converge with the expected accuracy order. Therefore, by taking larger N_x and smaller h_x, the

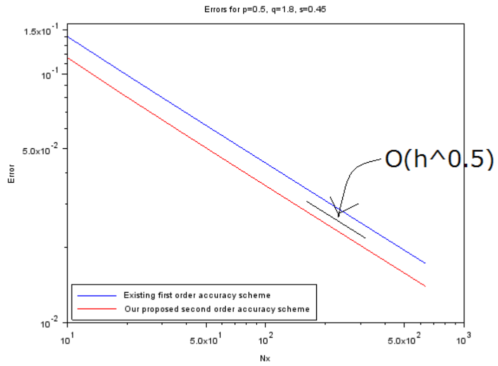


Figure 5.24: Errors of two numerical methods for $q = 1.8$, $p = 0.5$, $s = 0.45$

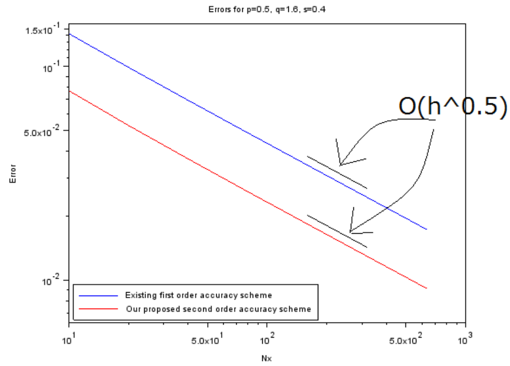


Figure 5.25: Errors of two numerical methods for $q = 1.6$, $p = 0.5$, $s = 0.4$

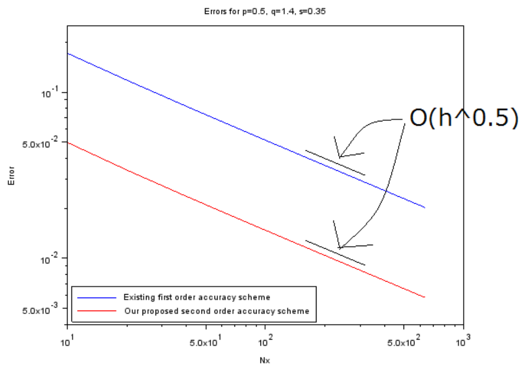


Figure 5.26: Errors of two numerical methods for $q = 1.4$, $p = 0.5$, $s = 0.35$

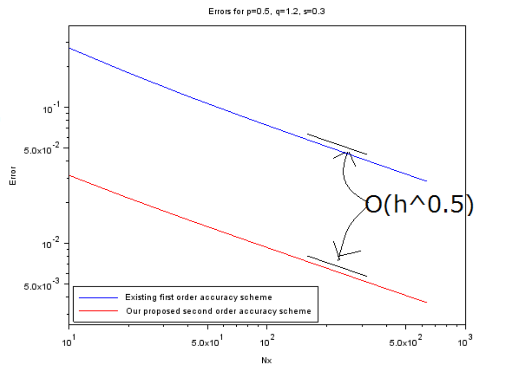


Figure 5.27: Errors of two numerical methods for $q = 1.2$, $p = 0.5$, $s = 0.3$

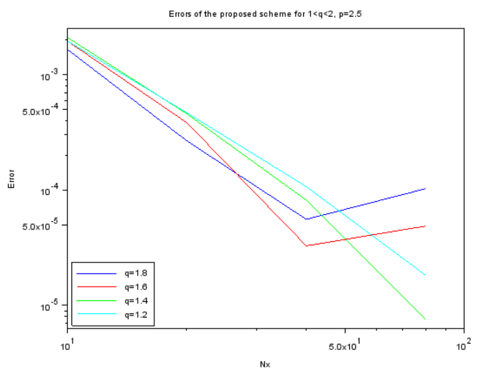


Figure 5.28: Errors of the author's proposed explicit scheme with various q for $p = 2.5$

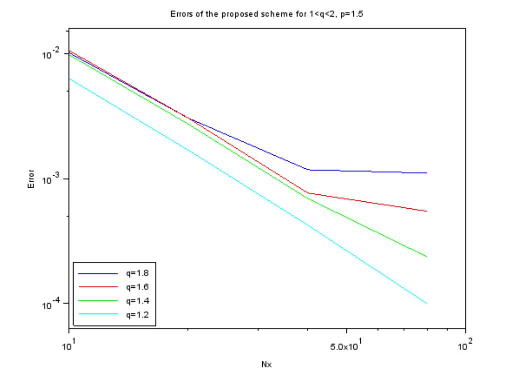


Figure 5.29: Errors of the author's proposed explicit scheme with various q for $p = 1.5$

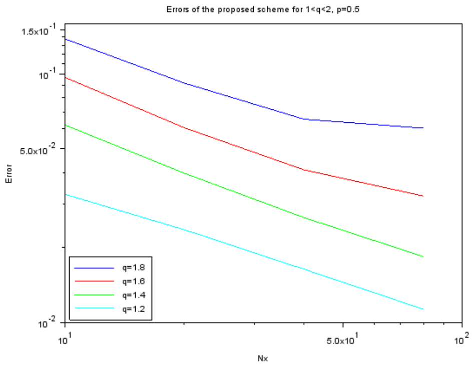


Figure 5.30: Errors of the author's proposed explicit scheme with various q for $p = 0.5$

expected accuracy order will be obtained. However, larger N_x requires smaller h_t, and this means the rapid increase of computational complexity. Therefore, explicit methods are not suitable for measuring errors accurately. In this section, the numerical experiments are done with implicit methods which do not impose the stability conditions on time step size h_t.

Next, the author makes experiments for $0 < q < 1$ with the same analytical solution and the force term. The existing finite difference methods proposed by M.M. Meerschaert and C. Tadjeran are not defined in $0 < q < 1$. Therefore, the author verify the accuracy only of the author's proposed implicit scheme. Figures 5.31, 5.32 and 5.33 are the results with $C = -100000$, $Nt = 1000$, $q = 0.8, 0.6, 0.4, 0.2$, $s = 0.2, 0.1, 0.0, -0.1$ for $p = 2.5, 1.5, 0.5$ respectively.

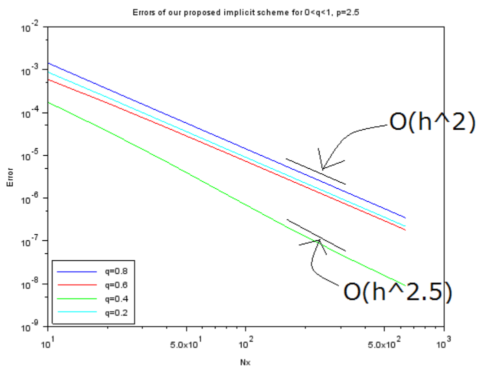


Figure 5.31: Errors of the author's proposed implicit scheme with various q for $p = 2.5$

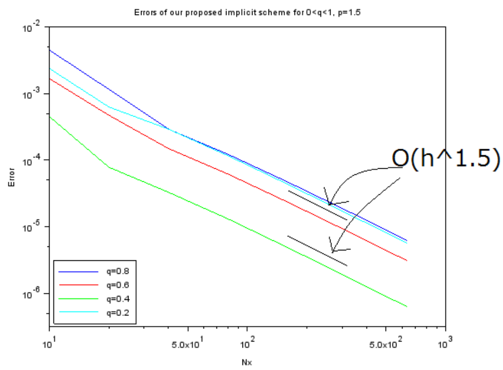


Figure 5.32: Errors of the author's proposed implicit scheme with various q for $p = 1.5$

Figure 5.31 indicates the accuracy order of out proposed implicit scheme is the second order accuracy. In addition, the result for $q = 0.4$ is influenced by the accuracy around boundaries. By the phenomenon of accuracy decaying, the accuracy around boundaries is $O(h_x^{2.5})$, and the result for $q = 0.4$ has a stronger effect of $O(h_x^{2.5})$ than $O(h_x^2)$ which is the accuracy of the author's proposed scheme. Figure 5.32 and 5.33 show the accuracy decaying happens in the computations. The expected accuracy order is the second order accuracy, but the accuracy de-

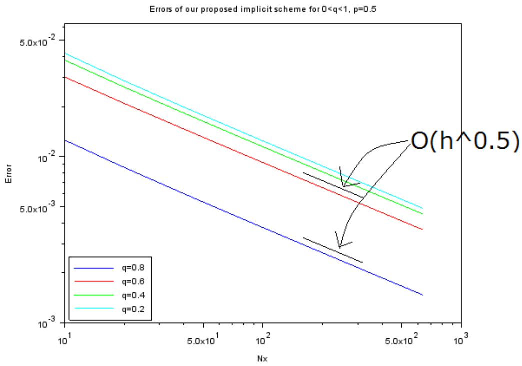


Figure 5.33: Errors of the author's proposed implicit scheme with various q for $p = 0.5$

cays to $O(h_x^{1.5})$ and $O(h_x^{0.5})$. From these results, the accuracy of the numerical solutions for $0 < q < 1$ also decreases depending on the form of the analytical solution.

Next, the author makes experiments in the case of non-zero Dirichlet boundary conditions. Let us consider the following two problems. Problem 1 is defined by the following analytical solution

$$u_1(x,t) = \exp(-t)x^2(1-x)^2 + 3(1-x)^2 - 2(1-x)^3, \ 0 \le x \le 1$$

and the force term

$$\begin{aligned} & f_1(x,t) \\ = \ & -\exp(-t)x^2(1-x)^2 - \frac{C}{2}\exp(-t)\left\{\frac{2\left(x^{2-q}+(1-x)^{2-q}\right)}{\Gamma(3-q)}\right. \\ & \left. -\frac{12\left(x^{3-q}+(1-x)^{3-q}\right)}{\Gamma(4-q)} + \frac{24\left(x^{4-q}+(1-x)^{4-q}\right)}{\Gamma(5-q)}\right\} \\ & -\frac{C}{2}\left\{\frac{x^{-q}}{\Gamma(1-q)} - \frac{6\left(x^{2-q}+(1-x)^{2-q}\right)}{\Gamma(3-q)} + \frac{12\left(x^{3-q}+(1-x)^{3-q}\right)}{\Gamma(4-q)}\right\}. \end{aligned}$$

The initial condition of Problem 1 is $u_1(x,0) = x^2(1-x)^2 + 3(1-x)^2 - 2(1-x)^3$, and the boundary conditions are $u_1(0,t) = 1$, $u_1(1,t) = 0$. Problem 2 is defined by the following analytical solution

$$u_2(x,t) = \exp(-t)x(1-x) + (1-x), \ 0 \le x \le 1$$

and the force term

$$\begin{aligned} & f_2(x,t) \\ = \ & -\exp(-t)x(1-x) - \frac{C}{2}\exp(-t)\left\{\frac{\left(x^{1-q}+(1-x)^{1-q}\right)}{\Gamma(2-q)} - \frac{2\left(x^{2-q}+(1-x)^{2-q}\right)}{\Gamma(3-q)}\right\} \\ & -\frac{C}{2}\left\{\frac{x^{-q}}{\Gamma(1-q)} - \frac{\left(x^{1-q}+(1-x)^{1-q}\right)}{\Gamma(2-q)}\right\}. \end{aligned}$$

The initial condition of Problem 2 is $u_2(x,0) = x(1-x) + (1-x)$, and the boundary conditions are $u_2(0,t) = 1$, $u_2(1,t) = 0$. This problem also has non-zero Dirichlet boundary conditions. All experiments are done for $0 \le t \le 1$. In the paper[21], M. Ilic and others mentioned that the matrix transform method cannot be applied to non-zero Dirichlet boundary conditions. Therefore, the author makes experiments by using existing first order accuracy implicit scheme (3.1) proposed by M.M. Meerschaert and C. Tadjeran and by using the author's proposed second order accuracy implicit scheme (5.6).

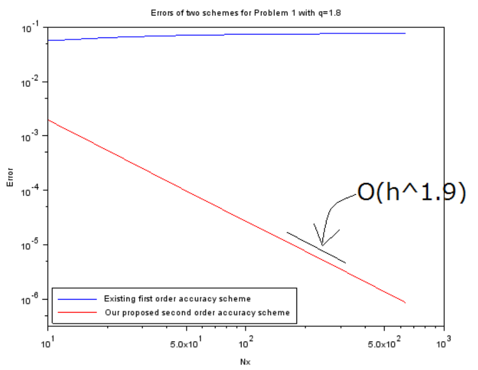


Figure 5.34: Errors of two scheme with Problem 1 for $q = 1.8$

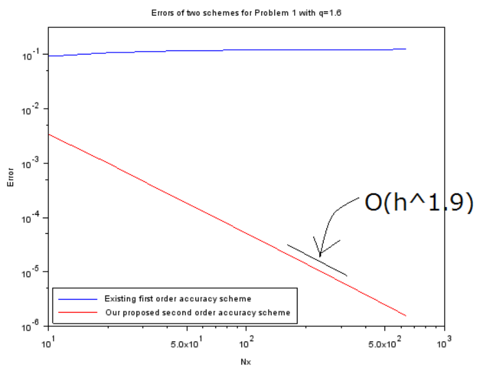


Figure 5.35: Errors of two scheme with Problem 1 for $q = 1.6$

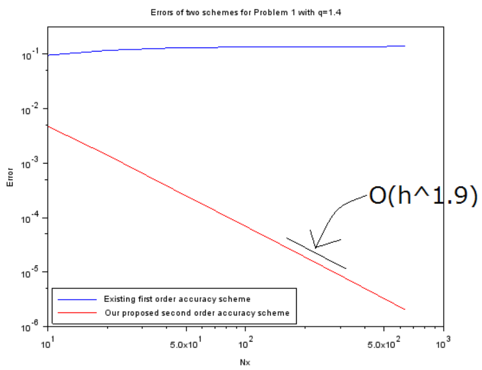


Figure 5.36: Errors of two scheme with Problem 1 for $q = 1.4$

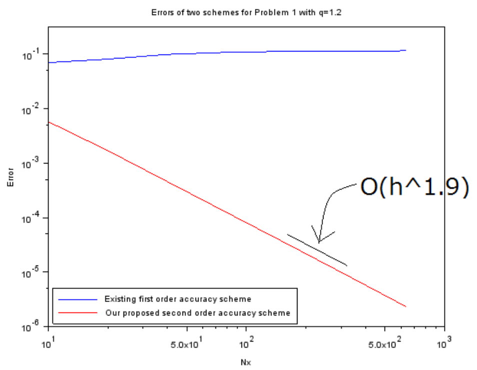


Figure 5.37: Errors of two scheme with Problem 1 for $q = 1.2$

Figures 5.34, 5.35, 5.36 and 5.37 show the errors of the existing first accuracy implicit scheme and the author's proposed second accuracy implicit schemes with $C = 100000$, $N_t = 1000$, $h_t = 1/1000$ for $q = 1.8, 1.6, 1.4, 1.2$ and $s = 0.45, 0.4, 0.35, 0.3$ respectively. These graphs indicate that the existing first accuracy scheme cannot compute with non-zero Dirichlet boundary condition, since the numerical solutions do not converge to the analytical solution. The existing first accuracy scheme does not employ the feature of error cancelling, so the accuracy order becomes $O(1)$ by the accuracy decaying. In contrast, the numerical solutions of the author's proposed scheme converge to the analytical solution with about second order accuracy. The author's proposed scheme employ the feature of error cancelling, and can analytically compute constant functions without errors. In addition, this analytical solution has the order $O(x^2)$ around boundaries. Therefore, the numerical solutions are not influenced by the accuracy decaying.

Figure 5.38 is the results of the author's proposed second order accuracy implicit scheme for Problem 1 with $C = -100000$, $N_t = 1000$, $h_t = 1/1000$ for $q = 0.8, 0.6, 0.4, 0.2$ and $s = 0.2, 0.1, 0.0, -0.1$ respectively. This graph shows

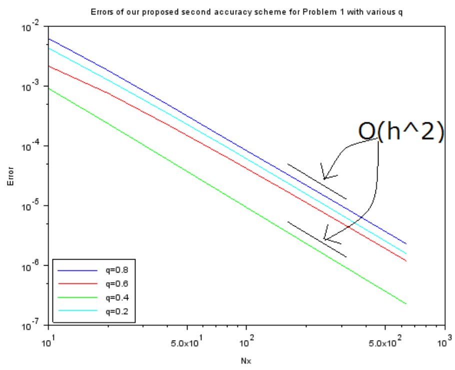


Figure 5.38: Errors of the author's proposed implicit scheme with Problem 1 and various q

that the author's proposed implicit scheme actually compute with second order accuracy for $0 < q < 1$ for non-zero Dirichlet boundary condition. In addition, the accuracy decaying does not happen.

Next, the author makes experiments for Problem 2. Figures 5.39, 5.40, 5.41 and 5.42 show the error of existing first order accuracy implicit scheme and the author's proposed second order accuracy implicit scheme with $C = 100000$, $N_t = 1000$, $h_t = 1/1000$ for $q = 1.8, 1.6, 1.4, 1.2$ and $s = 0.45, 0.4, 0.35, 0.3$ respectively.

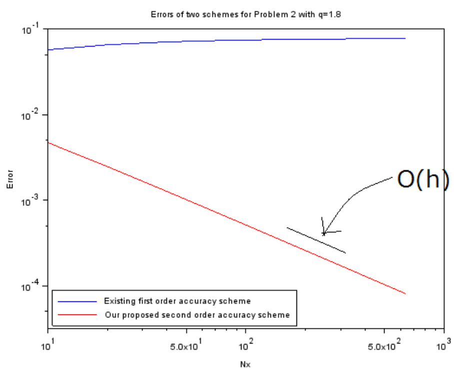


Figure 5.39: Errors of two scheme with Problem 2 for $q = 1.8$

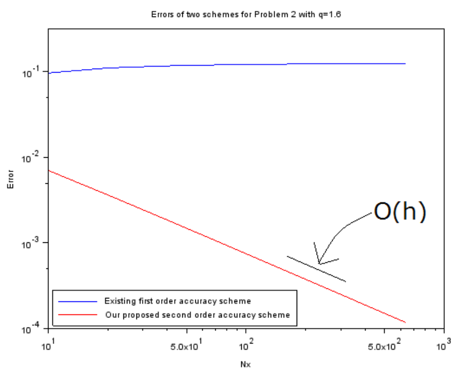
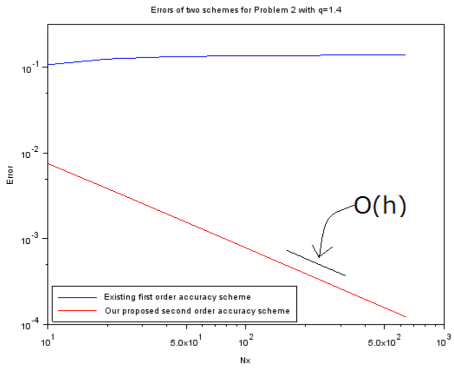


Figure 5.40: Errors of two scheme with Problem 2 for $q = 1.6$

In the same way of the results of Problem 1, the numerical solutions of existing scheme do not converge to the analytical solution. The numerical solutions of the author's proposed scheme converge not with the second order accuracy, but with the first order accuracy. This is because the accuracy decaying happens. The analytical solution has the order $O(x)$ around boundaries, so the accuracy decaying occurs and the accuracy order decreases from the second order accuracy $O(h_x^2)$ to $O(h_x)$.



