



Research and application of compact finite difference method of low reaction-diffusion equation

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ABSTRACT

The paper describes the theory of fractional derivative and specific application examples in the field of engineering sciences. On this basis, this paper mainly studies the low reaction-diffusion equations. First using compact operator, the paper constructs a higher-order finite difference scheme. Then the paper proves the existence and uniqueness of the difference solution by matrix method and analyzes the stability and convergence of the scheme by Fourier method.

Key words: Fractional Differential Equations, Low reaction-diffusion equations, Compact finite difference method, Fourier method

INTRODUCTION

Application of fractional differential equations in the field of engineering sciences is gradually expanded. Especially in recent years, application of fractional differential equations in the field of hydromechanics, viscoelasticity, rheology, fractional control systems and fractional controller, electroanalytical chemistry, electronic circuit and electrically conductive in biological system are more and more [1-3].

There are three fractional derivative definitions: Grinwald-letnikov (G-L) Definition[1], Riemann-Liouville (R-L) Definition[1] and Caputo Definition[2].

R-L Definition:

Let $\gamma \in (0,1), a, b \in \mathbb{R}, a < t < b, f(t)$ is continuous on $[a, b]$, the R-L fractional differential is ${}_a D_t^{1-\gamma} f(t) = \frac{1}{\Gamma(\gamma)} \frac{d}{dt} \int_a^t \frac{f(\tau)}{(t-\tau)^{1-\gamma}} d\tau$ where $\Gamma(\cdot)$ is Gamma function.

Caputo Definition: ${}_a D_t^\gamma f(t) = \frac{1}{\Gamma(1-\gamma)} \int_a^t f(s)(t-s)^{-\gamma} ds, 0 \leq t \leq T, 0 < \gamma < 1.$

When γ negative real number or positive integer, three definitions is can be converted to each other. G-L definition is generally used for discrete computing. R-L and Caputo definition are commonly used in the discussion of fractional differential equations.

APPLICATION EXAMPLE

(1) Promotion and application of Newton's law

Wasteland et al [5, 6] propose to Newton's second law of $f = ma$ instead of with $f = mx^{(a)} (x^{(a)} = D^a x, 1 < a < 2).$

(2) Conduction applications in biology

In the study of biological electrical conduction, experts give the transfer function $X(\omega) = X_0 \omega^{-\alpha}, (0 < \alpha < 1)$

where ω is current frequency, X_0 and α are constant and their values are associated with the cell type.

If we see the above formula as Laplace transform, i.e. $S^\alpha G(s) = G_0$, then L inverse transformation is fractional differential equation ${}_0 D_t^\alpha g(t) = 0, 0 < \alpha < 1$.

(3) Application of $PI^\lambda D^\mu$ controller

The function of $PI^\lambda D^\mu$ controller is $G(s) = \frac{\bar{U}(s)}{E(s)} = k_p + k_I s^{-\lambda} + k_D s^\mu$ where $\lambda, \mu > 0, k_p, k_I, k_D$ constants are and the output equation is $k_I D^{-\lambda} e(t) + k_D D^\mu e(t) + k_p e(t) = u(t)$.

For the above formula, if $\lambda = \mu = 1$, then it is the traditional PID controller; if $\lambda = 1, \mu = 0$, then it is PI controller; if $\lambda = 0, \mu = 1$, then it is PD controller; if $\lambda = \mu = 0$, we give a gain.

(4) Application of Fractional control system

The system equation of $PI^\lambda D^\mu$ controller is

$$\sum_{k=0}^n a_k D^{\beta_k} y(t) + k_p y(t) + k_I D^{-\lambda} y(t) + k_D D^\mu y(t) = k_p w(t) + k_I D^{-\lambda} w(t) + k_D D^\mu w(t)$$

$$G_{closed}(s) = \frac{k_p s^\lambda + k_I + k_D s^{\mu+\lambda}}{\sum_{k=0}^m a_k s^{\beta_k+\lambda} + k_p s^\lambda + k_I + k_D s^{\mu+\lambda}}$$

Where the transfer function is

$$\sum_{k=0}^n a_k D^{\beta_k} y(t) = k_p w(t) + k_I D^{-\lambda} w(t) + k_D D^\mu w(t)$$

If the system is open-loop system, then the differential equation is

COMPACT FINITE DIFFERENCE METHOD OF LOW REACTION-DIFFUSION EQUATION

Derivation of the equation

General reaction-diffusion equation set is the following:

$$\frac{\partial}{\partial t} a(x,t) = D \frac{\partial^2}{\partial x^2} a(x,t) - \kappa a(x,t)b(x,t) \tag{1}$$

$$\frac{\partial}{\partial t} b(x,t) = D \frac{\partial^2}{\partial x^2} b(x,t) - \kappa a(x,t)b(x,t) \tag{2}$$

