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博 士 学 位 论 文

分数阶动力方程的数值方法及其理论分析

Numerical Methods of the Fractional Kinetic Equations and Theoretical Analysis

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摘 要

分数阶动力方程近年来得到广泛的兴趣和关注。其主要原因是由于分数阶微积分理论自身的迅速发展，以及其在物理、化学、生物，环境科学，工程以及金融等各类学科中的广泛应用。分数阶动力方程为描述不同物质的记忆和继承性质提供了强有力的工具。

然而，分数阶动力方程的解析解是比较复杂的，多数解析解都包含了有级数形式或特殊函数。而且，多数分数阶动力方程的解不能显式地得到。这就促使我们必须考虑有效的数值方法。目前，关于分数阶动力方程的数值方法以及相关的稳定性和收敛性分析相当有限，而且很难得到。这些激励我们发展有效的数值方法解分数阶的微分方法。在本论文中，我们考虑两种类型的分数阶动力方程。第一类分数阶动力方程是带有扩散，对流-扩散以及Fokker-Planck类型的分数阶动力方程。其数值方法和理论分析将分别在第二章，第三章和第四章详细讨论。第二类分数阶动力方程是带有反常次扩散的分数阶动力方程。例如，反常次扩散方程，非线性反应次扩散方程，以及分数阶Cable方程。这些方程的数值方法和理论分析将在第五章，第六章和第七章进行讨论。所有上面提到的方程已经被用于描述受反常扩散和非指数松弛方式控制的复杂系统中的传输动力学。这些分数阶方程都可以从基本的随机游走和推广的控制方程中逐步地得到。

第一章，我们总结了分数阶计算理论的发展史，本论文讨论的问题的背景，以及有关分数阶动力方程的先前的工作。并给出了我们的研究工作以及论文的结构。

第二章, 我们考虑在有界区域上的空间-时间分数阶扩散方程。这个方程是从标准的扩散方程中，二阶空间导数由$\beta \in (1,2]$阶的Riemann-Liouville分数阶导数代替，一阶时间导数由$\alpha \in (0,1]$阶的Caputo分数阶导数代替得到。我们研究含有初边值问题的空间-时间分数阶扩散方程的显式差分格式和隐式差分格式。给出了方法的稳定性和收敛性结论。证明了隐式差分格式的无条件稳定性和收敛性，而显式差分格式的条件稳定性和收敛性。数值例子显示了反常扩散的性态。在这一章中，我们还考虑了有限区域上二维分数阶扩散方程。提出了求解二维

空间-时间分数阶扩散方程的隐式差分格式，讨论了这个隐式差分格式稳定性和收敛性。一些数值例子显示了这些技巧的应用。

第三章，我们考虑有限区域上的空间-时间分数阶对流-扩散方程。这个方程是从标准的对流-扩散方程中，一阶时间导数由$\alpha \in (0,1]$阶的Caputo分数阶导数代替, 一阶和二阶空间导数分别由$\beta \in (0,1]$阶和$\gamma \in (1,2]$阶的Riemann-Liouville分数阶导数代替得到。我们提出隐式和显式差分格式。利用数学归纳法，证明了这个隐式差分格式的无条件稳定性和收敛性，而显式差分格式的条件稳定性和收敛性。其数值结果和理论分析相符。

第四章，我们考虑有界区域上的空间-时间Fokker-Planck方程。这个方程是从标准的Fokker-Planck中，一阶时间导数由$\alpha \in (0,1]$阶的Caputo分数阶导数代替, 二阶空间导数由左Riemann-Liouville分数阶导数和右Riemann-Liouville分数阶导数代替得到。我们提出了计算有效的隐式数值方法。讨论了隐式数值方法的稳定性和收敛性。并给出了数值例子，这个数值结果与精确解相符。

第五章，我们考虑反常次扩散方程。提出了一种新隐式数值方法和两种改进收敛阶的技巧。利用能量不等式证明了这个新的隐式差分格式的稳定性和收敛性。我们给出一些数值例子。数值结果证实了我们的理论分析。这些方法也可以应用于其它类型的积分微分方程和高维问题。

第六章，我们考虑非线性反应-次扩散过程。我们提出了一种新的计算有效的数值方法去模拟该过程。首先，将非线性反应次扩散过程归结为一个等价方程。然后，我们提出一个隐式格式近似这个方程。接着利用新的能量方法给出稳定性和收敛性证明。最后一些数值例子显示这种方法的应用。这种方法和理论结果可以用于分数阶积分微分方程。

第七章，我们讨论的分数阶Cable方程。我们提出了隐式差分方法。利用能量方法讨论了稳定性和收敛性。我们还提出了有限元近似。建立了稳定性和误差估计，并导出收敛阶。数值例子证明了方法的有效性和理论结果的正确性。

关键词：分数阶动力方程；反常次扩散方程；有限差分方法；稳定性；收敛性；能量方法；有限元法

Abstract

Fractional kinetic equations have been of great interest recently. It is caused both by the intensive development of the theory of fractional calculus itself and by the applications of such constructions in various sciences such as physics, chemistry, biology, environmental sciences, engineering and finance. Fractional kinetic equations provide a powerful instrument for the description of memory and hereditary properties of different substances.