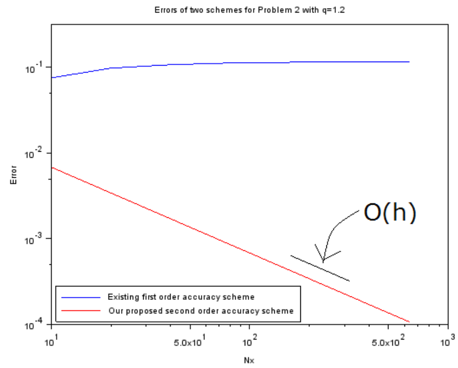


Figure 5.41: Errors of two scheme with Problem 2 for $q = 1.4$

Figure 5.42: Errors of two scheme with Problem 2 for $q = 1.2$

Figure 5.43 is the results of the author's proposed second order accuracy implicit scheme for Problem 2 with $C = -100000$, $N_t = 1000$, $h_t = 1/1000$ for $q = 0.8, 0.6, 0.4, 0.2$ and $s = 0.2, 0.1, 0.0, -0.1$ respectively. This graph indicates

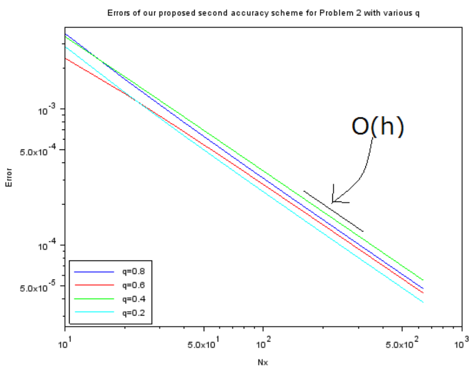


Figure 5.43: Errors of the author's proposed implicit scheme with Problem 2 and various q

that the accuracy decaying happens also for $0 < q < 1$. Therefore, the accuracy of the author's proposed scheme decreases from the second accuracy $O(h_x^2)$ to the first order accuracy $O(h_x)$.

5.2 Time-fractional partial differential equations

5.2.1 The author's proposed finite difference method

In this section, the author proposes the implicit high accuracy finite difference methods for one-dimensional time-fractional partial differential equations which is given by

$$ {}^{\mathrm{R}}_{t_0}D_t^q u(x,t) = C\frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), $$

for $0 < q < 1$, $t_0 \le t \le T$ and $L \le x \le R$. The constant $C > 0$ is a diffusion constant, and the function f is a force term. This equation also appears in the model to simulate physical phenomena, and there are many research to study about this equation. Existing finite difference methods to this equation employ Caputo derivative for time derivative, and have first order accuracy[67, 44, 28]. However, the author consider to use Riemann-Liouville derivative to apply the author's proposed formulae. It is not difficult to convert Riemann-Liouville derivative to Caputo derivative, so the author also try to develop schemes for Caputo derivative in the future task. Let N_t and N_x be the number of grid points for time and space respectively. In addition, let the time step size h_t be $h_t = (T - t_0)/N_t$, and let the space step size h_x be $h_x = (R - L)/N_x$. Let U_j^m denote an approximate solution $U_j^m \simeq u(jh_x, mh_t)$. Then, the author's proposed scheme is given by

$$\begin{aligned}
& \frac{h_t^{-q}}{\Gamma(-q)} \sum_{i=0}^{m-1} \frac{\Gamma(i-q)}{\Gamma(i+1)} \left\{ \frac{2+q}{2} U_j^{m-i} - \frac{q}{2} U_j^{m-i-1} \right\} \\
& + \frac{h_t^{-q}}{\Gamma(1-q)} U_j^0 \left\{ m^{-q} - \frac{\Gamma(m-q)}{\Gamma(m)} \right\} \\
= \; & C \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h_x^2} + f_j^m.
\end{aligned} \tag{5.31}$$

where $1 \le j \le N_x - 1$ and $1 \le m \le N_x$. This scheme also has the feature of error cancelling, and can compute constant functions. The matrix representation of the scheme (5.31) is given by $A\vec{U}^m = \vec{b}^{m-1}$ where $\vec{U}^m = (U_0^m, U_1^m, \dots, U_{N_x}^m)^T$. The entries $a_{i,j}$ of the matrix A are defined as

$$a_{i,j} = \begin{cases} 1, & i = j = 0 \ or \ i = j = N_x \\ 2r + \frac{2+q}{2}, & i = j, \ 1 \le i, j \le N_x - 1 \\ -r, & j = i-1 \ or \ j = i+1, \ 1 \le i \le N_x - 1 \\ 0, & otherwise \end{cases}$$

where $r = Ch_t/h_x^q$ The entries b_j^m of the vector $\vec{b}^m$ are defined as

$$\begin{aligned}
b_j^{m-1} \; = \; & \frac{q}{2} U_j^{m-1} - \sum_{i=1}^{m-1} g_i \left\{ \frac{2+q}{2} U_j^{m-i} - \frac{q}{2} U_j^{m-i-1} \right\} \\
& - U_j^0 \left\{ m^{-q} - \frac{\Gamma(m-q)}{\Gamma(m)} \right\} + h_t^q f_j^m
\end{aligned}$$

where g_n is $g_n = \Gamma(n-q)/(\Gamma(-q)\Gamma(n+1))$. This scheme indicates that the past information is required to calculate the present values.

5.2.2 Stability analysis

As mentioned above, the author apply the matrix method to the schemes for space-fractional partial differential equations. In a similar way, to analyze the stability of the scheme (5.31), the author uses the matrix method to the matrix A. If any eigenvalues λ of the matrix A satisfy $|\lambda| \ge 1$, this scheme is stable. Eigenvalues derived from the first and last column are exactly 1 by Gerschgorin's theorem. From the matrix representation of the scheme, we have

$$\begin{aligned}
& |\lambda - a_{i,i}| \le \sum_{j \ne i} |a_{j,i}| \\
= \; & |\lambda - 2r - \frac{2+q}{2}| \le 2r \\
\Rightarrow \; & \frac{2+q}{2} \le \lambda \le 4r + \frac{2+q}{2}.
\end{aligned}$$

Then, any eigenvalues λ are always more than 1, and this scheme is stable.

5.2.3 Numerical experiments

For the numerical experiments about the author's proposed second accuracy scheme, let us assume two problems. Problem 1 is defined by the following analytical solution

$$u_1(x,t) = t^p \sin(2\pi x),\ 0 \le x \le 1,$$

and the force term

$$f_1(x,t) = \frac{\Gamma(p+1)}{\Gamma(p-q+1)} t^{p-q} \sin(2\pi x) + 4C\pi^2 t^p \sin(2\pi x)$$

where the constant p is a factor which controls the order of the analytical solution at initial points. The initial condition of Problem 1 is $u(x,0) = 0$, and the boundary conditions are $u(0,t) = u(1,0) = 0$. Problem 2 is defined by the following analytical solution

$$u_2(x,t) = (t^p + 1)\sin(2\pi x),\ 0 \le x \le 1,$$

and the force term

$$\begin{aligned} & f_2(x,t) \\ = \ & \left\{ \frac{\Gamma(p+1)}{\Gamma(p-q+1)} t^{p-q} + \frac{t^{-q}}{\Gamma(1-q)} \right\} \sin(2\pi x) \\ & + 4C\pi^2 (t^p+1)\sin(2\pi x) \end{aligned}$$

where the constant p is a factor which controls the order of the analytical solution at initial points. The initial condition of Problem 1 is $u(x,0) = \sin(2\pi x)$, and the boundary conditions are $u(0,t) = u(1,0) = 0$.

Figure 5.44 is the analytical solution of Problem 1. Figures 5.45, 5.46 and 5.47 show the errors of the proposed scheme to Problem 1 for $q = 0.8$ in blue lines, $q = 0.6$ in red lines, $q = 0.4$ in green lines and $q = 0.2$ in cyan line with $C = 0.000001$, $N_x = 320$ for $p = 2.5, 1.5, 0.5$ respectively.

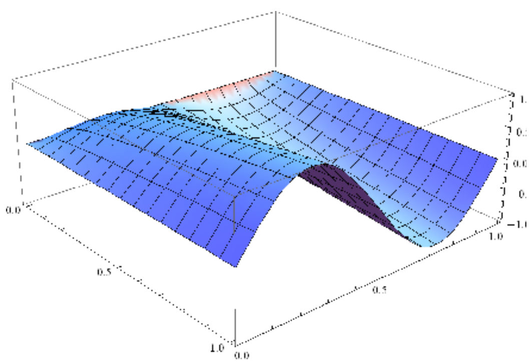


Figure 5.44: The analytical solution $u_1(x,t)$ of Problem 1

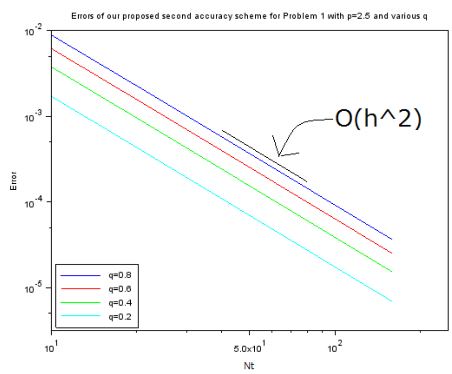


Figure 5.45: Errors of the proposed scheme with Problem 1 for $p = 2.5$

Figure 5.45 indicates that the proposed scheme computes actually with the second order accuracy if the accuracy decaying does not occur. On the other hand, Figures 5.46 and 5.47 show the influence of the accuracy decaying. In a

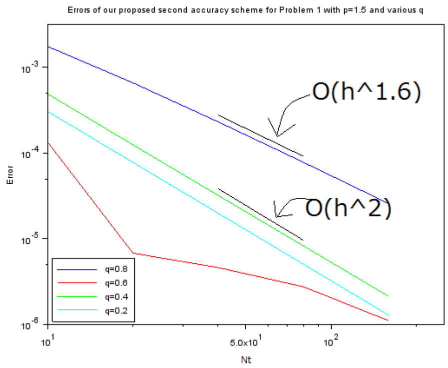


Figure 5.46: Errors of the proposed scheme with Problem 1 for $p = 1.5$

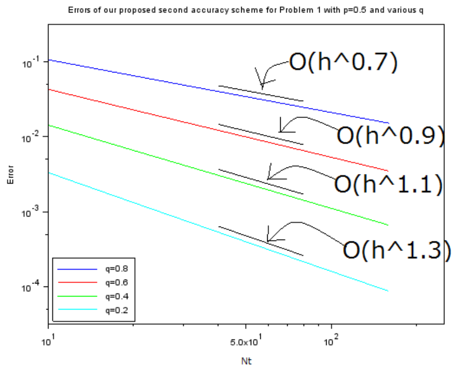


Figure 5.47: Errors of the proposed scheme with Problem 1 for $p = 0.5$

similar way of space-fractional partial differential equations, the accuracy decaying happens around initial points. Therefore, the accuracy around the initial boundary is $O(h_t^{1.5})$ for $p = 1.5$ and is $O(h_t^{0.5})$ for $p = 0.5$. The computations of the numerical solutions at $t = 1$ require the numerical solutions around initial points as the past information. Therefore, the results at $t = 1$ are also influenced by the accuracy decaying. Then, how much does the accuracy decay at $t = 1$? The notable points in Figures 5.46 and 5.47 are that the observed accuracy orders are represented with $O(h_t^{p+1-q})$. This relation is meaningful, but it is not easy to mathematically analyze the accuracy of the formula which contain the past information. In addition, time-fractional partial differential equations are similar not to space-fractional partial differential equations but to fractional ordinary differential equations which the author introduces in Chapter 7. This is because two equations include time fractional derivatives. Further error analysis of the author's proposed method is a future task.

Figure 5.48 is the analytical solution of Problem 2. Figures 5.49, 5.50 and 5.51 show the errors of the author's proposed scheme to Problem 2 for $q = 0.8$ in blue lines, $q = 0.6$ in red lines, $q = 0.4$ in green lines and $q = 0.2$ in cyan lines with $C = 0.000001$, $N_x = 320$ for $p = 2.5, 1.5, 0.5$ respectively.

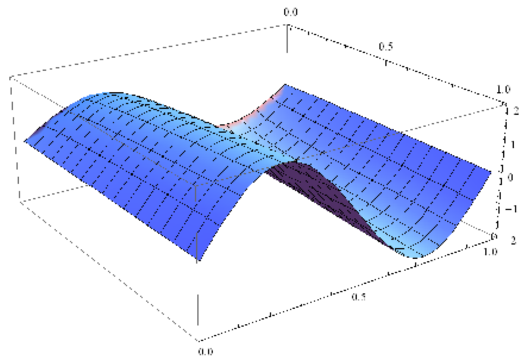


Figure 5.48: The analytical solution $u_1(x,t)$ of Problem 2

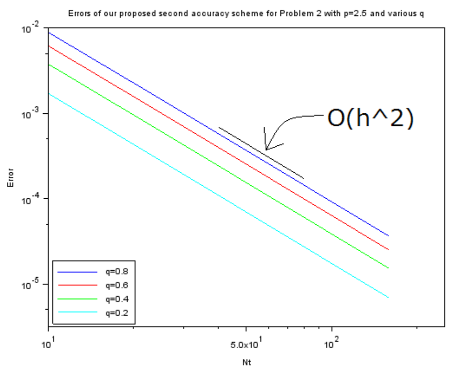


Figure 5.49: Errors of the proposed scheme with Problem 2 for $p = 2.5$

Figure 5.49, 5.50 and 5.51 indicates that the proposed scheme computes actu-

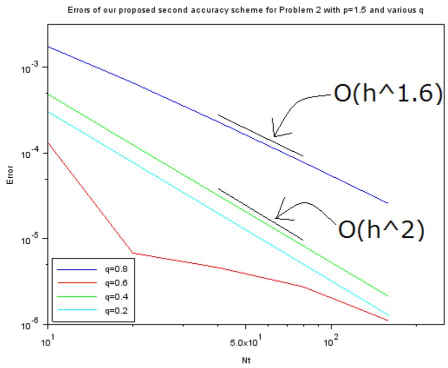


Figure 5.50: Errors of the proposed scheme with Problem 2 for $p = 1.5$

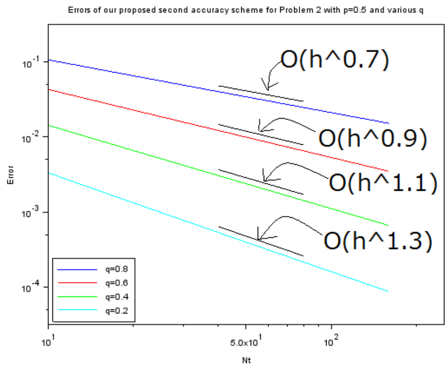


Figure 5.51: Errors of the proposed scheme with Problem 2 for $p = 0.5$

ally with the second order accuracy if the analytical solution contains a constant function. The proposed scheme can compute constants functions without errors, so the results of Problem 2 are almost the same to that of Problem 1. In Problem 2, the accuracy decaying happens in a similar way of Problem 1.

Chapter 6

Numerical solutions in the form of polynomial expansion for homogeneous parabolic fractional partial differential equations

6.1 Motivation

This section treat the following homogeneous parabolic fractional partial differential equations in bounded domain as

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= \frac{C}{2}\left[{}^{\mathrm{R}}_{-L}D^{q}_{x}u(x,t) + {}^{\mathrm{R}}_{x}D^{q}_{L}u(x,t)\right] \\ &= \frac{C}{2}\,{}_{-L}R^{q}_{L}u(x,t) \end{aligned} \tag{6.1}$$

where $1 < q < 2$ and $-L \leq x \leq L$. In the above equation, the operator ${}_{-L}R^{q}_{L}$ defined by the sum of right side and left side fractional derivative is called Riesz derivative. There are two motivations to develop the numerical solving method in the form of polynomial for this kind of equations. In Chapter 5, the author proposes finite difference methods for space-fractional partial differential equations. In addition, the author shows that the author's proposed schemes are second order accuracy but its accuracy decays depending on the analytical solution of equations. Then, there is a question. Does the analytical solution of the equation (6.1) have the form which causes the accuracy decaying? This is one of motivations, and the other motivation is to measure the error. In order to measure the error, we need to know the analytical solution, since the error is made from the comparison between the analytical solution and numerical solutions. Whether the accuracy decaying will happen depends on the form of the analytical solution at boundaries. However, to measure the error, we need to know the form of the analytical solution in the whole domain.

6.2 The author's proposed method in the form of polynomial expansion

The author's proposed method is similar to development of the analytical solution of integer order diffusion equations in a finite domain. In finite domain, the analytical solution of integer order diffusion equations is developed by using separation of variables. Then, we solve two kinds of differential equations about time and space individually. The solutions of differential equations about space are sine and cosine functions which become multiples of constants for second derivatives. In a similar way, the proposed method is to find odd and even functions which becomes multiples of constants for right side fractional derivative and left side fractional derivative. Firstly, the analytical solution of homogeneous parabolic fractional partial differential equations in finite domain is also developed by using separation of variables. Let us assume that the analytical solution $u(x,t)$ be represented as $u(x,t) = X(x)T(t)$. Then, by substituting this to Eq. (6.1), we have

$$\begin{aligned} X(x)T'(t) &= \frac{C}{2}\left[{}^{\mathrm{R}}_{L}D^{q}_{x}X(x) + {}^{\mathrm{R}}_{x}D^{q}_{R}X(x)\right]T(t) \\ \Rightarrow \quad \frac{T'(t)}{T(t)} &= \frac{C}{2}\frac{\left[{}^{\mathrm{R}}_{L}D^{q}_{x}X(x) + {}^{\mathrm{R}}_{x}D^{q}_{R}X(x)\right]}{X(x)} = -\mu \end{aligned}$$

where μ is a constant $\mu > 0$ which depends on neither t nor x. Then, we have the differential equations about t as

$$T'(t) = -\mu T(t).$$

The solution of the above equation is given by using an exponential function as

$$T(x) = A\exp(-\mu t)$$

where A is an integral constant. In regard to x, we have the following fractional differential equations as

$$\frac{C}{2}\left[{}^{\mathrm{R}}_{L}D^{q}_{x}X(x) + {}^{\mathrm{R}}_{x}D^{q}_{R}X(x)\right] = -\mu X(x). \tag{6.2}$$

This differential equation contain the two kinds of fractional derivative, so it is not easy to solve analytically. In integer order diffusion equations, the analytical solution about x is composed by the combination of sine and cosine functions. In a similar way, let us assume that the function $X(x)$ is odd or even function expanded at the center of domain. Here, we put the function $X(x)$ as an even function defined by

$$\begin{aligned} X_0(x) &= a_0 + a_2x^2 + a_4x^4 + \cdots \\ &= \sum_{k=0}^{\infty} a_{2k}x^{2k}. \end{aligned}$$

An odd function is defined by

$$\begin{aligned} X_1(x) &= a_1x + a_3x^3 + a_5x^5 + \cdots \\ &= \sum_{k=0}^{\infty} a_{2k+1}x^{2k+1}. \end{aligned}$$

The author call this even function $X_0(x)$ fractional cosine function, and call this odd function $X_1(x)$ fractional sine function in this thesis. By assuming that the function $X(x)$ can be expanded at the center of the domain, we can solve Eq. (6.1) by computing the coefficient a_k.