Where D is diffusion constant. When the particle movement and reactions are affected by the low diffusion factor, equation set can be developed in the following form

$$\frac{\partial}{\partial t} a(x,t) = {}_0 D_t^{1-\gamma} \left[\kappa_\gamma \frac{\partial^2}{\partial x^2} a(x,t) - \kappa a(x,t)b(x,t) \right] \tag{3}$$

$$\frac{\partial}{\partial t} b(x,t) = {}_0 D_t^{1-\gamma} \left[\kappa_\gamma \frac{\partial^2}{\partial x^2} b(x,t) - \kappa a(x,t)b(x,t) \right] \tag{4}$$

where κ_γ is diffusion coefficient, ${}_0 D_t^{1-\gamma} v(x,t)$ is $1-\gamma$ order fractional partial derivative defined by

$${}_0D_t^{1-\gamma}v(x,t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t \frac{v(x,\eta)}{(t-\eta)^{1-\gamma}} d\eta \tag{5}$$

By decoupling operation, Chen, Liu and Burrage[3] simplified the formula (3) and (4) for the following low-reaction-diffusion equation:

$$\frac{\partial}{\partial t}u(x,t) = {}_0D_t^{1-\gamma}[\kappa_\gamma \frac{\partial^2}{\partial x^2}u(x,t) - \kappa_\gamma u(x,t)] + f(x,t), 0 < t < T, 0 < x < L \tag{6}$$

where $0 < \gamma < 1$, $\kappa_\gamma > 0$ is general diffusion coefficient, $k > 0$ is bimolecular reaction rate constant. Dirichlet boundary and initial conditions of (6) are

$$u(0,t) = \phi(t), 0 < t \leq T \tag{7}$$

$$u(L,t) = \varphi(t), 0 < t \leq T \tag{8}$$

$$u(x,0) = \varpi(x), 0 < x \leq L \tag{9}$$

For the initial boundary value problem of this equation, Chen et al[3] gave implicit difference scheme and explicit difference scheme. They respectively proved the stability of the format and discussed solvability of implicit difference scheme.

Format construction

In order to obtain the numerical solution of the above equation, we introduce the general mesh generation:

$$(x_j, t_k), x_j = jh, j = 0, 1, \dots, M, t_k = k\tau, k = 0, 1, \dots, N$$

where M, N are positive integer, $h = L/M$ is spatial orientation step, $\tau = T/N$ is time orientation step.

Let u_j^k denote the exact solution in (x_j, t_k) point and U_j^k denote the difference solution of this point. By the G-L formula, we obtain:

$${}_0D_t^{1-\gamma}f(t) = \frac{1}{\tau^{1-\gamma}} \sum_{k=0}^{[t/\tau]} \lambda_l f(t - k\tau) + O(\tau) \tag{10}$$

Where

$$\lambda_l = (-1)^l \binom{1-\gamma}{l}, l = 0, 1, \dots \tag{11}$$

We use compact operator $\frac{\delta_x^2}{h^2 \left(1 + \frac{1}{12} \delta_x^2\right)}$ to approach $\frac{\partial^2 u}{\partial x^2}$ and then we get compact difference scheme for (6)-(9):

$$\mu = \kappa_\gamma \frac{\tau^\gamma}{h^2}, \nu = \kappa \tau^\gamma$$

Due to $\lambda_0 = 1$, in the network point $(x_j, t_k), j = 1, 2, \dots, M-1, k = 0$, we get

$$\begin{cases} \frac{U_j^k - U_j^{k-1}}{\tau} = \tau^{\gamma-1} \sum_{l=0}^k \lambda_l \left[\kappa_\gamma \frac{\partial_x^2}{h^2 \left(1 + \frac{1}{12} \delta_x^2\right)} U_j^{k-l} - k U_j^{k-l} \right] + f_j^k, \\ U_j^0 = \varpi(x_j), \quad j = 0, 1, 2, \dots, M, \\ U_j^0 = \phi(t_k), U_M^k = \psi(t_k), k = 1, 2, \dots, N \end{cases} \tag{12}$$