However, many analytical solutions for the fractional kinetic equations are complicated, which include the complicated series or especial function. Moreover, analytic solutions of most fractional kinetic equations cannot be obtained explicitly. At present numerical methods and analysis of stability and convergence for fractional partial differential equations are quite limited and difficult to derive. This motivates us to develop effective numerical methods for the fractional differential equations. In this thesis, we consider two kind of fractional kinetic equations. The first kind of the fractional kinetic equations is the fractional kinetic equations of the diffusion, diffusion-advection, and Fokker-Planck type. Numerical methods and theoretical analysis for the fractional kinetic equations are discussed in Chapters 2, 3 and 4, respectively. The second kind of the fractional kinetic equations is the fractional kinetic equations of anomalous subdiffusion type, such as the anomalous subdiffusion equation, a nonlinear fractional reaction-subdiffusion process and the fractional cable equation. Numerical methods and theoretical analysis for the fractional kinetic equations are discussed in Chapters 5, 6 and 7, respectively. These fractional kinetic equations above-mentioned have been presented as a useful approach for the description of transport dynamics in complex systems which are governed by anomalous diffusion and non-exponential relaxation patterns. These fractional equations can be derived asymptotically from basic random walk models, and from a generalised master equation.

In the first chapter, we summarize the history of the theory of fractional calculus,

the background and significance of this dissertation, and the previous works about the fractional kinetic equations. Our research group and the framework of this thesis are given.

In Chapter 2, we consider a space-time fractional diffusion equation on a finite domain. The equation is obtained from the standard diffusion equation by replacing the second-order space derivative by a Riemann-Liouville fractional derivative of order $\beta \in (1,2]$, and the first-order time derivative by a Caputo fractional derivative of order $\alpha \in (0,1]$. An implicit and an explicit difference approximations for the space-time fractional diffusion equation with initial and boundary values are investigated. Stability and convergency results for the methods are discussed. Using mathematical induction, we prove that the implicit difference method is unconditionally stable and convergent, but the explicit difference method is conditionally stable and convergent. Some numerical results show the system exhibits anomalous diffusive behaviour. In this chapter, we also consider a two-dimensional fractional diffusion equation on a finite domain. We examine an implicit difference approximation to solve the space-time fractional diffusion equation. Stability and convergency of the method are discussed. Some numerical examples are presented to show the application of the present technique.

In Chapter 3, we consider a space-time fractional advection dispersion equation on a finite domain. This equation is obtained from the standard advection-dispersion equation by replacing the first-order time derivative by the Caputo fractional derivative of order $\alpha \in (0,1]$, and the first-order and second-order space derivatives by the Riemman-Liouville fractional derivatives of order $\beta \in (0,1]$ and of order $\gamma \in (1,2]$, respectively. n implicit and an explicit difference approximations is proposed. Using mathematical induction, we prove that the implicit difference method is unconditionally stable and convergent, but the explicit difference method is conditionally stable and convergent. Numerical results are in good agreement with theoretical analysis.

In Chapter 4, we consider a space-time fractional Fokker-Planck equation on a finite domain. This equation is obtained from the standard Fokker-Planck equation by replacing the first-order time derivative by the Caputo fractional derivative, the second-order space derivative by the left and right Riemann–Liouville fractional derivatives. We propose a computationally effective implicit numerical method to solve this equation. Stability and convergence of the methods are discussed. Numerical example is given, which is in good agreement with the exact solution.

In Chapter 5, we consider anomalous subdiffusion equation. A new implicit numerical method and two solution techniques for improving the order of convergence of the implicit numerical method for solving the anomalous subdiffusion equation are proposed. The stability and convergence of the new implicit numerical method are investigated by the energy method. Some numerical examples are given. The numerical results demonstrate the effectiveness of theoretical analysis. These methods and supporting theoretical results can also be applied to other fractional integro-differential equations and higher-dimensional problems.

In Chapter 6, a nonlinear fractional reaction-subdiffusion process is considered. We propose a new computationally efficient numerical method to simulate the process. Firstly, the nonlinear fractional reaction-subdiffusion equation is decoupled, which is equivalent to solving a nonlinear fractional reaction-subdiffusion equation. Secondly, we propose an implicit numerical method to approximate this equation. Thirdly, the stability and convergence of the method are discussed using a new energy method. Finally, some numerical examples are presented to show the application of the present technique. This method and supporting theoretical results can also be applied to fractional integro-differential equations.

In Chapter 7, a fractional cable equation is discussed. An implicit difference method is proposed. The stability and convergence of the method are discussed using an energy method. Moreover, we also propose the finite element approximation of the fractional cable equation. The stability and error estimates are established. We derive the convergent order of the method. Numerical examples are presented which demonstrate the effectiveness of the methods and confirm the theoretical analysis.

Key words: fractional kinetic equation; anomalous subdiffusion equation; finite difference method; stability; convergency; the energy method; finite element method

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