Before substituting $X_0(x)$ and $X_1(x)$ to Eq. (6.2), let us consider the fractional derivative for the polynomial x^n where n is a positive integer $n = 0, 1, 2, 3, \cdots$. From the definition of Riemann-Liouville definition, we have

$$\begin{aligned} & {}^{\mathrm{R}}_{-L}D^{q}_{x}x^{n} \\ = \; & \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \int_{-L}^{x} \frac{\xi^n}{(x-\xi)^{q-1}}d\xi. \end{aligned}$$

By applying changing variable as $\tau = x - \xi$, we have

$$\begin{aligned}
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \int_0^{x+L} \frac{(x-\tau)^n}{\tau^{q-1}} d\tau \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \int_0^{x+L} \sum_{k=0}^{n} x^{n-k}(-1)^k \tau^{k+1-q}\binom{n}{k} d\tau \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \left[\sum_{k=0}^{n}\binom{n}{k} x^{n-k}(-1)^k \frac{\tau^{k+2-q}}{k+2-q}\right]_0^{x+L} \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \sum_{k=0}^{n}\binom{n}{k} x^{n-k}(-1)^k \frac{(x+L)^{k+2-q}}{k+2-q} \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \left\{x^n \frac{(x+L)^{2-q}}{2-q} - n x^{n-1}\frac{(x+L)^{3-q}}{3-q} + \cdots + (-1)^n \frac{(x+L)^{n+2-q}}{n+2-q}\right\}.
\end{aligned}$$

Then, we have the fractional derivative of $X_0(x)$ as

$$\begin{aligned}
&{}_{-L}^{\mathrm{R}}D_x^q X_0(x) \\
&= \left[\frac{d}{dx}\right]^2 \frac{1}{\Gamma(2-q)}\left[L^{2-q}\left\{\frac{a_0}{2-q} + \frac{a_2}{4-q}L^2 + \dots\right\}\right. \\
&\quad + \left(\frac{x}{L}\right) L^{2-q}\left\{a_0\frac{1-q}{1-q} + a_2 L^2 \frac{1-q}{3-q} + a_4 L^4 \frac{1-q}{5-q} + \dots\right\} \\
&\quad + \left(\frac{x}{L}\right)^2 L^{2-q}\left\{a_0\frac{(1-q)(-q)}{2(-q)} + a_2 L^2 \frac{(1-q)(-q)}{2(2-q)} + a_4 L^4 \frac{(1-q)(-q)}{2(4-q)} + \dots\right\} \\
&\quad + \left(\frac{x}{L}\right)^3 L^{2-q}\left\{a_0\frac{(1-q)(-q)(-1-q)}{6(-1-q)} + a_2 L^2 \frac{(1-q)(-q)(-1-q)}{6(1-q)} + \dots\right\} \\
&\quad + \dots \\
&\quad + \left(\frac{x}{L}\right)^n L^{2-q}\frac{\Gamma(2-q)}{\Gamma(n+1)\Gamma(2-n-q)} \sum_{k=0}^{\infty} \frac{a_{2k}L^{2k}}{2-n-q+2k} \\
&\quad \left. + \dots \right].
\end{aligned}$$

Next, let us consider the left fractional derivative for the polynomial x^n. Here, we have

$$\begin{aligned}
&{}_x^{\mathrm{R}}D_L^q x^n \\
&= \frac{1}{\Gamma(2-q)}\left[-\frac{d}{dx}\right]^2 \int_x^L \frac{\xi^n}{(\xi - x)^{q-1}} d\xi.
\end{aligned}$$

By applying changing variable as $\tau = \xi - x$, we have

$$\begin{aligned}
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \int_0^{L-x} \frac{(x+\tau)^n}{\tau^{q-1}} d\tau \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \int_0^{L-x} \sum_{k=0}^{n} x^{n-k} \tau^{k+1-q}\binom{n}{k} d\tau \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \left[\sum_{k=0}^{n}\binom{n}{k} x^{n-k} \frac{\tau^{k+2-q}}{k+2-q}\right]_0^{L-x} \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \sum_{k=0}^{n}\binom{n}{k} x^{n-k} \frac{(L-x)^{k+2-q}}{k+2-q} \\
&= \frac{1}{\Gamma(2-q)}\left[\frac{d}{dx}\right]^2 \left\{x^n \frac{(L-x)^{2-q}}{2-q} + n x^{n-1}\frac{(L-x)^{3-q}}{3-q} + \frac{n(n-1)}{2} x^{n-2}\frac{(L-x)^{4-q}}{4-q} + \dots\right\}.
\end{aligned}$$

Then, we have the left fractional derivative to X_0 as

$$\begin{aligned}
&{}^{\mathrm{R}}_{x}D^{q}_{L}X_0(x)\\
=\; & \left[\frac{d}{dx}\right]^2 \frac{1}{\Gamma(2-q)} \left[L^{2-q}\left\{\frac{a_0}{2-q}+\frac{a_2}{4-q}L^2+\dots\right\}\right.\\
& -\left(\frac{x}{L}\right)L^{2-q}\left\{a_0\frac{1-q}{1-q}+a_2L^2\frac{1-q}{3-q}+a_4L^4\frac{1-q}{5-q}+\dots\right\}\\
& +\left(\frac{x}{L}\right)^2L^{2-q}\left\{a_0\frac{(1-q)(-q)}{2(-q)}+a_2L^2\frac{(1-q)(-q)}{2(2-q)}+a_4L^4\frac{(1-q)(-q)}{2(4-q)}+\dots\right\}\\
& -\left(\frac{x}{L}\right)^3L^{2-q}\left\{a_0\frac{(1-q)(-q)(-1-q)}{6(-1-q)}+a_2L^2\frac{(1-q)(-q)(-1-q)}{6(1-q)}+\dots\right\}\\
& +\dots\\
& +(-1)^n\left(\frac{x}{L}\right)^nL^{2-q}\frac{\Gamma(2-q)}{\Gamma(n+1)\Gamma(2-n-q)}\sum_{k=0}^{\infty}\frac{a_{2k}L^{2k}}{2-n-q+2k}\\
& \left.+\dots\right].
\end{aligned}$$

Therefore, we obtain

$$\begin{aligned}
&\frac{C}{2}\left[{}^{\mathrm{R}}_{-L}D^{q}_{x}X_0(x)+{}^{\mathrm{R}}_{x}D^{q}_{L}X_0(x)\right]\\
=\; & \left[\frac{d}{dx}\right]^2 \frac{C}{\Gamma(2-q)} \left[L^{2-q}\left\{\frac{a_0}{2-q}+\frac{a_2}{4-q}L^2+\dots\right\}\right.\\
& +\left(\frac{x}{L}\right)^2L^{2-q}\left\{a_0\frac{(1-q)(-q)}{2(-q)}+a_2L^2\frac{(1-q)(-q)}{2(2-q)}+a_4L^4\frac{(1-q)(-q)}{2(4-q)}+\dots\right\}\\
& +\dots\\
& +\left(\frac{x}{L}\right)^{2m}L^{2-q}\frac{\Gamma(2-q)}{\Gamma(2m+1)\Gamma(2-2m-q)}\sum_{k=0}^{\infty}\frac{a_{2k}L^{2k}}{2-2m-q+2k}\\
& \left.+\dots\right]\\
=\; & \frac{C}{\Gamma(2-q)}\left[L^{-q}\left\{a_0\frac{(1-q)(-q)}{(-q)}+a_2L^2\frac{(1-q)(-q)}{(2-q)}+a_4L^4\frac{(1-q)(-q)}{(4-q)}+\dots\right\}\right.\\
& +\left(\frac{x}{L}\right)^2L^{-q}\left\{a_0\frac{(1-q)(-q)(-1-q)(-2-q)}{2(-2-q)}+a_2L^2\frac{(1-q)(-q)(-1-q)(-2-q)}{2(-q)}+\dots\right\}\\
& +\dots\\
& +\left(\frac{x}{L}\right)^{2m}L^{-q}\sum_{k=0}^{\infty}\frac{a_{2k}L^{2k}\Gamma(2-q)}{(2k-2m-q)\Gamma(2m+1)\Gamma(-2m-q)}\\
& \left.+\dots\right].
\end{aligned}$$

By substituting to Eq. (6.2), we obtain the following relation for each term

$$-\mu a_{2m}x^{2m}=\left(\frac{x}{L}\right)^{2m}L^{-q}\sum_{k=0}^{\infty}\frac{Ca_{2k}L^{2k}}{(2k-2m-q)\Gamma(2m+1)\Gamma(-2m-q)}$$

where m is a non-negative integer. Let b_k be $b_k = a_kL^k$, and applying Euler's reflection formula to $\Gamma(2m+1)\Gamma(-2m-q)$, we have the following system of equations

$$
\begin{aligned}
-b_0\frac{\Gamma(1)}{\Gamma(1+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_0}{q}+\frac{b_2}{q-2}+\frac{b_4}{q-4}+\dots \\
-b_2\frac{\Gamma(3)}{\Gamma(3+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_0}{q+2}+\frac{b_2}{q}+\frac{b_4}{q-2}+\dots \\
-b_4\frac{\Gamma(5)}{\Gamma(5+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_0}{q+4}+\frac{b_2}{q+2}+\frac{b_4}{q}+\dots \\
\vdots &= \vdots \\
-b_{2m}\frac{\Gamma(2m+1)}{\Gamma(2m+1+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_0}{q+2m}+\frac{b_2}{q+2m-2}+\dots. \qquad (6.3)
\end{aligned}
$$

Next, let us consider about the odd function $X_1(x)$. In the same way to the function $X_0(x)$, we obtain

$$
\begin{aligned}
&\frac{C}{2}\left[{}^{\mathrm{R}}_{-L}D^q_x X_1(x)+{}^{\mathrm{R}}_{x}D^q_L X_1(x)\right] \\
= \ &\frac{C}{\Gamma(2-q)}\left[\left(\frac{x}{L}\right)L^{-q}\sum_{k=0}^{\infty}\frac{a_{2k+1}L^{2k+1}\Gamma(2-q)}{(2k-q)\Gamma(2)\Gamma(-1-q)}\right. \\
&+\left(\frac{x}{L}\right)^3 L^{-q}\sum_{k=0}^{\infty}\frac{a_{2k+1}L^{2k+1}\Gamma(2-q)}{(2k-2-q)\Gamma(4)\Gamma(-3-q)} \\
&+\dots \\
&+\left(\frac{x}{L}\right)^{2m+1} L^{-q}\sum_{k=0}^{\infty}\frac{a_{2k+1}L^{2k+1}\Gamma(2-q)}{(2k-2m-q)\Gamma(2m+2)\Gamma(-2m-1-q)} \\
&\left.+\dots\right].
\end{aligned}
$$

From Eq. (6.2), we have the following relation for each term

$$
-\mu a_{2m+1}x^{2m+1}=\left(\frac{x}{L}\right)^{2m+1}L^{-q}\sum_{k=0}^{\infty}\frac{Ca_{2k+1}L^{2k+1}}{(2k-2m-q)\Gamma(2m+2)\Gamma(-2m-1-q)}
$$

where m is a non-negative integer. Let b_k be $b_k=a_kL^k$, and applying Euler's reflection formula to $\Gamma(2m+2)\Gamma(-2m-1-q)$, we have the following system of equations

$$
\begin{aligned}
-b_1\frac{\Gamma(2)}{\Gamma(2+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_1}{q}+\frac{b_3}{q-2}+\frac{b_5}{q-4}+\dots \\
-b_3\frac{\Gamma(4)}{\Gamma(4+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_1}{q+2}+\frac{b_3}{q}+\frac{b_5}{q-2}+\dots \\
-b_5\frac{\Gamma(6)}{\Gamma(6+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_1}{q+4}+\frac{b_3}{q+2}+\frac{b_5}{q}+\dots \\
\vdots &= \vdots \\
-b_{2m+1}\frac{\Gamma(2m+2)}{\Gamma(2m+2+q)}\frac{\mu\pi L^q}{C\sin(q\pi)} &= \frac{b_1}{q+2m}+\frac{b_3}{q+2m-2}+\dots. \qquad (6.4)
\end{aligned}
$$

Now, we obtain two infinite size of equations (6.3) and (6.4). Then, how can we solve them? The author suggests the following two points for this question. First point is the approximation to a finite size. In the beginning, we cannot solve infinite size problems by using computers. It is required that the approximation from infinite size system of equations to finite size. In this thesis, let N denote the size of approximated system of equations. Then, by this approximation, we obtain a finite number of approximated coefficients $b_{k,N}$ and an approximation μ_N to μ. In addition, let the approximation function $X_{0,N}(x)$ to $X_0(x)$ be

$$X_{0,N}(x) = \sum_{k=0}^{N-1} a_{2k}x^{2k},$$

and let the approximation function $X_{1,N}(x)$ to $X_1(x)$ be

$$X_{1,N}(x) = \sum_{k=0}^{N-1} a_{2k+1}x^{2k+1}.$$

Then, we obtain not $X_0(x)$ and $X_1(x)$ but approximated functions $X_{0,N}(x)$ and $X_{1,N}(x)$. However, even approximated functions have many significant properties in order to understand homogeneous parabolic fractional partial differential equations (6.1). Second point is uniqueness of the coefficients b_k. When we solve Eqs. (6.3) or (6.4), the values of coefficients b_k cannot be uniquely decided unless we decide just two values before solving. This fact is shown from the number of variables and equations. In this thesis, we decide μ and b_0 in Eq. (6.3) and μ and b_1 in Eq. (6.4) before solving. The proposed method simply puts $b_0 = 1$ and $b_1 = 1$. However, the value of μ cannot be decided without consideration, since μ has a mathematical meaning. The author suggests two methods to decide the value of μ.

Eigenvalues method

One is to use the property that μ is the eigenvalue of the Riesz derivative operator. Equation (6.2) can be represented with Riesz operator as

$$-\mu X(x) = \frac{C}{2} {}_{-L}R_L^q X(x).$$

Then, it is interpreted that the function $X(x)$ is an eigenfunction and μ is an eigenvalue. Therefore, the approximated eigenvalue μ_N can be calculated as the eigenvalues of eigenfunctions $X_{0,N}(x)$ and $X_{1,N}(x)$ by computing the eigenvalues of the following matrix

$$\begin{pmatrix}
-\frac{\Gamma(1+q)\sin(q\pi)}{q\Gamma(1)\pi L^q} & -\frac{\Gamma(1+q)\sin(q\pi)}{(q-2)\Gamma(1)\pi L^q} & \cdots & -\frac{\Gamma(1+q)\sin(q\pi)}{(q-2N)\Gamma(1)\pi L^q} \\
-\frac{\Gamma(3+q)\sin(q\pi)}{(q+2)\Gamma(3)\pi L^q} & -\frac{\Gamma(3+q)\sin(q\pi)}{q\Gamma(3)\pi L^q} & \cdots & -\frac{\Gamma(3+q)\sin(q\pi)}{(q-2N+2)\Gamma(3)\pi L^q} \\
-\frac{\Gamma(5+q)\sin(q\pi)}{(q+4)\Gamma(5)\pi L^q} & -\frac{\Gamma(5+q)\sin((q+2)\pi)}{(q+2)\Gamma(5)\pi L^q} & \cdots & -\frac{\Gamma(5+q)\sin(q\pi)}{(q-2N+4)\Gamma(5)\pi L^q} \\
\vdots & \vdots & \ddots & \vdots \\
-\frac{\Gamma(2N+1+q)\sin(q\pi)}{(q+2N)\Gamma(2N+1)\pi L^q} & -\frac{\Gamma(2N+1+q)\sin(q\pi)}{(q+2N-2)\Gamma(2N+1)\pi L^q} & \cdots & -\frac{\Gamma(2N+1+q)\sin(q\pi)}{(q)\Gamma(2N+1)\pi L^q}
\end{pmatrix}$$

for $X_{0,N}$ and the following matrix

$$\begin{pmatrix}
-\frac{\Gamma(2+q)\sin(q\pi)}{q\Gamma(2)\pi L^q} & -\frac{\Gamma(2+q)\sin(q\pi)}{(q-2)\Gamma(2)\pi L^q} & \cdots & -\frac{\Gamma(2+q)\sin(q\pi)}{(q-2N)\Gamma(2)\pi L^q} \\
-\frac{\Gamma(4+q)\sin(q\pi)}{(q+2)\Gamma(4)\pi L^q} & -\frac{\Gamma(4+q)\sin(q\pi)}{q\Gamma(4)\pi L^q} & \cdots & -\frac{\Gamma(4+q)\sin(q\pi)}{(q-2N+2)\Gamma(4)\pi L^q} \\
-\frac{\Gamma(6+q)\sin(q\pi)}{(q+4)\Gamma(6)\pi L^q} & -\frac{\Gamma(6+q)\sin((q+2)\pi)}{(q+2)\Gamma(6)\pi L^q} & \cdots & -\frac{\Gamma(6+q)\sin(q\pi)}{(q-2N+4)\Gamma(6)\pi L^q} \\
\vdots & \vdots & \ddots & \vdots \\
-\frac{\Gamma(2N+2+q)\sin(q\pi)}{(q+2N)\Gamma(2N+2)\pi L^q} & -\frac{\Gamma(2N+2+q)\sin(q\pi)}{(q+2N-2)\Gamma(2N+2)\pi L^q} & \cdots & -\frac{\Gamma(2N+2+q)\sin(q\pi)}{(q)\Gamma(2N+2)\pi L^q}
\end{pmatrix}$$

for $X_{1,N}$.

Search method

The other method to decide the value of μ_N is to search the appropriate value in order to satisfy the boundary condition. In this thesis, we assume the zero Dirichlet boundary condition for Eq. (6.1), so the appropriate value of μ_N is searched by solving the following system of equations under the assumption $b_{0,N} = 1$ and $b_{1,N} = 1$

$$\begin{pmatrix} \frac{1}{q} + \frac{\frac{1}{q-2}}{\frac{\Gamma(3)\mu\pi L^q}{\Gamma(3+q)\sin(q\pi)}} & \frac{\frac{1}{q-4}}{\frac{1}{q-2}} & \cdots & \frac{\frac{1}{q-2N}}{\frac{1}{q-2N+2}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{q+2N-4} & \frac{1}{q+2N-6} & \cdots & \frac{1}{q-2} \end{pmatrix} \begin{pmatrix} b_{2,N} \\ b_{4,N} \\ \vdots \\ b_{2N,N} \end{pmatrix} = \begin{pmatrix} -\frac{1}{q} - \frac{\Gamma(1)\mu\pi L^q}{\Gamma(1+q)\sin(q\pi)} \\ -\frac{1}{q+2} \\ \vdots \\ -\frac{1}{q+2N-2} \end{pmatrix}$$

and

$$\begin{pmatrix} \frac{1}{q} + \frac{\frac{1}{q-2}}{\frac{\Gamma(4)\mu\pi L^q}{\Gamma(4+q)\sin(q\pi)}} & \frac{\frac{1}{q-4}}{\frac{1}{q-2}} & \cdots & \frac{\frac{1}{q-2N}}{\frac{1}{q-2N+2}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{q+2N-4} & \frac{1}{q+2N-6} & \cdots & \frac{1}{q-2} \end{pmatrix} \begin{pmatrix} b_{3,N} \\ b_{5,N} \\ \vdots \\ b_{2N+1,N} \end{pmatrix} = \begin{pmatrix} -\frac{1}{q} - \frac{\Gamma(2)\mu\pi L^q}{\Gamma(2+q)\sin(q\pi)} \\ -\frac{1}{q+2} \\ \vdots \\ -\frac{1}{q+2N-2} \end{pmatrix}$$

so that the coefficients $b_{k,N}$ satisfy respectively the following boundary conditions

$$X_{0,N}(-L) = X_{0,N}(L) = \sum_{k=0}^{N-1} b_{2k,N} = 0$$

and

$$X_{1,N}(-L) = X_{1,N}(L) = \sum_{k=0}^{N-1} b_{2k+1,N} = 0.$$

The author introduces the two methods to decide the approximated values μ_N and coefficients $b_{k,N}$. However, the values calculated with two methods are different because of difference of the objectives. This thesis mainly uses the latter method. This is because the approximated function $X_{0,N}(x)$ and $X_{1,N}(x)$ satisfy zero Dirichlet boundary conditions with high accuracy. It is very important to satisfy the boundary condition for studying the properties of Eq. (6.1) and for utilizing the method to solve equations. Therefore, to calculate μ_N, the author apply the method which uses the boundary conditions in this thesis.