Let $P = \tau \left(\frac{1}{12} f_0^k + \frac{5}{6} f_1^k + \frac{1}{12} f_2^k \right)$, $Q = \tau \left(\frac{1}{12} f_{M-2}^k + \frac{5}{6} f_{M-1}^k + \frac{1}{12} f_M^k \right)$, we get

$$F^k = \begin{pmatrix} \left(\mu - \frac{\nu}{12} \right) \sum_{l=0}^{k-2} \lambda_{k-1} U_0^l + \left(\frac{1}{12} + \mu \lambda_1 - \lambda_1 \frac{\nu}{12} \right) U_0^{k-1} - \left(\frac{1}{12} - \mu + \frac{\nu}{12} \right) U_0^k + P \\ \tau \left(\frac{1}{12} f_1^k + \frac{5}{6} f_2^k + \frac{1}{12} f_3^k \right) \\ \vdots \\ \tau \left(\frac{1}{12} f_{M-3}^k + \frac{5}{6} f_{M-2}^k + \frac{1}{12} f_{M-1}^k \right) \\ \left(\mu - \frac{\nu}{12} \right) \sum_{l=0}^{k-2} \lambda_{k-1} U_M^l + \left(\frac{1}{12} + \mu \lambda_1 - \lambda_1 \frac{\nu}{12} \right) U_M^k - \left(\frac{1}{12} - \mu + \frac{\nu}{12} \right) U_M^k + Q \end{pmatrix}$$

Theorem 3.1 Difference scheme (14) has the unique solution.

Proof: Obviously, constant matrix A is strictly diagonally dominant matrix for any $\mu = K_\gamma \frac{\tau^{\gamma-1}}{h^2} > 0$. Then A is nonsingular. So the solution of this compact format is being and unique [4-8].

Local truncation error: In the formula (10), let $t = k\tau$, $f(t) = 1$, we get $\frac{(k\tau)^{\gamma-1}}{\Gamma(\gamma)} = \frac{t^{\gamma-1}}{\Gamma(\gamma)} =_0 D_t^{1-\gamma} 1 = \tau^{\gamma-1} \sum_{l=0}^k \lambda_l + O(\tau)$.

So for any $t < T$, the local truncation error of (12) is

$$R_j^k = \left(\frac{u_j^k - u_j^{k-1}}{t} - \frac{\partial u}{\partial t} \Big|_j^k \right) +_0 D_t^{1-\gamma} \left[\kappa_\gamma \frac{\partial^2}{\partial x^2} u(x,t) - \kappa u(x,t) \right] \Big|_j^k - \tau^{\gamma-1} \sum_{l=0}^k \lambda_l \left(\frac{\partial^2 u}{\partial x^2} - \kappa u \right) \Big|_j^{k-1} + \kappa_\gamma \tau^{\gamma-1} \sum_{l=0}^k \lambda_l \left(\frac{\partial^2}{\partial x^2} u(x,t) \Big|_j^{k-1} - \frac{\delta_x^2}{h^2 (1 + \frac{\delta_x^2}{12})} u_j^{k-1} \right) = O(\tau) + \kappa_\gamma \tau^{\gamma-1} \sum_{l=0}^k \lambda_l \left(-\frac{\delta_x^6 u_j^k}{240 h^2} + \dots \right) = O(\tau) + O(h^4)$$

Theoretical analysis: We use Fourier method to discuss the stability of difference scheme. Let U_j^k be the approximate solution of (12), $\rho_j^k = U_j^k - U_j^{k-1}, 1 \leq j \leq M-1, 0 \leq k \leq N$ and the corresponding vector $\rho^k = (\rho_1^k, \rho_2^k, \dots, \rho_{M-1}^k)^T$. Then we get

$$\begin{aligned} & \left(\frac{1}{12} - \mu + \frac{\nu}{12} \right) \rho_{j-1}^k + \left(\frac{5}{6} + 2\mu + \frac{5\nu}{6} \right) \rho_j^k + \left(\frac{1}{12} - \mu + \frac{\nu}{12} \right) \rho_{j+1}^k \\ & = \left(\frac{1}{12} + \lambda_1 \mu - \lambda_1 \frac{\nu}{12} \right) \rho_{j-1}^{k-1} + \left(\frac{5}{6} - 2\lambda_1 \mu - \lambda_1 \frac{5\nu}{6} \right) \rho_j^{k-1} + \left(\frac{1}{12} + \lambda_1 \mu - \lambda_1 \frac{\nu}{12} \right) \rho_{j+1}^{k-1} \\ & + \sum_{l=0}^{k-2} \lambda_{k-1} \left(\mu - \frac{\nu}{12} \right) \rho_{j+1}^l - \sum_{l=0}^{k-2} \lambda_{k-1} \left(2\mu - \frac{5\nu}{6} \right) \rho_j^l + \sum_{l=0}^{k-2} \lambda_{k-1} \left(\mu - \frac{\nu}{12} \right) \rho_{j-1}^l \end{aligned} \tag{15}$$