6.3 Experiments about the analytical solution of homogeneous parabolic fractional differential equations

6.3.1 The value of μ_N

Firstly, the author finds the value of μ_N from Dirichlet boundary conditions as $X_{0,N}(L) = X_{0,N}(-L) = 0$ or $X_{1,N}(L) = X_{1,N}(-L) = 0$. Here, the author shows the graph between the value of μ_N and the value of $X_{0,N}(L)$ and $X_{1,N}(L)$ at boundary. In this section, all numerical experiments are done with $L = 1$ and $C = 1$.

Figure 6.1 is the result of $X_{0,N}(x)$ and $X_{1,N}(x)$ for $q = 1.999, 1.5$ and $N = 250$. For $q = 2$, $X_0(x)$ is equal to cosine function and $X_1(0)$ is equal to sine function. This means that, for $q = 2$, the boundary values $X_0(L) = \cos(L)$ and $X_1(L) =$

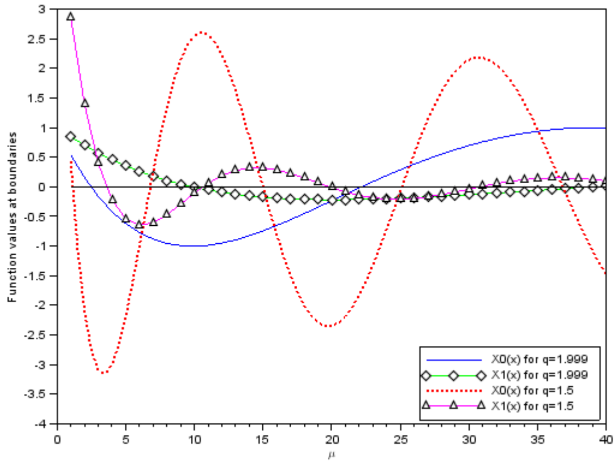


Figure 6.1: μ and the boundary value for $q = 1.999$ and $q = 1.5$

$\sin(L)$ are equal to 0 as $X_0(L) = \cos(L) = 0$ with $\mu = \left(\frac{\pi}{2}\right)^2, \left(\frac{3\pi}{2}\right)^2, \left(\frac{5\pi}{2}\right)^2, \cdots$ for $X_0(x)$ and equal to 0 as $X_1(x) = \sin(x) = 0$ with $\mu = \pi^2, (2\pi)^2, (4\pi)^2, \cdots$. Then, solutions of Figure 6.1 for $q = 1.999$ are almost the same to that of $q = 2$, so the boundary values change smoothly for fractional order q.

Figure 6.1 also indicates that there is an infinite number of solutions also for $q = 1.5$. This means that there are infinitely many μ's which satisfies zero Dirichlet boundary conditions.

Next, the author shows a table about μ_N satisfying zero Dirichlet boundary conditions as $\sum_{k=0}^{N-1} b_{2k} = 0$ and $\sum_{k=0}^{N-1} b_{2k+1} = 0$. By searching μ_N, we find a number of μ_N which satisfies zero Dirichlet boundary conditions. Here, the author names those a number of constants μ_N as $\mu_N^1, \mu_N^2, \mu_N^3, \cdots$ in ascending order, and name a number of constants μ as $\mu^1, \mu^2, \mu^3, \cdots$ in ascending order. In addition to μ_N^k, the author shows the condition number for $N = 2000$. Table

	$N = 500$	$N = 1000$	$N = 2000$	cond
μ_N^1	1.130029051	1.129817357	1.129711482	$2.73D+1$
μ_N^2	6.786741644	6.785470455	6.784834629	$2.98D+1$
μ_N^3	14.98880218	14.98599539	14.98459126	$4.00D+2$
μ_N^4	25.10321624	25.09851688	25.09616549	$7.74D+3$
μ_N^5	36.81942307	36.81253291	36.80908449	$1.64D+5$
μ_N^6	49.94244694	49.93310483	49.92842798	$3.58D+6$
μ_N^7	64.33501130	64.32298259	64.31695923	$7.98D+7$
μ_N^8	79.89371594	79.87878788	79.87130725	$1.80D+9$
μ_N^9	96.53546256	96.51757714	96.50477259	$4.07D+10$
μ_N^{10}	114.2388000	114.2553959	114.2624102	$9.49D+11$

Table 6.1: μ_N^k satisfying zero Dirichlet boundary conditions for $X_{0,N}(x) = 0$ with $q = 1.5$

6.1 represents that the values of μ_N^k converge to constants μ^k by increasing the matrix size N. In the case of $X_{1,N}(x)$, Table 6.2 shows that the values of μ_N^k also converge to constant μ^k by increasing N. However, the condition number for solving a system of equations becomes larger by increasing N. Therefore, it is difficult to calculate more μ_N^k by using the proposed method.

	$N = 500$	$N = 1000$	$N = 2000$	cond
μ_N^1	3.579130385	3.578460938	3.578125862	$2.43D + 1$
μ_N^2	10.62386207	10.62187537	10.62088084	$3.92D + 1$
μ_N^3	19.83130712	19.82759963	19.82574334	$3.71D + 2$
μ_N^4	30.77568662	30.76993499	30.76705459	$5.38D + 3$
μ_N^5	43.21505649	43.20698319	43.20293908	$8.99D + 4$
μ_N^6	56.98739769	56.97675610	56.97142387	$1.62D + 6$
μ_N^7	71.97429293	71.96085834	71.95412424	$3.08D + 7$
μ_N^8	88.08400917	88.06762385	88.05947939	$6.03D + 8$
μ_N^9	105.2520790	105.2219068	105.2324051	$1.21D + 10$
μ_N^{10}	123.5144476	123.5410414	123.5372264	$2.56D + 11$

Table 6.2: μ_N^k satisfying zero Dirichlet boundary conditions for $X_{1,N}(x) = 0$ with $q = 1.5$

6.3.2 Fractional cosine and sine functions and Riesz derivative

By computing appropriate μ_N^k, the author can define fractional sine and cosine. In this paper, the author calls even function $X_{0,N}(x)$ with μ_N^k '$fcos_{k,N}(x)$' and calls odd function $X_{1,N}(x)$ with μ_N^k '$fsin_{k,N}(x)$'. Additionally, under the limitation $N \to \infty$, the values of μ_N^k converge to μ^k, so the author calls even function $X_0(x)$ with μ^k '$fcos_k(x)$' and calls odd function $X_1(x)$ with μ^k '$fsin_k(x)$'.

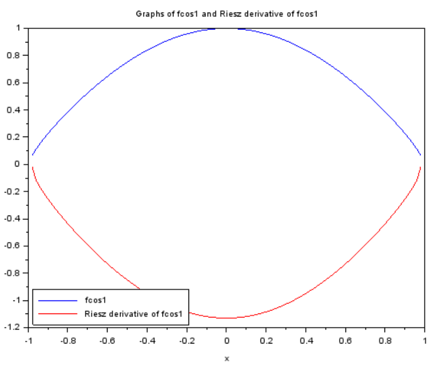


Figure 6.2: $fcos_{1,1000}$ and Riesz derivative of $fcos_{1,1000}$

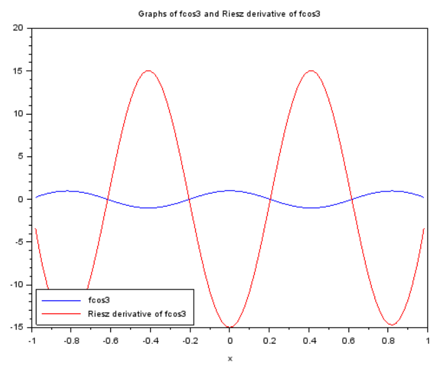


Figure 6.3: $fcos_{3,1000}$ and Riesz derivative of $fcos_{3,1000}$

Figures 6.2, 6.3, 6.4 and 6.5 show the function $fcos_{k,1000}(x)$ and Riesz derivative

$$\frac{1}{2}\left[{}_{-1}^{\mathrm{R}}D_x^q fcos_{k,1000}(x) + {}_{x}^{\mathrm{R}}D_1^q fcos_{k,1000}(x)\right]$$

for $k = 1, 3, 5, 7$. In this section, fractional derivatives in Riesz derivative are calculated with the author's proposed second accuracy formula (4.10) with 500 points. From Eq. (6.2), functions $X(x)$ become $-\mu$ times by q-th order Riesz derivative. In the same way, the function $fcos_{k,1000}(x)$ actually becomes $-\mu_{1000}^k$

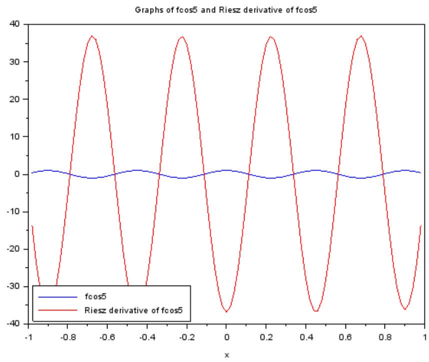


Figure 6.4: $fcos_{5,1000}$ and Riesz derivative of $fcos_{5,1000}$

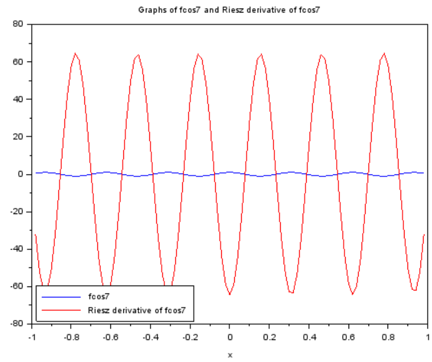


Figure 6.5: $fcos_{7,1000}$ and Riesz derivative of $fcos_{7,1000}$

times by applying Riesz derivative. By incrementing k of μ^k_{1000}, the number of extremum of the function increases, and the number of local maxima in the graph also increases.

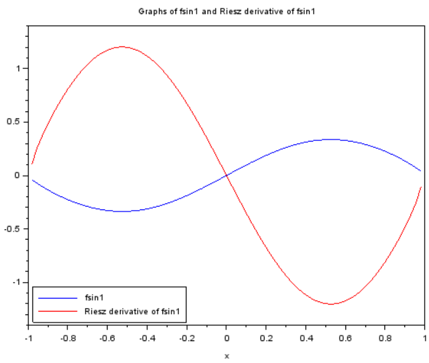


Figure 6.6: $fsin_{1,1000}$ and Riesz derivative of $fsin_{1,1000}$

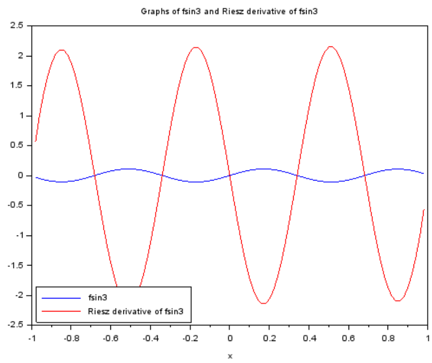


Figure 6.7: $fsin_{3,1000}$ and Riesz derivative of $fsin_{3,1000}$

Figure 6.6, 6.7, 6.8 and 6.9 show the function $fsin_{k,1000}(x)$ and Riesz derivative of the function $fsin_{k,1000}(x)$ for $k = 1, 3, 5, 7$. Functions $fcos_{k,1000}(x)$ also $-\mu^k_{1000}$ times by applying Riesz derivative. In contrast to $fcos_{k,1000}(x)$, the numerical results show functions $fsin_{k,1000}(x)$ are odd functions.

6.3.3 Other properties

First derivative

In this section, the author calculates first derivative of $X_{0,N}(x)$ and $X_{1,N}(x)$. Especially, the author shows the experimental results for $fcos_{1,1000}(x)$ and $fsin_{1,1000}(x)$. The function $fcos_{1,1000}(x)$ is the function $X_{0,1000}(x)$ with μ^1_{1000}, and the function $fsin_{1,1000}(x)$ is the function $X_{1,1000}(x)$ with μ^1_{1000}. The reason why the author uses only $fcos_{1,1000}(x)$ and $fsin_{1,1000}(x)$ is that functions calculated by μ^k_{1000} with larger k have more errors around boundaries as mentioned in the above section. Both $fcos_{1,1000}(x)$ and $fsin_{1,1000}(x)$ are given with the form of polynomials, so

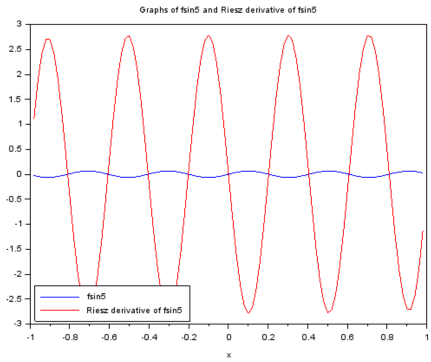


Figure 6.8: $fsin_{5,1000}$ and Riesz derivative of $fsin_{5,1000}$

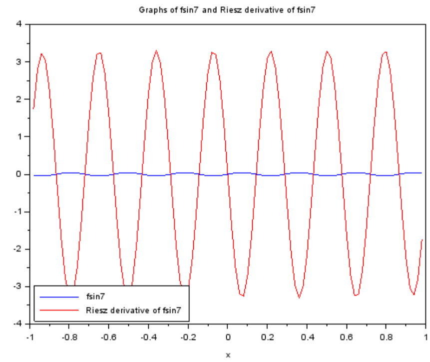


Figure 6.9: $fsin_{7,1000}$ and Riesz derivative of $fsin_{7,1000}$

we can calculate first derivative analytically.
Figure 6.10 shows that first derivatives diverge at boundaries for $fcos_{1,1000}(x)$

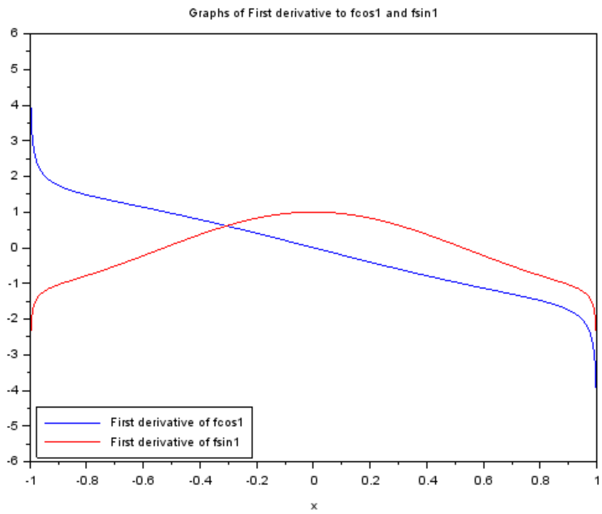


Figure 6.10: Graph of first derivative of $fcos_{1,1000}$ and first derivative of $fsin_{1,1000}$

and $fsin_{1,1000}(x)$. This means that both functions cannot be represented by polynomials at boundaries, and are not differentiable. In addition, this is equivalent to that the analytical solution of homogeneous parabolic fractional differential equations have the form which causes the accuracy decaying. The divergence of first derivative around boundaries indicates the functions have the order $O(x^p)$, $0 < p < 1$ around boundaries. Then, when we solve the equations by using finite difference methods, the accuracy decaying happens and the accuracy order becomes low.

Orthogonality

If we use $fcos_{k,N}$ and $fsin_{k,N}$ for series expansion like cosine and sine functions, $fcos_{k,N}$ and $fsin_{k,N}$ should have the orthogonality. In addition, Riesz derivative is the summation of right and left derivative and seems to be the adjoint operator. Therefore, those functions are estimated to be orthogonal. In this section, the author shows the orthogonality by calculating the following inner product by using trapezoidal rule with 1000 points,

$$\int_{-L}^{L} f(x)g(x)dx.$$

Because functions $fcos_{k,N}$ are even functions and functions $fsin_{k,N}$ are odd functions, the multiple of $fcos_{m,N}(x)$ and $fsin_{m,N}(x)$ is odd function and the inner product is always 0. Therefore, the author numerically calculates the inner product of $fcos_{m,1000}(x)fcos_{n,1000}(x)$ and $fsin_{m,1000}(x)fsin_{n,1000}(x)$.

Table 6.3 shows the value of inner product for $fcos_{m,1000}(x)$ and $fcos_{n,1000}(x)$.

	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$
$n=1$	1.079D+0	3.883D-7	-5.586D-7	7.029D-7	-8.387D-7
$n=2$	3.883D-7	9.866D-1	1.272D-6	-1.614D-6	1.935D-6
$n=3$	-5.586D-7	1.272D-6	1.004D+0	2.388D-6	-2.872D-6
$n=4$	7.029D-7	-1.614D-6	2.388D-6	9.977D-1	3.678D-6
$n=5$	-8.387D-7	1.935D-6	-2.872D-6	3.678D-6	1.001D+0

Table 6.3: Inner product of $fcos_{m,1000}(x)$ and $fcos_{n,1000}(x)$

For $m \neq n$, the values of inner product are small and near to 0. For $m = n$, the values of inner product are almost 1. Therefore, the results indicate that functions $fcos_{k,1000}(x)$ have orthogonality and are normalized. From Tab. 6.4,

	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$
$n=1$	1.170D-1	4.491D-8	-3.959D-8	3.620D-8	-3.382D-8
$n=2$	4.491D-8	2.692D-2	3.213D-8	-2.950D-8	2.765D-8
$n=3$	-3.959D-8	3.213D-8	1.175D-2	2.637D-8	-2.476D-8
$n=4$	3.620D-8	-2.950D-8	2.637D-8	6.531D-3	2.287D-8
$n=5$	-3.382D-8	2.765D-8	-2.476D-8	2.287D-8	4.155D-3

Table 6.4: Inner product of $fsin_{m,1000}(x)$ and $fsin_{n,1000}(x)$

we can estimate that functions $fsin_{k,1000}(x)$ also have orthogonality, but are not normalized.

6.3.4 Series expansion and solutions of fractional diffusion equation

To solve diffusion equations, we have to expand a function, which is defined by an initial condition, by using orthogonal functions. In the above section, the author shows the orthogonality of $fcos_k(x)$ and $fsin_k(x)$. Therefore, let us make series expansion by using $fcos_{k,1000}(x)$ and numerically solve a homogeneous parabolic fractional differential equation in this section. Firstly, let us expand the following function step function

$$f(x) = \begin{cases} 1 & -0.5 < x < 0.5 \\ 0 & x \leq -0.5, 0.5 \leq x \end{cases}$$

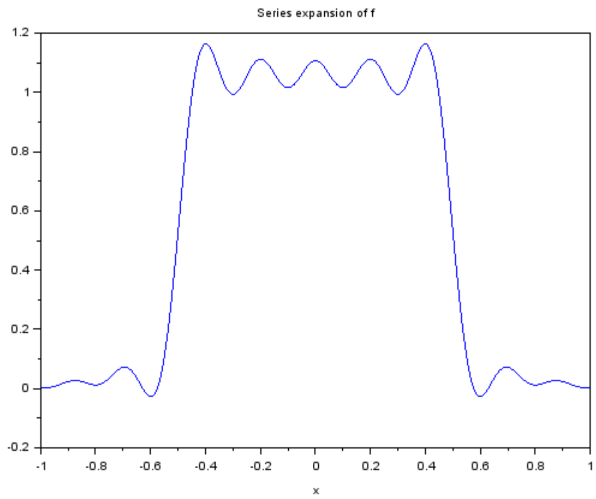


Figure 6.11: Graph of series expansion of a step function by using $fcos_{k,1000}(x)$, $1 \leq k \leq 10$

by using functions of $fcos_{1,1000}, fcos_{2,1000}, \cdots, fcos_{10,1000}$. This step function is expanded as

$$f(x) \simeq \sum_{k=1}^{10} C_k fcos_{k,1000}(x)$$
$$C_k = \int_{-1}^{1} f(x) fcos_k(x) dx.$$

The integrals in the above expression are computed by using trapezoidal rule with 1000 points. Figure 6.11 is the result of series expansion of the step function. Because of orthogonality, the step function can be expanded just like we expand with trigonometric functions.

Next, we solve a fractional diffusion equation with the initial condition $P(x, 0) = 1 - x^2$ and the boundary conditions $P(-1, t) = P(1, t) = 0$. Because the initial condition function is the even function, the function $P(x, 0)$ is expanded only with even functions $fcos_{k,1000}(x)$. Then, the solution is calculated by

$$P(x,t) \simeq \sum_{k=1}^{10} C_k \exp(-\mu_k t) fcos_{k,1000}(x)$$
$$C_k = \int_{-1}^{1} P(x, 0) fcos_{k,1000}(x) dx.$$

The integrals in the above expression are also computed by using trapezoidal rule with 1000 points. Figure 6.12 and 6.13 show the numerical result until $t = 1$. By using the proposed method, we can actually compute numerical solutions for this problem.

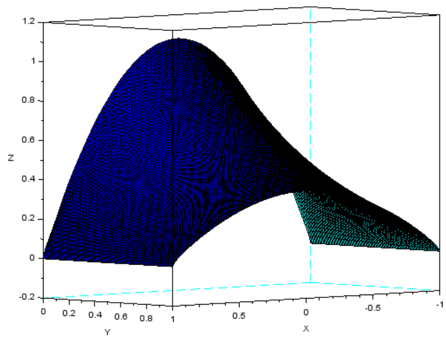


Figure 6.12: Numerical result to the function $P(x,t)$

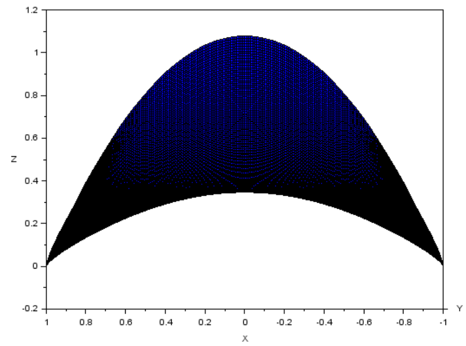


Figure 6.13: Numerical result to the function $P(x,t)$

Chapter 7

Fractional ordinary differential equations

7.1 Difference between Caputo type and Riemann-Liouville type fractional ordinary differential equations

Fractional ordinary differential equations are used in many fields, for example, control system, simulation of viscosity models and so on. This thesis treats the following fractional ordinary differential equations with Caputo definition

$$ {}^{\mathrm{C}}_{t_0}D_t^q y(t) = f(t, y) $$

where the fractional calculus order q is $0 < q < 1$ and t_0 denotes an initial point. The function f is a known function, and the function y is an unknown function. In contrast, Riemann-Lioville type fractional ordinary differential equations are defined by

$$ {}^{\mathrm{R}}_{t_0}D_t^q y(t) = f(t, y). $$

Then, from a reason, we motivated to solve not Riemann type fractional ordinary differential equations, but Caputo type. The reason is that the applications must assume fractional derivative as initial conditions when we choose Caputo type equations. This reason is also pointed out in a related work[13]. However, it is not shown why Caputo type equations require fractional derivatives as initial conditions in mathematical expressions. Therefore, the author firstly shows we have to impose initial conditions of fractional derivatives on Riemann-Liouville type equations. For $m-1 < q < m$ and $m = \lceil q \rceil$, the Riemann-Liouville type fractional ordinary differential equations are given by

$$ {}^{\mathrm{R}}_{t_0}D_t^q y(t) = f(t, y). $$

Integrating both side, we have

$$ {}^{\mathrm{R}}_{t_0}D_t^{q-1} y(t) - {}^{\mathrm{R}}_{t_0}D_t^{q-1} y(t_0) = {}_{t_0}D_t^{-1} f(t, y). $$

Repeating the integration, we have

$$ {}^{\mathrm{R}}_{t_0}D_t^{q-m+1} y(t) = \sum_{k=1}^{m-1} \frac{{}^{\mathrm{R}}_{t_0}D_t^{q-k} y(t_0)}{\Gamma(m-k)} (t - t_0)^{m-1-k} + {}_{t_0}D_t^{-m+1} f(t, y). $$

Applying fractional integral to both side, we obtain

$$ {}_{t_0}D_t^{-q+m-1} \left[\frac{d}{dt}\right] {}^{\mathrm{R}}_{t_0}D_t^{q-m} y(t) = \sum_{k=1}^{m-1} \frac{{}^{\mathrm{R}}_{t_0}D_t^{q-k} y(t_0)}{\Gamma(q-k+1)} (t - t_0)^{q-k} + {}_{t_0}D_t^{-q} f(t, y). $$

Here, let $Y(t)$ be defined by $Y(t) = {}^{\mathrm{R}}_{t_0}D_t^{q-m}y(t)$, and applying the exchange rule, we have

$$\begin{aligned}
& {}_{t_0}D_t^{-q+m-1}\left[\frac{d}{dt}\right]Y(t) \\
= & \left[\frac{d}{dt}\right]{}_{t_0}D_t^{-q+m-1}y(t) - \frac{Y(t_0)}{\Gamma(q-m+1)}(t-t_0)^{q-m} \\
= & \left[\frac{d}{dt}\right]{}_{t_0}D_t^{-1}Y(t) - \frac{Y(t_0)}{\Gamma(q-m+1)}(t-t_0)^{q-m} \\
= & \; y(t) - \frac{{}^{\mathrm{R}}_{t_0}D_t^{q-m}y(t_0)}{\Gamma(q-m+1)}(t-t_0)^{q-m}.
\end{aligned}$$

Therefore, we obtain the solution for Riemann-Liouville type fractional ordinary differential equations

$$y(t) = \sum_{k=1}^{m} \frac{{}^{\mathrm{R}}_{t_0}D_t^{q-m}y(t_0)}{\Gamma(q-m+1)}(t-t_0)^{q-m} + {}_{t_0}D_t^{-q}f(t,y).$$

This solution contains fractional derivative terms as ${}^{\mathrm{R}}_{t_0}D_t^{q-m}y(t_0)$. However, the physical meaning of fractional derivatives are not trivial, and in most cases there is not any measurement method for fractional derivative. Hence, many applications employ Caputo type fractional ordinary differential equations, and this thesis also treats them. Next, the author shows the solution for Caputo type fractional ordinary differential equations with $m-1 < q < m$ and $m = \lceil q \rceil$. Applying fractional integral to both side, we have

$$\begin{aligned}
& {}_{t_0}D_t^{-q}\,{}^{\mathrm{C}}_{t_0}D_t^{q}y(t) = {}_{t_0}D_t^{-q}f(t,y) \\
\Rightarrow \; & {}_{t_0}D_t^{-m}y^{(m)}(t)dt = {}_{t_0}D_t^{-q}f(t,y) \\
\Rightarrow \; & {}_{t_0}D_t^{-m+1}\left[y^{(m-1)}(t) - y^{(m-1)}(t_0)\right] = {}_{t_0}D_t^{-q}f(t,y)
\end{aligned}$$

Then, it holds

$$y(t) = \sum_{k=0}^{m-1} \frac{y^{(k)}(t_0)}{k!}(t-t_0)^k + \frac{1}{\Gamma(q)}\int_{t_0}^{t} \frac{f(u,y)}{(t-u)^{1-q}}du. \tag{7.1}$$

This solution actually does not include fractional derivatives as initial conditions but integer order derivatives. From this property, Caputo type fractional ordinary differential equations are preferred. The solution is developed, but the problem is how to compute the integral in Eq. (7.1). In the next section, the author introduces the two numerical computational method for fractional ordinary differential equations. They have a different method to compute the integral in Eq. (7.1). Depending on the way of approximation of the integral, the accuracy and the stability change.

7.2 The author's proposed explicit numerical computational method for fractional ordinary differential equations

7.2.1 Existing methods and the author's proposed methods

In the above section, the solutions for Caputo type fractional differential equations are developed. This section introduces the numerical computational methods for the solution. Let t_n be a grid point about time, and t_0 is the initial point.

Let y_n be a numerical solution of $y(t_n)$, and let y_0 be an initial condition as $y_0 = y(t_0)$. In addition, let h be a step size, and we put $t_n = t_0 + nh$. As a existing method, the predictor-corrector method has been proposed by K. Diethelm, N.J. Ford, A.D. Freed[13]. For $0 < q < 1$, this method is given by

$$\begin{aligned} & y_n \\ = \quad & y_0 + \frac{h^q}{\Gamma(2+q)} f(t_n, y_n^P) + \frac{h^q}{\Gamma(q+2)} \sum_{j=0}^{n-1} a_{j,n} f(t_j, y_j) \end{aligned}$$

where the coefficients $a_{j,n}$ are defined by

$$a_{j,n} = \begin{cases} (n-1)^{q+1} - (n-1-q)n^q, & j = 0 \\ (n-j+1)^{q+1} - 2(n-j)^{q+1} + (n-j-1)^{q+1}, & 1 \le j \le n-1 \\ 1, & j = n \end{cases}$$

and the predictor term y_n^P is defined by

$$y_n^P = y_0 + \frac{h^q}{\Gamma(1+q)} \sum_{j=0}^{n-1} \{(n-j)^q - (n-1-j)^q\} f(t_j, y_j).$$

This scheme can be represented by changing the order of summations as

$$\begin{aligned} & y_n \\ = \quad & y_0 + \frac{h^q}{\Gamma(2+q)} \left[f(t_n, y_n^P) + q f(t_{n-1}, y_{n-1}) \right] \\ & + \frac{h^q}{\Gamma(2+q)} \sum_{j=1}^{n-1} \left[f(t_{n-j}, y_{n-j}) \left\{ -(1+q) j^q + (j+1)^{1+q} - j^{1+q} \right\} \right. \\ & \left. - f(t_{n-1-j}, y_{n-1-j}) \left\{ -(1+q)(j+1)^q + (j+1)^{1+q} - j^{1+q} \right\} \right] \end{aligned}$$

where y_n^P is defined by

$$y_n^P = y_0 + \frac{h^q}{\Gamma(1+q)} \sum_{j=0}^{n-1} f(t_{n-1-j}, y_{n-1-j}) \{(j+1)^q - j^q\}.$$

Therefore, it is shown that predictor-corrector method consists of the combination of the second accuracy formula (4.12) and the first order accuracy formula (4.11). If ${}^{\mathrm{C}}_{t_0}D^q_t y(t) \in C^2[t_0, T]$ then, the accuracy of the predictor-corrector method is given by

$$\max_{0 \le j \le n} |y(t_j) - y_j| = O(h^{1+q}).$$

The author's proposed method also employ the predictor-corrector method, but uses the third order accuracy formula (4.13). The author's proposed method is given for $n \geq 2$ by

$$
\begin{aligned}
& y_n \\
= \; & y_0 + \frac{h^q}{\Gamma(q)} \left[A_0 f(t_n, y_n^P) + B_0 \left\{ \frac{3}{2} f(t_n, y_n^P) - 2f(t_{n-1}, y_{n-1}) + \frac{1}{2} f(t_{n-2}, y_{n-2}) \right\} \right. \\
& \quad \left. + C_0 \left\{ f(t_n, y_n^P) - 2f(t_{n-1}, y_{n-1}) + f(t_{n-2}, y_{n-2}) \right\} \right] \\
& + \frac{h^q}{\Gamma(q)} \sum_{j=1}^{n-2} [A_j f(t_{n-j}, y_{n-j}) \\
& \quad + B_j \left\{ \frac{3}{2} f(t_{n-j}, y_{n-j}) - 2f(t_{n-j-1}, y_{n-j-1}) + \frac{1}{2} f(t_{n-j-2}, y_{n-j-2}) \right\} \\
& \quad + C_j \{ f(t_{n-j}, y_{n-j}) - 2f(t_{n-j-1}, y_{n-j-1}) + f(t_{n-j-2}, y_{n-j-2}) \}] \\
& + \frac{h^q}{\Gamma(q)} [A_{n-1} f(t_1, y_1) \\
& \quad + B_{n-1} \left\{ 3f(t_1, y_1) - 4f(t_{1/2}, y_{1/2}) + f(t_0, y_0) \right\} \\
& \quad + C_{n-1} \left\{ 2f(t_1, y_1) - 4f(t_{1/2}, y_{1/2}) + 2f(t_0, y_0) \right\}] .
\end{aligned}
\tag{7.2}
$$

The coefficients A_j, B_j, C_j are defined by

$$
\begin{aligned}
A_j &= \frac{(j+1)^q}{q} - \frac{j^q}{q} \\
B_j &= -\frac{(j+1)^q}{q} + \frac{(j+1)^{q+1}}{q(q+1)} - \frac{j^{q+1}}{q(q+1)} \\
C_j &= \frac{(j+1)^q}{2q} - \frac{(j+1)^{q+1}}{q(q+1)} + \frac{(j+1)^{q+2}}{q(q+1)(q+2)} - \frac{j^{q+2}}{q(q+1)(q+2)}.
\end{aligned}
$$

The predictor term y_n^P is given by

$$
\begin{aligned}
& y_n^P \\
= \; & y_0 + \frac{h^q}{\Gamma(q)} [A_0 f(t_{n-1}, y_{n-1}) \\
& \quad + (A_0 + B_0) \{ 3f(t_{n-1}, y_{n-1}) - 4f(t_{n-2}, y_{n-2}) + f(t_{n-3}, y_{n-3}) \} \\
& \quad \left. + \left(\frac{A_0}{2} + B_0 + C_0 \right) \{ 2f(t_{n-1}, y_{n-1}) - 4f(t_{n-2}, y_{n-2}) + 2f(t_{n-3}, y_{n-3}) \} \right] \\
& + \frac{h^q}{\Gamma(q)} \sum_{j=1}^{n-2} [A_j f(t_{n-j}, y_{n-j}) \\
& \quad + B_j \left\{ \frac{3}{2} f(t_{n-j}, y_{n-j}) - 2f(t_{n-j-1}, y_{n-j-1}) + \frac{1}{2} f(t_{n-j-2}, y_{n-j-2}) \right\} \\
& \quad + C_j \{ f(t_{n-j}, y_{n-j}) - 2f(t_{n-j-1}, y_{n-j-1}) + f(t_{n-j-2}, y_{n-j-2}) \}] \\
& + \frac{h^q}{\Gamma(q)} [A_{n-1} f(t_1, y_1) \\
& \quad + B_{n-1} \left\{ 3f(t_1, y_1) - 4f(t_{1/2}, y_{1/2}) + f(t_0, y_0) \right\} \\
& \quad + C_{n-1} \left\{ 2f(t_1, y_1) - 4f(t_{1/2}, y_{1/2}) + 2f(t_0, y_0) \right\}] .
\end{aligned}
\tag{7.3}
$$

This method requires the computation for the values of $y_{1/2} \simeq y(t_0 + h/2)$ and y_1 as the preparation. Their values are computed by a different method. The numerical solution y_1 is computed by

$$\begin{aligned} & y_1 \\ = \; & y_0 + \frac{h^q}{\Gamma(1+q)} \left\{ \frac{q}{2(1+q)} f(t_0, y_0) \right. \\ & \left. + \frac{2+q}{2(1+q)} f\left(t_0 + \frac{2}{2+q} h, y_0 + \frac{2}{2+q} y_0^1 + \frac{2}{(2+q)^2} y_0^2 \right) \right\}. \end{aligned} \tag{7.4}$$

The numerical solution $y_{1/2}$ is computed by

$$\begin{aligned} & y_{1/2} \\ = \; & y_0 + \left(\frac{h}{2}\right)^q \frac{1}{\Gamma(1+q)} \left\{ \frac{q}{2(1+q)} f(t_0, y_0) \right. \\ & \left. + \frac{2+q}{2(1+q)} f\left(t_0 + \frac{1}{2+q} h, y_0 + \frac{2}{2+q} y_{1/2}^1 + \frac{2}{(2+q)^2} y_{1/2}^2 \right) \right\}. \end{aligned}$$

The values of y_1^1, $y_{1/2}^1$ are computed by

$$\begin{aligned} & y_1^1 \\ = \; & \frac{18 \cdot 12^q - 64 \cdot 8^q + 45 \cdot 6^q + 3 \cdot 4^q - 36 \cdot 3^q + 7 \cdot 2^q}{3 \cdot (2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_0 \\ & + \frac{-8 \cdot 2^q (6^q - 3 \cdot 4^q + 2 \cdot 3^q)}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{1/4} + \frac{2(12^q - 9 \cdot 4^q + 8 \cdot 3^q)}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{2/4} \\ & - \frac{8 \cdot 2^q (2^q - 2)(2^q - 1)}{3 \cdot (2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{3/4} \\ & + \frac{3 \cdot 2^q - 4 \cdot 3^q + 6^q}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{4/4} \end{aligned} \tag{7.5}$$

$$\begin{aligned} & y_{1/2}^1 \\ = \; & \frac{18 \cdot 12^q - 64 \cdot 8^q + 45 \cdot 6^q + 3 \cdot 4^q - 36 \cdot 3^q + 7 \cdot 2^q}{3 \cdot (2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_0 \\ & + \frac{-8 \cdot 2^q (6^q - 3 \cdot 4^q + 2 \cdot 3^q)}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{1/8} + \frac{2(12^q - 9 \cdot 4^q + 8 \cdot 3^q)}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{2/8} \\ & - \frac{8 \cdot 2^q (2^q - 2)(2^q - 1)}{3 \cdot (2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{3/8} \\ & + \frac{3 \cdot 2^q - 4 \cdot 3^q + 6^q}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{4/8} \end{aligned} \tag{7.6}$$

where K_x is defined as

$$K_x = y_0 + (xh)^q f(t_0, y_0)/\Gamma(1+q).$$

In a similar way, the values of y_1^2, $y_{1/2}^2$ are computed by

$$\begin{aligned} & y_1^2 \\ = \; & \frac{24 \cdot 12^q - 64 \cdot 8^q + 36 \cdot 6^q + 24 \cdot 4^q - 24 \cdot 3^q + 4 \cdot 2^q}{3 \cdot (2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_0 \\ & + \frac{-16 \cdot (12^q - 2 \cdot 8^q + 6^q)}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{1/4} + \frac{8(12^q - 3 \cdot 4^q + 2 \cdot 3^q)}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{2/4} \\ & - \frac{16 \cdot 2^q (2 \cdot 2^q - 1)(2^q - 1)}{3 \cdot (2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{3/4} \\ & + \frac{4 \cdot 2^q - 8 \cdot 3^q + 4 \cdot 6^q}{(2^q - 1)(2^q - 4 \cdot 3^q + 4 \cdot 4^q - 6^q)} K_{4/4} \end{aligned} \tag{7.7}$$

and

$$
\begin{aligned}
& y_{1/2}^2 \\
= & \frac{24\cdot 12^q - 64\cdot 8^q + 36\cdot 6^q + 24\cdot 4^q - 24\cdot 3^q + 4\cdot 2^q}{3\cdot(2^q-1)(2^q-4\cdot 3^q+4\cdot 4^q-6^q)}K_0 \\
& + \frac{-16\cdot(12^q - 2\cdot 8^q + 6^q)}{(2^q-1)(2^q-4\cdot 3^q+4\cdot 4^q-6^q)}K_{1/8} + \frac{8(12^q - 3\cdot 4^q + 2\cdot 3^q)}{(2^q-1)(2^q-4\cdot 3^q+4\cdot 4^q-6^q)}K_{2/8} \\
& - \frac{16\cdot 2^q(2\cdot 2^q-1)(2^q-1)}{3\cdot(2^q-1)(2^q-4\cdot 3^q+4\cdot 4^q-6^q)}K_{3/8} \\
& + \frac{4\cdot 2^q - 8\cdot 3^q + 4\cdot 6^q}{(2^q-1)(2^q-4\cdot 3^q+4\cdot 4^q-6^q)}K_{4/8}. \qquad (7.8)
\end{aligned}
$$

7.2.2 Derivation of the accuracy order

The author's proposed method is based on the third order accuracy formula (4.13) and (4.7). The formula (4.7) is given by using coefficients A_j, B_j, C_j as

$$
\begin{aligned}
& {}_{t_0}D_t^{-q} f(t,y) \\
= & \frac{h^q}{\Gamma(q)} \sum_{j=0}^{N-1} \big[f(t-jh, y(t-jh))A_j + hf'(t-jh, y(t-jh))B_j \\
& + h^2 f''(t-jh, y(t-jh))C_j \big] + O\left(\frac{1}{N^3}\right)
\end{aligned}
$$

where $q > 0$. The author's proposed method approximate the integral in Eq. (7.1) by using this formula (4.7). Eqs (7.2) and (7.3) are obtained by applying Taylor expansion to f, f', f'' by seeing them as one variable function about t, and have third order accuracy. Then, the author shows how to develop y_1. The value of y_1 is computed like Runge-Kutta method in Eq. (7.4). For y_1, the analytical solution (7.1) is given by

$$
\begin{aligned}
& y(t_1) - y_0 \\
= & \frac{1}{\Gamma(q)} \int_{t_0}^{t_1} \frac{f(u, y(u))}{(t_1-u)^{1-q}} du.
\end{aligned}
$$

Here, let us consider to expand this integral like the derivation of Runge-Kutta method. Applying Taylor expansion to f around t_0 and y_0, we have

$$
\begin{aligned}
= & \frac{1}{\Gamma(q)} \int_{t_0}^{t_1} (t_1-u)^{q-1} \bigg\{ f(t_0, y_0) + (u-t_0)\frac{\partial f}{\partial t} + (y(u)-y_0)\frac{\partial f}{\partial y} \\
& + \frac{(u-t_0)^2}{2}\frac{\partial^2 f}{\partial t^2} + (u-t_0)(y(u)-y_0)\frac{\partial^2 f}{\partial t \partial y} + \frac{(y(u)-y_0)^2}{2}\frac{\partial^2 f}{\partial y^2} + \dots \bigg\} du
\end{aligned}
$$

Here, $y(u) - y_0$ can be approximated by Taylor expansion as

$$
y(u) - y_0 = (u-t_0)y'(t_0) + \frac{(u-t_0)^2}{2}y''(t_0) + \dots.
$$

By substituting the above expression, we have

$$
\begin{aligned}
& y(t_1) - y_0 \\
= \quad & \frac{1}{\Gamma(q)} \int_{t_0}^{t_1} (t_1 - u)^{q-1} \left\{ f(t_0, y_0) + (u - t_0) \frac{\partial f}{\partial t} \right. \\
& + \left((u - t_0) y'(t_0) + \frac{(u - t_0)^2}{2} y''(t_0) \right) \frac{\partial f}{\partial y} + \frac{(u - t_0)^2}{2} \frac{\partial^2 f}{\partial t^2} \\
& \left. + (u - t_0)((u - t_0) y'(t_0)) \frac{\partial^2 f}{\partial t \partial y} + \frac{(u - t_0) y'(t_0)}{2} \frac{\partial^2 f}{\partial y^2} + \ldots \right\} du \\
= \quad & \frac{1}{\Gamma(q)} \left[\frac{h^q}{q} f(t_0, y_0) + \frac{h^{1+q}}{q(1+q)} \frac{\partial f}{\partial t} + \frac{h^{1+q}}{q(1+q)} y'(t_0) \frac{\partial f}{\partial y} \right. \\
& + \frac{h^{2+q}}{q(1+q)(2+q)} y''(t_0) \frac{\partial f}{\partial y} + \frac{h^{2+q}}{q(1+q)(2+q)} \frac{\partial^2 f}{\partial t^2} \\
& \left. + \frac{2h^{2+q}}{q(1+q)(2+q)} y'(t_0) \frac{\partial^2 f}{\partial t \partial y} + \frac{h^{2+q}}{q(1+q)(2+q)} (y'(t_0))^2 \frac{\partial^2 f}{\partial y^2} \right] \\
& + O(h^{3+q})
\end{aligned} \tag{7.9}
$$

Here, by folding the above expression with Taylor expansion, we have

$$
\begin{aligned}
& y_1 \\
= \quad & y_0 + \frac{h^q}{\Gamma(1+q)} \left\{ \frac{q}{2(1+q)} f(t_0, y_0) \right. \\
& \left. + \frac{2+q}{2(1+q)} f\left(t_0 + \frac{2}{2+q} h, y_0 + \frac{2}{2+q} y'(t_0) h + \frac{2}{(2+q)^2} y''(t_0) h^2 \right) \right\} \\
& + O(h^{3+q}).
\end{aligned}
$$

Expression (7.9) is a series expansion of the integral in Eq. (7.1) for $n = 1$. If we can expand the integral for $n = 2, 3, 4, \ldots$, we may construct a similar method to Runge-Kutta method. However, it is difficult because of two reasons. One reason is fractional derivatives require the past information. In integer order calculus, differentiations are the local phenomena, and the next node is calculated only with the present node. Yet, fractional differentiations have a interval like integrals, and by only the present node, we cannot compute the next node. Therefore, numerical methods for fractional ordinary differential equations are more similar to the computation of integral than Runge-Kutta method. Second reason is that the difference of Taylor expansion. The above expression contains the first order derivative and the second order derivative of y, and those values are computed by using an initial condition and total differentiation of f. For example, for first degree ordinary differential equations, $y'(t_0)$ is given as a part of equation to solve. However, in fractional ordinary differential equations, $y'(t_0)$ is not a part of given equation, and it is not easy to calculate $y'(t_0)$. From the expression (7.9), the values of $y'(t_0)$ and $y''(t_0)$ must be numerically computed with second order and first order accuracy respectively. Let us consider that the value of $y'(t_0)$ is numerically computed by using a difference method as

$$
y'(t_0) = \frac{a_0 y(t_0) + a_1 y\left(t_0 + \frac{h}{4}\right) + a_2 y\left(t_0 + \frac{2h}{4}\right) + a_3 y\left(t_0 + \frac{3h}{4}\right) + a_4 y(t_1)}{h}.
$$

If we know the exact values of $y(t_0 + mh/4)$, $m = 1, 2, 3, 4$, $y'(t_0)$ can be computed with the second accuracy for $a_0 = -3, a_1 = 0, a_2 = 4, a_3 = 0, a_4 = -1$. However, we do not know even the exact values of $y(t_0 + mh/4)$. Therefore, we have to compute $y(t_0+kh/4)$ with at least third order accuracy. Then, firstly, let consider to approximate the values of $y(t_0+mh/4)$ with the accuracy order $O(h^{3+q})$. Let $K_{m/4}$ be defined as

$$K_{m/4} = y_0 + \frac{1}{\Gamma(1+q)}\left(\frac{kh}{4}\right)^q f(t_0, y_0).$$

This approximation is given by taking only first term of the expression (7.9), and the accuracy is $O(h^{1+q})$. The value K_x can be calculated only from t_0 and y_0. In addition, the value of $y(t_0+xh)$ is given by using the expression (7.9) as

$$\begin{aligned} & y(t_0+xh) \\ = \;& K_x + \frac{1}{\Gamma(q)}\left[\frac{(xh)^{1+q}}{q(1+q)}\frac{\partial f}{\partial t} + \frac{(xh)^{1+q}}{q(1+q)}y'(t_0)\frac{\partial f}{\partial y} + \frac{(xh)^{2+q}}{q(1+q)(2+q)}y''(t_0)\frac{\partial f}{\partial y}\right. \\ & \left. + \frac{(xh)^{2+q}}{q(1+q)(2+q)}\frac{\partial^2 f}{\partial t^2} + \frac{2(xh)^{2+q}}{q(1+q)(2+q)}y'(t_0)\frac{\partial^2 f}{\partial t \partial y} + \frac{(xh)^{2+q}}{q(1+q)(2+q)}(y'(t_0))^2\frac{\partial^2 f}{\partial y^2}\right] \\ & + O(h^{3+q}). \end{aligned}$$

By transformation, we have

$$\begin{aligned} & K_x \\ \simeq \;& y(t_0+xh) - \frac{1}{\Gamma(q)}\left[\frac{(xh)^{1+q}}{q(1+q)}\frac{\partial f}{\partial t} + \frac{(xh)^{1+q}}{q(1+q)}y'(t_0)\frac{\partial f}{\partial y}\right. \\ & + \frac{(xh)^{2+q}}{q(1+q)(2+q)}y''(t_0)\frac{\partial f}{\partial y} + \frac{(xh)^{2+q}}{q(1+q)(2+q)}\frac{\partial^2 f}{\partial t^2} \\ & \left. + \frac{2(xh)^{2+q}}{q(1+q)(2+q)}y'(t_0)\frac{\partial^2 f}{\partial t \partial y} + \frac{(xh)^{2+q}}{q(1+q)(2+q)}(y'(t_0))^2\frac{\partial^2 f}{\partial y^2}\right] \end{aligned} \tag{7.10}$$

Therefore, by combination of K_x such that we eliminate the terms except $y(t_0+xh)$, we obtain $y'(t_0)$ with high accuracy. That is, we approximate $y'(t_0)$ by the following expression

$$y'(t_0) = \frac{a_0K_0 + a_1K_{1/4} + a_2K_{2/4} + a_3K_{3/4} + a_4K_{4/4}}{h} + O(h^{3+q}).$$

Then, the coefficients a_m can be computed from the following system of equations

$$\begin{aligned} a_0 + a_1 + a_2 + a_3 + a_4 &= 0 \\ a_1 + 2a_2 + 3a_3 + 4a_4 &= 4 \\ a_1 + 4a_2 + 9a_3 + 16a_4 &= 0 \\ a_1 + 2^{1+q}a_2 + 3^{1+q}a_3 + 4^{1+q}a_4 &= 0 \\ a_1 + 2^{2+q}a_2 + 3^{2+q}a_3 + 4^{2+q}a_4 &= 0. \end{aligned}$$

First two equations are for difference method to compute $y'(t_0)$, and last three equations are for eliminating terms except $y(t_0+xh)$ in the expression (7.10). By solving this system of equations, we have the expression (7.5) as the approximation of $y'(t_0)$. In a similar way, the value of $y''(t_0)$ is numerically computed as

$$y''(t_0) = \frac{b_0K_0 + b_1K_{1/4} + b_2K_{2/4} + b_3K_{3/4} + b_4K_{4/4}}{h} + O(h^{3+q}).$$

The coefficients b_m can be computed from the following system of equations

$$\begin{aligned} b_0 + b_1 + b_2 + a_3 + b_4 &= 0 \\ b_1 + 2b_2 + 3b_3 + 4b_4 &= 0 \\ b_1 + 4b_2 + 9b_3 + 16b_4 &= 16 \\ b_1 + 2^{1+q}b_2 + 3^{1+q}b_3 + 4^{1+q}b_4 &= 0 \\ b_1 + 2^{2+q}b_2 + 3^{2+q}b_3 + 4^{2+q}b_4 &= 0. \end{aligned}$$

By solving this system of equations, we have the expression (7.7). The expressions (7.6) and (7.8) are obtained by approximating $y'(t_0)$ and $y''(t_0)$ by using $K_0, K_{1/8}, K_{2/8}, K_{3,8}, K_{4/8}$. Therefore, it is shown that the author's proposed method has third order accuracy, and the accuracy of this the author's proposed method is given by the following theorem.

Theorem 7.2.1 *If* ${}_{t_0}^{\mathrm{C}}D_t^q y(t) \in C^2[t_0, T]$ *then, the accuracy of the proposed method is*

$$|y(T) - y_N| = O(h^3)$$

for $N \to \infty$, $h = T/N$.

7.2.3 Stability of existing method and the author's proposed method

In the previous section, the author proposed third order accuracy numerical method. The accuracy of this method is higher than that of the existing method. However, the stability is another significant factor when equations are numerically solved. If a method is unstable, its numerical solutions diverge also in ordinary differential equations. However, experimental results in Section 7.4 show that the existing method and the author's proposed method are stable. Therefore, the author tries to prove the stability of the existing method and the author's proposed method in this section. The stability of numerical methods for ordinary differential equations are analyzed by substituting a test function to numerical schemes. This stability analysis method is similar to Von Neumann stability analysis, and uses the following function as a test function in integer order differential equations

$$y'(t) = -ky(t), \;\; k > 0.$$

The solution of this equation is $y(t) = y_0 \exp(-kt)$. Existing method and the author's proposed method are similar to linear multi-step method. Therefore, let us consider the stability analysis of linear multi-step method as an example. By applying integral to both side of a first order ordinary differential equation, a multi-step method is given

$$\begin{aligned} \int_{t_{n-1}}^{t_{n+1}} y'(t)dt &= \int_{t_{n-1}}^{t_{n+1}} f(t, y)dt \\ \Rightarrow \;\; y_{n+1} - y_{n-1} &= 2hf(t_n, y_n) \end{aligned}$$

where the integral about f is approximated by using mid-point rule. Then, by substituting a test function, we have

$$y_{n+1} - y_{n-1} = -2khy_n.$$

The characteristic equation of the above equation is given by

$$\lambda^2 + 2kh\lambda - 1 = 0$$

Let λ_m be the m-th root of the above equation. Then, the condition that linear multi-step methods are stable is: all roots λ_m satisfy $|\lambda_m| \leq 1$. The above characteristic equation has a solution which is less than -1. Therefore, this linear multi-step method is unstable. If a linear multi-step method is stable, there exists a stability region. This region is defined by the area which the numerical solutions do not diverge. Numerical methods are compared with the stability region, and generally higher order accuracy methods have narrower stability region in linear multi-step methods.

Next, let us analyze the stability of existing method and the author's proposed method. For predictor-corrector method, it is sufficient to analyze only predictor term, since the corrector scheme as implicit scheme is more stable than the predictor scheme as explicit scheme in general. As a test function, the author employ the solution of the following fractional ordinary differential equations as

$$
{}_{t_0}^{\mathrm{C}}D_t^q y(t) = -ky(t).
$$

The solution is given by

$$
y(t) = 1 - \frac{k(t-t_0)^q}{\Gamma(q+1)} + \frac{k^2(t-t_0)^{2q}}{\Gamma(2q+1)} - \frac{k^3(t-t_0)^{3q}}{\Gamma(3q+1)} + \dots .
$$

By substituting the solution to the predictor term of existing method, we have

$$
\begin{aligned}
y_n^P - y_0 &= -\frac{kh^q}{\Gamma(1+q)} \sum_{j=0}^{n-1} \left\{(n-j)^q - (n-1-j)^q\right\} y_j \\
\Rightarrow \quad \lambda^n &+ \alpha \sum_{j=0}^{n-1} \left\{(n-j)^q - (n-1-j)^q\right\} \lambda^j - 1 = 0
\end{aligned}
$$

where $\alpha = kh^q/\Gamma(1+q)$. Figure 7.1 is the graph of the absolute value of the

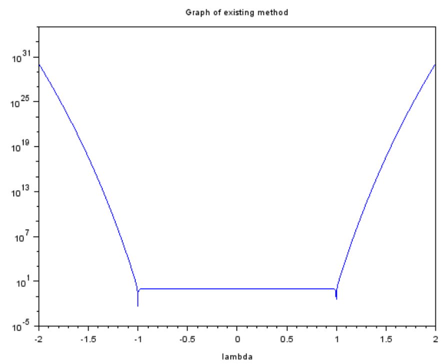


Figure 7.1: Graph of characteristic equation for existing method

following characterestic equation

$$
f(\lambda) = \lambda^n + \alpha \sum_{j=0}^{n-1} \left\{(n-j)^q - (n-1-j)^q\right\} \lambda^j - 1
$$

where $\alpha = 0.1$, $n = 100$, $q = 0.2$. This result shows that the all roots λ_m satisfy $|\lambda_m| \leq 1$, and the existing method is stable. Next, let us analyze the stability of the author's proposed method. By substituting the solution to the predictor term of the author's proposed method, we have

$$
\begin{aligned}
& y_n^P - y_0 \\
= \; & \frac{kh^q}{\Gamma(q)} \Bigg[y_{n-1} \left(-5A_0 - 5B_0 - 2C_0 - A_1 - \frac{3}{2}B_1 - C_1 \right) \\
& + y_{n-2} \left(6A_0 + 8B_0 + 4C_0 + 2B_1 + 2C_1 - A_2 - \frac{3}{2}B_2 - C_2 \right) \\
& + y_{n-3} \left(-2A_0 - 3B_0 - 2C_0 - \frac{1}{2}B_1 - C_1 + 2B_2 + 2C_2 - A_3 - \frac{3}{2}B_3 - C_3 \right) \\
& + \sum_{j=4}^{n-2} y_{n-j} \left(-\frac{1}{2}B_{j-2} - C_{j-2} + 2B_{j-1} + 2C_{j-1} - A_j - \frac{3}{2}B_j - C_j \right) \\
& + y_1 \left(-\frac{1}{2}B_{n-3} - C_{n-3} + 2B_{n-2} + 2C_{n-2} - A_{n-1} - 3B_{n-1} - 2C_{n-1} \right) \\
& + y_{1/2} \left(4B_{n-1} + 4C_{n-1} \right) \\
& + y_0 \left(-\frac{1}{2}B_{n-2} - C_{n-2} - B_{n-1} - 2C_{n-1} \right) \Bigg].
\end{aligned}
$$

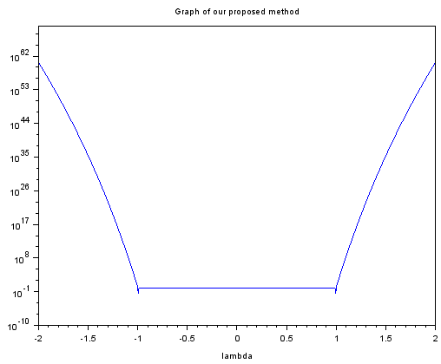


Figure 7.2: Graph of characteristic equation for the author's proposed method

Figure 7.2 is the graph of the absolute value of the following characteristic equation with $\alpha = 0.1$, $n = 100$, $q = 0.2$,

$$
\begin{aligned}
& f(\lambda) \\
= \; & \lambda^{2n} - 1 - \alpha \left[\lambda^{2(n-1)} \left(-5A_0 - 5B_0 - 2C_0 - A_1 - \frac{3}{2}B_1 - C_1 \right) \right. \\
& + \lambda^{2(n-2)} \left(6A_0 + 8B_0 + 4C_0 + 2B_1 + 2C_1 - A_2 - \frac{3}{2}B_2 - C_2 \right) \\
& + \lambda^{2(n-3)} \left(-2A_0 - 3B_0 - 2C_0 - \frac{1}{2}B_1 - C_1 + 2B_2 + 2C_2 - A_3 - \frac{3}{2}B_3 - C_3 \right) \\
& + \sum_{j=4}^{2(n-2)} \lambda^{n-j} \left(-\frac{1}{2}B_{j-2} - C_{j-2} + 2B_{j-1} + 2C_{j-1} - A_j - \frac{3}{2}B_j - C_j \right) \\
& + \lambda^2 \left(-\frac{1}{2}B_{n-3} - C_{n-3} + 2B_{n-2} + 2C_{n-2} - A_{n-1} - 3B_{n-1} - 2C_{n-1} \right) \\
& + \lambda \left(4B_{n-1} + 4C_{n-1} \right) \\
& \left. + \left(-\frac{1}{2}B_{n-2} - C_{n-2} - B_{n-1} - 2C_{n-1} \right) \right].
\end{aligned}
$$

where we put $y_m = \lambda^{2m}$ in order to avoid $y_{1/2} = \lambda^{1/2}$ by putting $y_m = \lambda^m$. From this graph, the author's proposed method seems to be stable. However, there are three problems for this stability analysis. One is the solution of the test function. The solution of the test function takes 1 at $t = t_0$ for $0 < q < 1$. Though the solution converges for $t \to \infty$, the undifferentiability around $t = t_0$ may cause the problem for this stability analysis. Second problem is the author's proposed method changes the form depending on the value of n. This means the number of step depends on n. The third problem is the treatment of $y_{1/2}$. To convert to the characteristic equation, we put y_m to λ^{2m}. Then, there is also a problem that we can simply put $y_{1/2}$ to λ. It is required to prove this conversion is allowable. These three problems remain in the stability analysis of the author's proposed method, and they are future tasks.

7.3 The author's proposed implicit numerical computational method for fractional ordinary differential equations using Lagrange interpolate polynomial

In the previous section, the author introduces the explicit numerical computational methods, but the accuracy of each explicit method is not so higher than that of implicit methods. This section shows the author's proposed implicit method which employs Lagrange interpolate polynomials. This method is a sort of collocation methods, and defines the analytical solution as

$$y(t) = \sum_{i=0}^{n} c_i P_i(t), \quad t_0 \le t \le L \tag{7.11}$$

where c_i are unknown constants and $P_i(t)$ are Lagrange polynomials whose sample points are Chebyshev nodes s_i. Therefore, $P_i(t)$ is given by

$$P_i(t) = \prod_{j \neq i} \frac{t - s_j}{s_i - s_j}.$$

The existing method which is explained in Chapter 3 employs Jacobi polynomials as orthogonal polynomials[4]. In contrast, this method employs Lagrange polynomials as interpolate polynomials. By increasing the number of degree of polynomials, Runge's phenomenon occurs and errors also increase for equally distance grids. To avoid Runge's phenomenon, the author uses Chebyshev nodes. It is well known that the errors produced by increasing the number of degree can be decreased by using Chebyshev nodes. Next, let us compare the existing method based on Jacobi polynomials and the author's proposed method. In the existing method, the solution is assumed as the following function

$$\tilde{y}_n(x) = a + \sum_{i=0}^{n} c_i x^q J_i^{(0,q)}\left(\frac{2x}{L} - 1\right),$$

where $J_i^{(0,q)}$ is a Jacobi polynomial. This means that if the analytical solution has the form $y(x) = x^q \sum_{i=0}^{n} x^i$ as shifted polynomials, this existing method can compute the solution analytically. In contrast, the author's proposed method can compute analytically if the analytical solution consist of polynomials whose degree is less than or equal to n. These two methods assume different solution functions, so if the analytical solution can be represented with finite degree polynomials, the accuracy of the author's proposed method is better than that of the existing method. In contrast, the accuracy of the existing method is better if the analytical solution can be represented with finite degree shifted polynomial as $y(t) = t^q + t^{1+q} + t^{2+q}$. In the previous section, the explicit numerical methods are introduced. They assume that the fractional derivative of the analytical solution is continuous differentiable as ${}_{t_0}^{\mathrm{C}}D_t^q y(t) \in C^2[t_0, T]$ to obtain the expected accuracy. This means that explicit methods assume that the analytical solutions can be represented with shifted polynomials. The author's proposed implicit method assumes the different type analytical solution. Therefore, by having the author's proposed implicit method, we have one more choice for solving ordinary differential equations. Especially, in fractional calculus, we have to treat more sorts of functions than in integer order calculus. Therefore, by proposing the author's implicit method, we can treat various assumptions, and apply numerical methods to more applications.

As a collocation method, the numerical solution can be computed by substituting the assumed solution (7.11). Then, we have

$$\sum_{i=0}^{n} c_i P_i(t) = y_{t_0} + \frac{1}{\Gamma(q)} \int_{t_0}^{t} (t-u)^{q-1} f\left(u, \sum_{i=0}^{n} c_i P_i(u)\right) du.$$

By putting $t = s_k$, we obtain

$$c_k - y_0 = \frac{1}{\Gamma(q)} \int_{t_0}^{s_k} (s_k - u)^{q-1} f\left(u, \sum_{i=0}^{n} c_i P_i(u)\right) du.$$

This integral includes the singularity at the kernel, and has a form suitable to Gauss-Jacobi quadrature. Firstly, we apply changing variables $\xi = 2(u-t_0)/(s_k - t_0) - 1$ as a preparation

$$\begin{aligned} & c_k - y_0 \\ = \; & \frac{1}{\Gamma(q)} \int_{-1}^{1} \left(\frac{s_k - t_0}{2}\right)^q (1-\xi)^{q-1} f\left(\tilde{\xi}, \sum_{i=0}^{n} c_i P_i(\tilde{\xi})\right) d\xi, \end{aligned}$$

where $\tilde{\xi}$ is defined by

$$\tilde{\xi} = \frac{\xi + 1}{2}(s_k - t_0) + t_0.$$

Let w_i be a i-th weight of Gauss-Jacobi quadrature, and let τ_i be a i-th node of Gauss-Jacobi quadrature. Then, we obtain equations

$$\begin{aligned} & c_k - y_0 \\ = & \frac{1}{\Gamma(q)} \left(\frac{s_k - t_0}{2} \right)^q \sum_{i=0}^{n} w_i f \left(\tilde{\tau}_i, \sum_{i=0}^{n} c_i P_i(\tilde{\tau}_i) \right) \end{aligned}$$

for $0 \leq k \leq n$. By solving this non-linear system of equations, the coefficients c_k are computed. Note that the number of nodes of Chebyshev nodes is the same to that of Gauss-Jacobi quadrature. By increasing the number of Gauss-Jacobi nodes, the accuracy improve. However, the number of Gauss-Jacobi nodes of the existing method is the same to the number of polynomials which consist of the solution function[4]. Thus, for the comparison, the author set the same number.

7.4 Experiments about fractional ordinary differential equations

7.4.1 Preparation of experiments

Problems

For the numerical experiments, the author sets four problems. All experiments are done with $t_0 = 0$, $L = T = 1$ and $0 < q < 1$. In Problem 1, let the solution function y be

$$y(t) = t^q - t^{1+q},$$

and a function f be

$$f(t, y) = \Gamma(1 + q) - \Gamma(2 + q) t^{1-q} (y + t^{1+q}).$$

In addition, the initial condition is $y(0) = 0$. This problem assumes that ${}_0^{\mathrm{C}}D_t^q y(t)$ is infinitely many times continuously differentiable. This property enables to obtain the expected accuracy of existing and the author's proposed explicit methods. In addition, note that the assumed solution function of existing implicit method using Jacobi polynomials exactly expresses this analytical solution for $n \geq 1$. This means the error of the existing implicit method for this problem is derived only from computational errors.

In Problem 2, the analytical function is given by

$$y(t) = t - t^2.$$

The function f is given by

$$f(t, y) = \frac{1}{\Gamma(2 - q)} t^{1-q} - \frac{2}{\Gamma(3 - q)} t^{1-q} (y + t^2),$$

and the initial condition is $y(0) = 0$. In contrast to Problem 1, the analytical solution is infinitely many times continuously differentiable. This means that this problem is not suitable for the existing and the author's proposed explicit method, and the author's proposed implicit method with Lagrange polynomial analytically solves it for $n \geq 2$.

Problem 3 is defined by the following analytical solution

$$y(t) = t^8 - 3t^{4+q/2} + \frac{9}{4} t^q,$$

and the function f

$$f(t,y) = \frac{40320}{\Gamma(9-q)}t^{8-q} - 3\frac{\Gamma(5+q/2)}{\Gamma(5-q/2)}t^{4-q/2} + \frac{9}{4}\Gamma(q+1) + \left(\frac{3}{2}t^{q/2} - t^4\right)^3 - y^{3/2}$$

with the initial condition $y(0) = 0$. This problem is cited from the paper by K. Diethelm, N.J. Ford and A.D. Freed[13].

In addition to Problem 3, Problem 4 is also cited from the papers by K. Diethelm and others[13, 4]. Let the analytical solution be

$$y(t) = 1 - \frac{t^q}{\Gamma(q+1)} + \frac{t^{2q}}{\Gamma(2q+1)} - \frac{t^{3q}}{\Gamma(3q+1)} + \dots,$$

and let the function f be

$$f(t,y) = -y.$$

The initial condition is $y(0) = 1$. This analytical solution can be represented with Mittag-Leffler function as

$$y(t) = E_{q,1}(-x^q) = \sum_{k=0}^{\infty} \frac{(-x^q)^k}{\Gamma(kq+1)}.$$

This equation is also a homogeneous equation.

Measurement of errors

For the numerical experiments about explicit methods, the author measures the error at a terminal point. Explicit methods compute the numerical solutions from an initial point to a terminal point step by step. Therefore, errors are accumulated at the terminal point. In addition, in order to check the stability, we should measure the error at the terminal point. The terminal point is set depending on the problem.

For implicit methods, the author employs different measurements to explicit methods. First measurement is cited from the paper[4]. Let e be a error with the first measurement given by

$$e = \max_{1 \geq j \geq 10000} |y(t_j) - y_N(t_j)|, \ t_j = \frac{L - t_0}{10000} j$$

for $j = 1, 2, \dots, 10000$. This measurement approximates a maximum error in an interval. The author propose the second measurement which is given by

$$E = \sum_{j=1}^{10000} h|y(t_j) - y_N(t_j)|, \ t_j = hj, \ h = \frac{L - t_0}{10000}.$$

This measurement numerically integrate errors between the analytical solution and numerical solutions, and can be called an average error.

7.4.2 Accuracy of the explicit methods for fractional ordinary differential equations

In this subsection, the author shows the numerical results about explicit existing method and the author's proposed method.

Figures 7.3, 7.4, 7.5 and 7.6 show the errors of explicit existing method and the author's proposed method for Problem 1 with various q. All experiments are

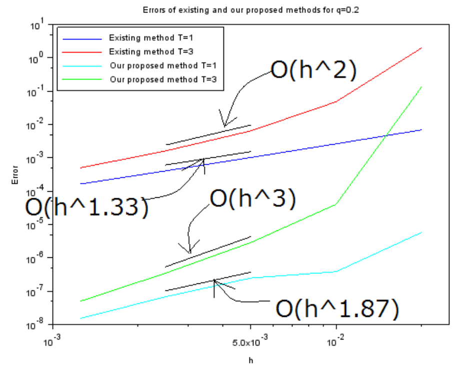


Figure 7.3: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.2$

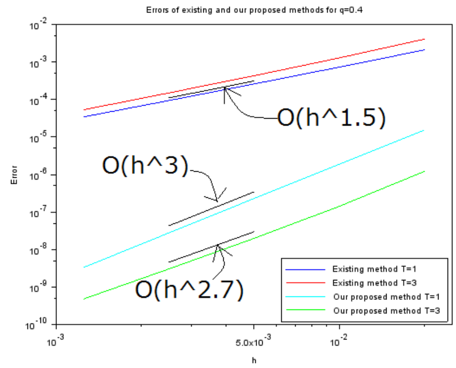


Figure 7.4: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.4$

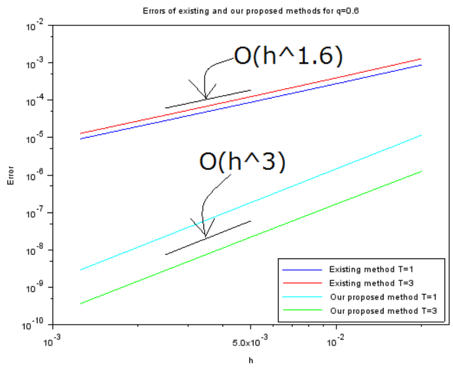


Figure 7.5: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.6$

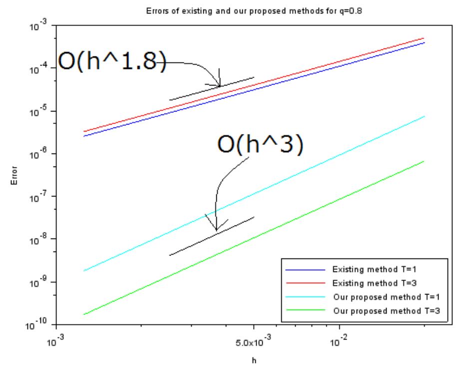


Figure 7.6: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.8$

done with two terminal points $T = 1$ and $T = 3$. If ${}_{t_0}^{C}D_t^q y(t) \in C^2[t_0, T]$, it is proven that the accuracy of the existing method is $O(h^{1+q})$ by K. Diethelm, N.J. Ford and A.D. Freed[13]. If ${}_{t_0}^{C}D_t^q y(t) \in C^\infty[t_0, T]$, it is proved that the accuracy of the author's proposed method is $O(h^3)$. Actually, Figures 7.5 and 7.6 exactly show the expected accuracy order. In addition, Fig. 7.4 represents that the expected accuracy order is almost obtained. However, Obtained accuracy orders in Figure 7.3 are not the same to the expected accuracy orders. This reason is that the stability becomes worse for small q. Table 7.1 shows the errors of

	h=0.02	h=0.01	h=0.005	h=0.0025	h=0.00125
Existing	5.287D+96	7.719D+172	9.321D+305	Nan	Nan
Proposed	2.277D+160	3.492D+295	Nan	Nan	Nan

Table 7.1: Errors of existing and the author's proposed methods for $q = 0.1$ and $T = 5$.

existing and the author's proposed methods for $q = 0.1$ and $T = 5$. This table represents that the numerical solutions diverge to ∞, and indicates that existing method and the author's proposed method are not stable in this case. For small q and large T, errors increase and the accuracy orders decay.

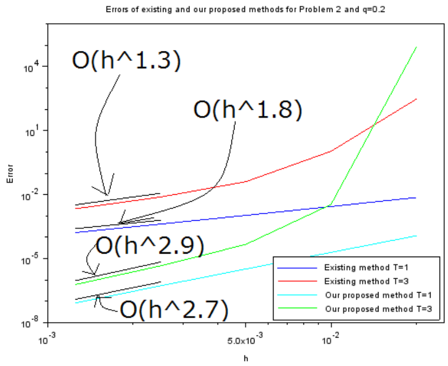


Figure 7.7: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.2$

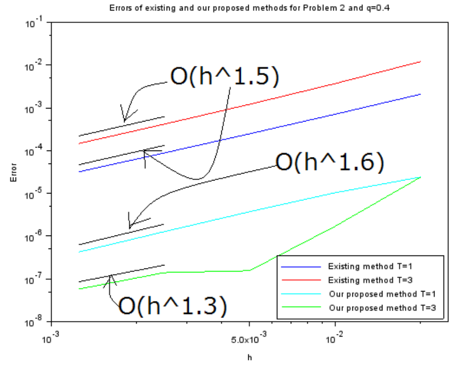


Figure 7.8: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.4$

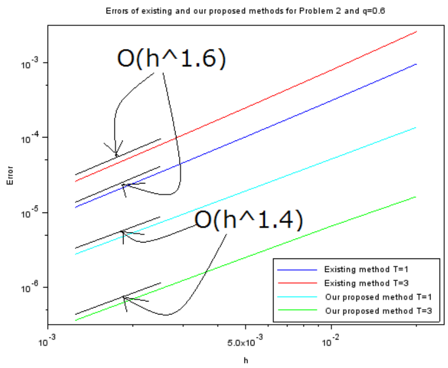


Figure 7.9: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.6$

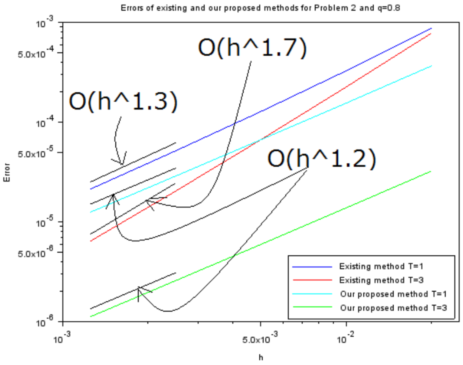


Figure 7.10: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.8$

Figures 7.7, 7.8, 7.9 and 7.10 show the errors for Problem 2 for $T = 1, 3$ with various q. For $q = 0.2$, the accuracy order is not firm because of the stability of numerical methods. In addition, the numerical experiments about the existing method is not firm neither in any q. However, for large q, the numerical results of the author's proposed method show the accuracy order decrease from $O(h^3)$ to $O(h^{2-q})$. In Problem 2, the differentiated function of the analytical function is given by

$$ {}_0^{\mathrm{C}}D_t^q y(t) = t^{1-q}/\Gamma(2-q) - 2t^{2-q}/\Gamma(3-q). $$

As mentioned in Chapter 4, the author's proposed third accuracy formula (4.7) calculate for this function with $O(h^{2-q})$. Therefore, the accuracy order of the author's proposed explicit method for fractional ordinary differential equations is also $O(h^{2-q})$, since this method employs the formula (4.7).

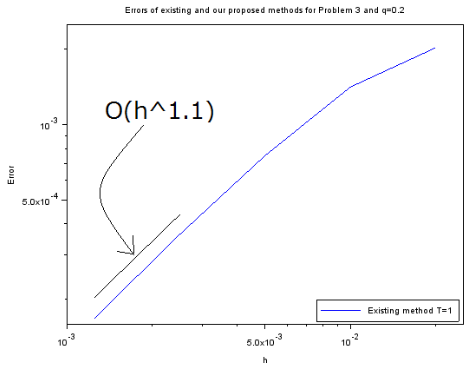


Figure 7.11: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.2$

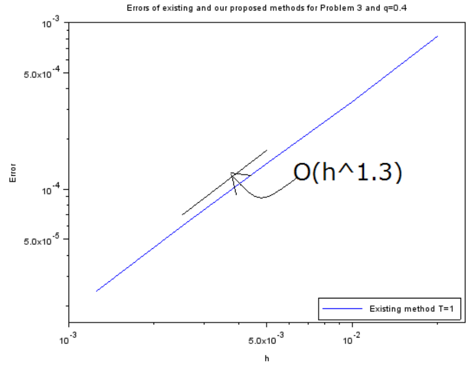


Figure 7.12: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.4$

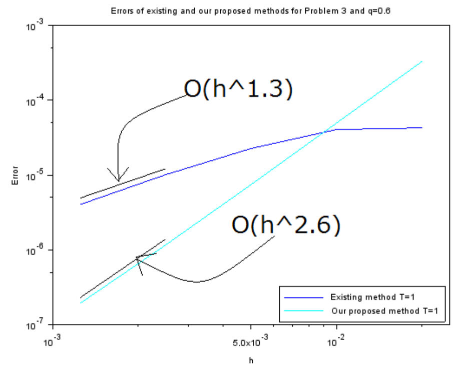


Figure 7.13: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.6$

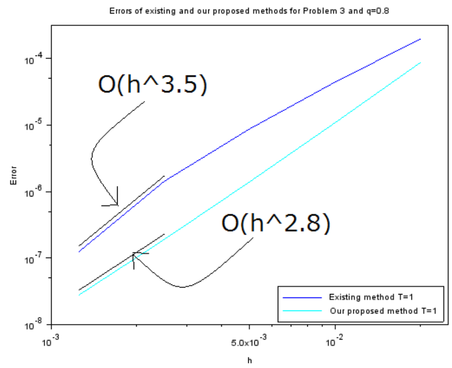


Figure 7.14: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.8$

Figures 7.11, 7.12, 7.13 and 7.14 show the errors of the existing method and the author's proposed method for Problem 3 and $T = 1$ with various q. In all experiments, the numerical solutions diverge to Nan for $T = 3$, so the graphs are not shown. Additionally, the numerical results of the author's proposed method for $T = 1$ and $q = 0.2$ diverge to Nan in Figure 7.11, and the results of the author's proposed method for $T = 1$ and $q = 0.4$ become complex numbers because a negative number is substituted to y. Therefore, those results are also not shown. In Problem 3, it holds ${}_0^{\mathrm{C}}D_t^q y(t) \in C^3[0, T]$. Therefore, the accuracy decaying does not happen in contrast to Problem 2, and the obtained accuracy orders are near to the expected accuracy order if the computations are done stably. However, these figures show the stability of the existing method and the author's proposed method for this problem is bad, and the numerical solutions are not firm for h. Depending on the problems, the stability of the existing method and the author's proposed method is changed. Because of the stability problem, the numerical results do not decrease along to the expected accuracy order.

Figure 7.15, 7.16, 7.17 and 7.18 show the errors of the existing and the author's proposed methods for Problem 4 and $T = 1$ and $T = 3$. Because of the accuracy

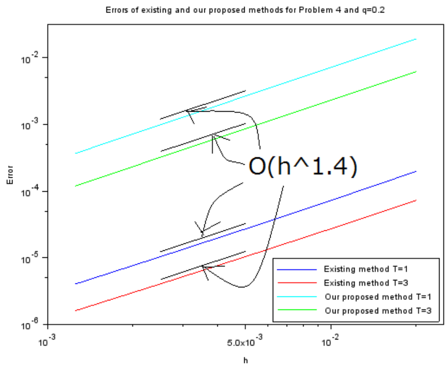


Figure 7.15: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.2$

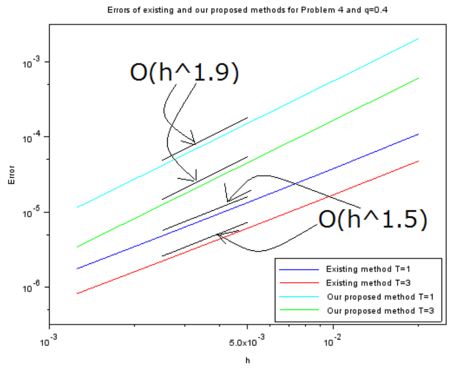


Figure 7.16: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.4$

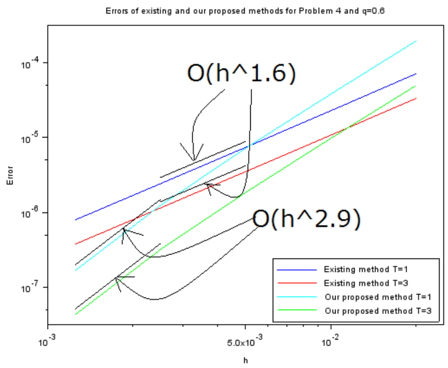


Figure 7.17: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.6$

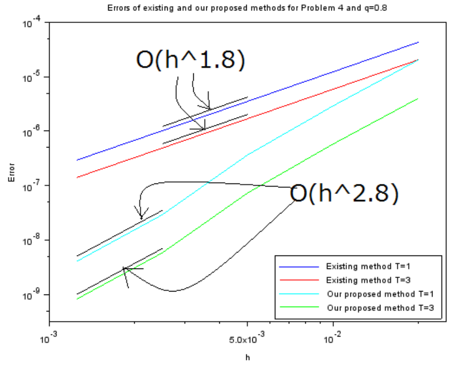


Figure 7.18: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.8$

decaying with the term $-t^q/\Gamma(q+1)$, the expected accuracy order is $O(h^{1+q})$ for both methods. However, the obtained accuracy orders are higher than the author expected. The possible reason is that the time step size is too large. By taking smaller h, the expected accuracy order may be obtained, but the computational complexity of the existing and the author's proposed methods are larger than that of Runge-Kutta methods or linear multi-step methods for integer order ordinary differential equations. The predictor-corrector methods for fractional ordinary differential equations have to compute each numerical solution from an initial point. In integer order calculus, differentiation is a local phenomenon, so the numerical methods do not consider the information from the initial point. To create the numerical methods with less computational complexity is a future task.

7.4.3 Accuracy of the implicit methods for fractional ordinary differential equations

This section shows the numerical experiments of three methods, the existing method using Jacobi polynomial, the existing method using double exponential transform and the author's proposed methods using Lagrange polynomial. All non-linear equations in those methods are solved by using Newton's method. The values of the weights and nodes of Gauss-Jacobi quadrature is cited from a website[7].

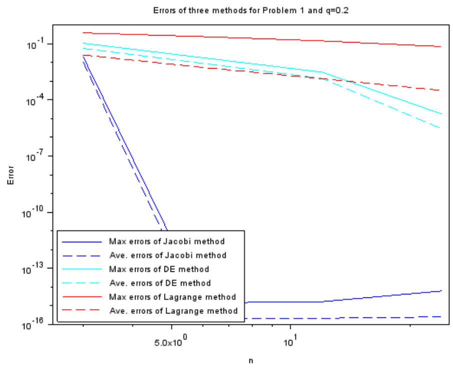


Figure 7.19: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.2$

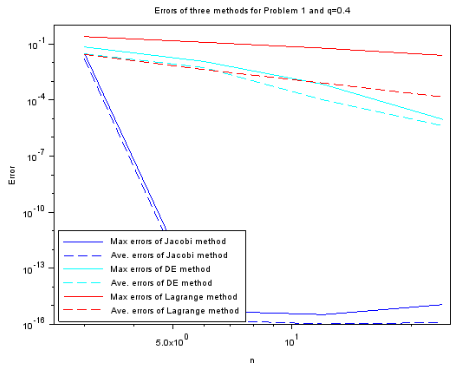


Figure 7.20: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.4$

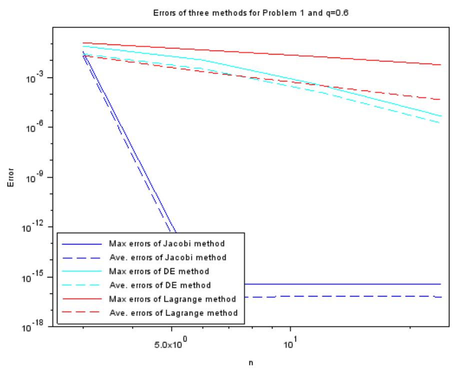


Figure 7.21: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.6$

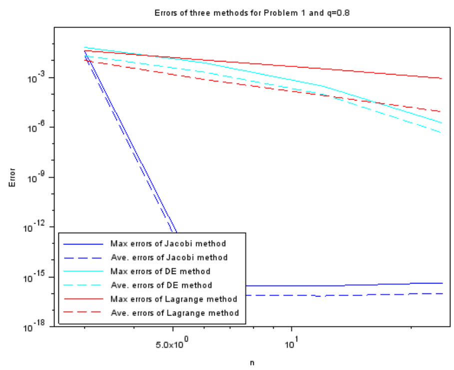


Figure 7.22: Errors of existing and the author's proposed methods for Problem 1 with $q = 0.8$

Figures 7.19, 7.20, 7.21 and 7.22 show the max errors and average errors of three methods with Problem 1. The solution function has the suitable form to apply the numerical method using Jacobi polynomial. Therefore, the errors of the Jacobi method are smaller than others.

Figures 7.23, 7.24, 7.25 and 7.26 show the max errors and average errors of three methods with Problem 2. The solution function of Problem 2 has the suitable form to apply the author's proposed method using Lagrange polynomial. For $n > 1$, the solution of the author's method can express the analytical solution. However, because of the error of integration, the accuracy is worse than that of double exponential transform method for $q = 0.6, 0.8$ and larger N. Caputo derivative of the analytical solution y in Problem 2 is undifferentiable at $x = 0$. Thus, the existing explicit method and the author's proposed explicit method for fractional ordinary differential equations introduced in this thesis cause the

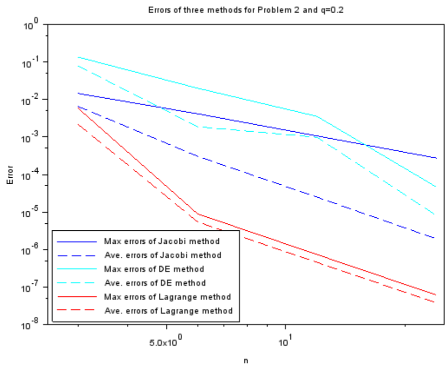


Figure 7.23: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.2$

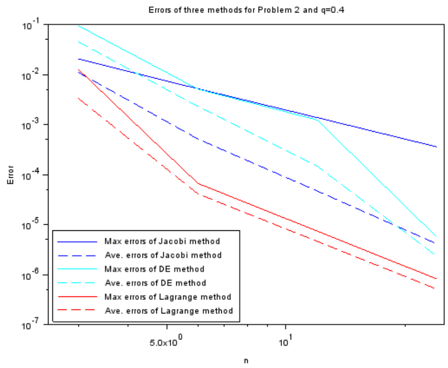


Figure 7.24: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.4$

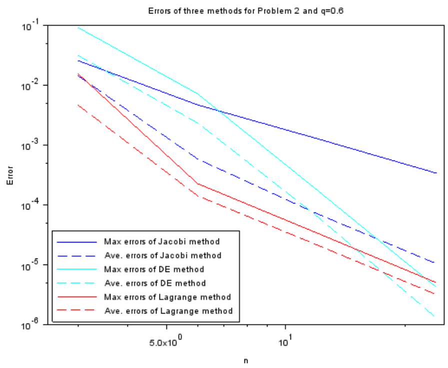


Figure 7.25: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.6$

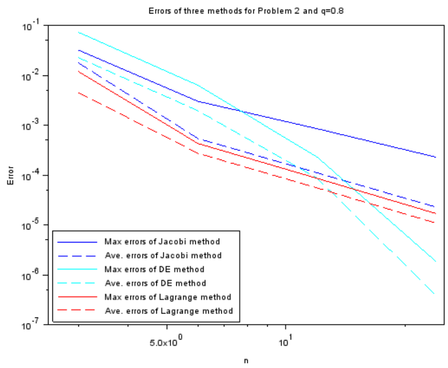


Figure 7.26: Errors of existing and the author's proposed methods for Problem 2 with $q = 0.8$

accuracy decaying. Yet, this results show the author's proposed implicit method is good at such problems. Therefore, when we try to solve fractional ordinary differential equations, we can treat a problem, which it is difficult to solve with explicit methods, by using the author's implicit method with small N.

Figures 7.27, 7.28, 7.29 and 7.30 present the max errors and average errors of three methods for Problem 3. Since the numerical solutions of double exponential transform become the complex numbers, the author does not show its results. The analytical solution of this problem consists of the combination of polynomial and not polynomial term. However, the minimum order term is $9t^q/4$, and it is indicated that this problem fits to the method using Jacobi polynomial. Actually, the errors of Jacobi method are smaller than that of Lagrange method.

Figures 7.31, 7.32, 7.33 and 7.34 present the max errors and average errors of three methods for Problem 4. This problem is not suitable for Lagrange method, since the solution cannot be represented with finite degree polynomial. In contrast, double exponential transform method solves this problem with high accuracy order. The errors of double exponential transform method decrease more rapidly than any other methods.

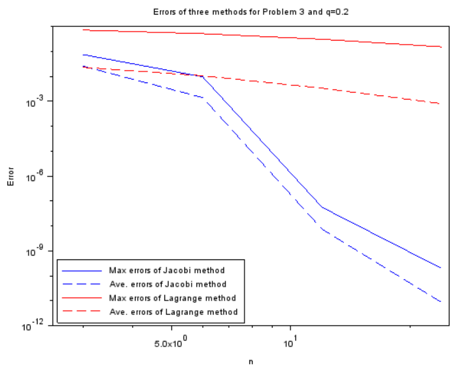


Figure 7.27: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.2$

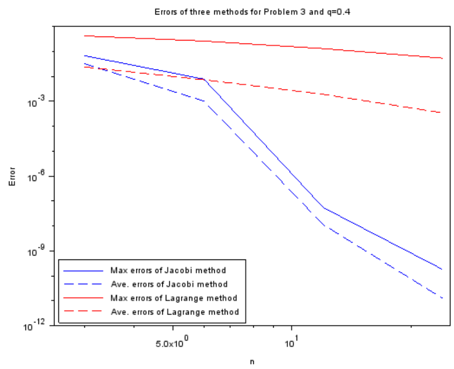


Figure 7.28: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.4$

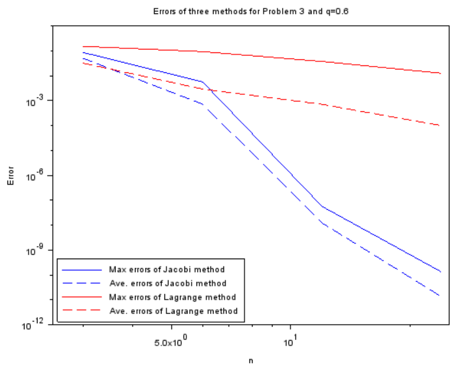


Figure 7.29: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.6$

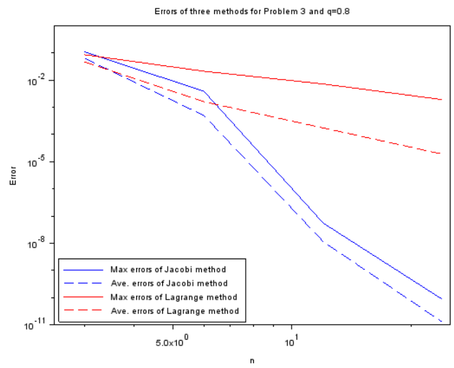


Figure 7.30: Errors of existing and the author's proposed methods for Problem 3 with $q = 0.8$

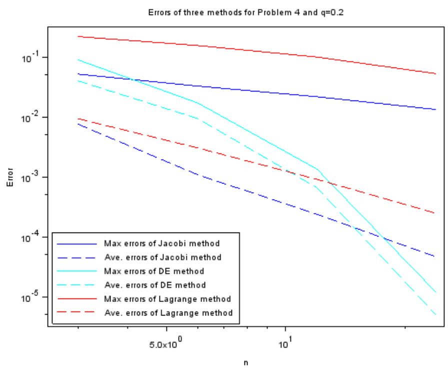


Figure 7.31: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.2$

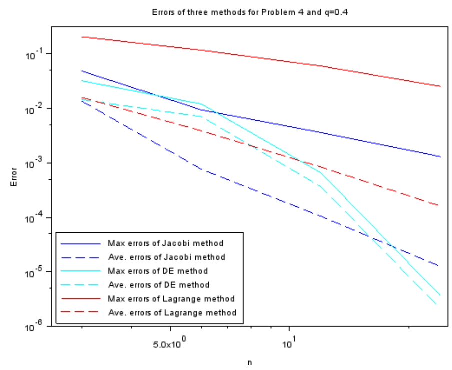


Figure 7.32: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.4$

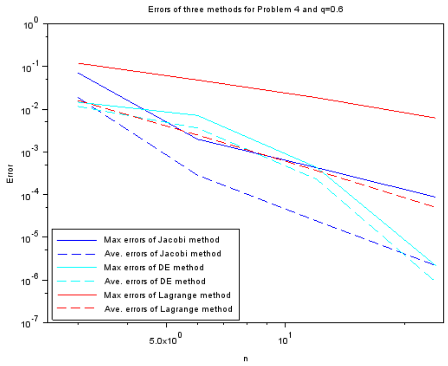


Figure 7.33: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.6$

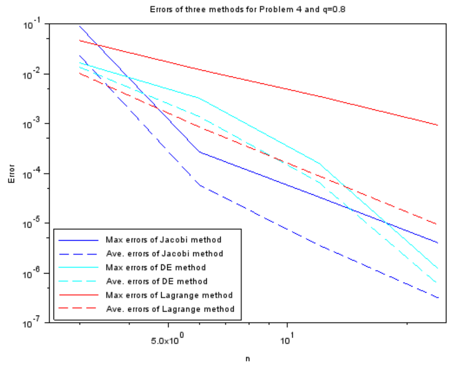


Figure 7.34: Errors of existing and the author's proposed methods for Problem 4 with $q = 0.8$

Chapter 8

Conclusion

This thesis has proposed new numerical methods for three problems. One is a finite difference method for space-fractional partial differential equations. The author's proposed finite difference methods have four improvements comparing to the existing method. First improvement is the accuracy order. The existing methods have only the first order accuracy about space, and the author's proposed methods have the second order accuracy about space. By using the author's proposed methods, errors decrease more rapidly than the existing methods. However, this accuracy order may decay if the analytical solution has the form which is expanded with low order around boundaries. This accuracy decaying happens both in the existing methods and the author's proposed methods. Second improvement is the stability condition. The stability condition about time step size of the author's proposed methods is less strict than that of the existing method. However, the author's proposed schemes contain the parameter s. To be stable, we have to select a proper value of the parameter s. Otherwise, the author's proposed schemes become unstable even if the time step size is sufficiently small. The third improvement is the boundary conditions. The existing methods cannot handle non-zero Dirichlet boundary conditions. If the analytical solution takes non-zero values at boundaries, the numerical solutions of the existing methods do not converge to the analytical solution. In contrast, the author's proposed schemes have the feature of error cancelling. Therefore, the numerical solutions of the author's proposed schemes actually converge to the analytical solution for non-zero Dirichlet boundary conditions. The fourth improvement is that the author's proposed methods can be applied to the case $0 < q < 1$. The existing methods cannot deal with the case $0 < q < 1$. Then, the author has made stability analysis to such a case by using Gerschgorin's theorem, and has shown the stability condition.

This thesis also has treated the numerical solutions in the form of polynomial expansion for homogeneous parabolic fractional partial differential equations. This approach is based on new idea, and there does not exist related works as far as the author knows. In this problem, the author has tried to lead the analytical solution by expanding even and odd function like integer order diffusion equations. In integer order diffusion equations with zero Dirichlet boundary conditions, the analytical solution can be expressed with the combination of orthogonal functions, sine and cosine functions. In a similar way, the author has proposed the numerical methods by computing the even and odd functions, and has shown their orthogonality. Those functions are analytically developed by solving infinite size of a system of equation. In the experiments, the numerical solutions are calculated in the form of polynomial expansion by solving approximated finite system of equations. However, the author could not find the general forms of such polynomials. To find the general forms is the future task.

This thesis also has discussed the numerical methods for fractional ordinary differential equations. The author has proposed a higher accuracy computational method than the existing method. The existing method has the accuracy order $O(h^{1+q})$, and the author's proposed method has the accuracy order $O(h^3)$. Actually, in almost experiments, results of the author's proposed method have been more accurate than the existing method. However, experimental results also have shown the stability of the author's proposed method is lower than that of the existing method, and the expected accuracy order cannot be obtained in many cases. In addition, the computational complexity is larger than the integer order linear multi-step method. As future tasks, the author considers to make more detailed stability analysis, and to apply the parallelization in order to obtain the results with smaller h. The author also has proposed the implicit method using Lagrange interpolate polynomial. This method accurately can solve the problem which causes the accuracy decaying in the explicit methods. This means that the author's proposed method gives us a choice which we can select the numerical method depending on problems. In addition, the author has made experiments of the double exponential transform method. This method has been already proposed, but the experiments about this method have never been done. The author has shown that double exponential transform method has much better accuracy order depending on problems.

The author has discussed high accuracy numerical computational methods about fractional differential equations. The author predicts fractional differential equations become more popular and more research fields employ them. Then, by given high accuracy numerical computational methods, this thesis will help the utilization and understanding of fractional differential equations.

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