where $j = 1, 2, \dots, M-1, k = 1, 2, \dots, N$. Let $\rho_j^k = d_k e^{i\sigma j h}$ and put it into (15). We get
For $k = 1$:

$$\left(1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2} + 4\mu \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3} \sin^2 \frac{\sigma h}{2} \right) d_1 = \left[4\mu(1-\gamma) \sin^2 \frac{\sigma h}{2} + \nu(1-\gamma) + \frac{\nu}{3}(\gamma-1) \sin^2 \frac{\sigma h}{2} \right] d_0$$

For $2 \leq k \leq N$

$$\begin{aligned} & \left(1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2} + 4\mu \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3} \sin^2 \frac{\sigma h}{2}\right) d_k \\ &= \left[4\mu(1-\gamma) \sin^2 \frac{\sigma h}{2} + \nu(1-\gamma) + \frac{\nu}{3}(\gamma-1) \sin^2 \frac{\sigma h}{2}\right] d_{k-1} \\ &+ \sum_{l=0}^{k-2} \left[-4\mu(1-\gamma) \sin^2 \frac{\sigma h}{2} - \nu + \frac{\nu}{3}(\gamma-1) \sin^2 \frac{\sigma h}{2}\right] \lambda_{k-1} d_l \end{aligned} \tag{16}$$

In order to prove the stability of format, we introduce the following lemma.

Lemma 2.1[4] The constant $\lambda_l (l = 0, 1, \dots)$ satisfies

$$(1) \lambda_0 = 1, \lambda_1 = \gamma - 1, \lambda_l < 0, l = 1, 2, \dots$$

$$(2) \sum_{l=0}^{\infty} \lambda_l = 0, \quad \text{for all } n \geq 1, -\sum_{l=1}^n \lambda_l < 1$$

Lemma 2.2 Assume $d_k (1 \leq k \leq N)$ satisfies (16). So for $0 < \gamma < 1$, we get $|d_k| \leq |d_0|, k = 1, 2, \dots, N$.

Proof: We use mathematical induction to prove. When $k = 1$, we have

$$|d_1| \leq \left| \frac{4\mu \sin^2 \frac{\sigma h}{2} + \nu(1-\gamma) \left(1 - \sin^2 \frac{\sigma h}{2}\right)}{1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2} + 4\mu \sin^2 \frac{\sigma h}{2} + \nu \left(1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2}\right)} \right| |d_0| \leq |d_0|$$

Assume we have $|d_n| \leq |d_0|, 1 \leq n \leq k-1$. So for $n = k$, from (15) we can get

$$\begin{aligned} |d_k| &\leq \left| \frac{4\mu \sin^2 \frac{\sigma h}{2} + \nu(1-\gamma) + \frac{\nu}{3}(\gamma-1) \sin^2 \frac{\sigma h}{2}}{1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2} + 4\mu \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3} \sin^2 \frac{\sigma h}{2}} \right| |d_0| + \left| \frac{4\mu(1-\gamma) \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3}(\gamma-1) \sin^2 \frac{\sigma h}{2}}{1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2} + 4\mu \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3} \sin^2 \frac{\sigma h}{2}} \right| \left(\sum_{l=0}^{k-1} |\lambda_{k-l}| - |\lambda_1| \right) |d_0| \\ &\leq \left| \frac{4\mu(1-\gamma) \sin^2 \frac{\sigma h}{2} + \nu(1-\gamma) - \frac{\nu}{3}(\gamma-1) \sin^2 \frac{\sigma h}{2}}{1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2} + 4\mu \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3} \sin^2 \frac{\sigma h}{2}} \right| |d_0| + \left| \frac{4\mu(1-\gamma) \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3}(\gamma-1) \sin^2 \frac{\sigma h}{2}}{1 - \frac{1}{3} \sin^2 \frac{\sigma h}{2} + 4\mu \sin^2 \frac{\sigma h}{2} + \nu - \frac{\nu}{3} \sin^2 \frac{\sigma h}{2}} \right| (1 - (1-\gamma)) |d_0| \leq |d_0| \end{aligned}$$

Theorem 3.2 Difference scheme (12) is unconditionally stable for $0 < \gamma < 1$.

Proof: From Lemma 2.2 and Parsifal's inequality, we can get

$$\begin{aligned} \|U^k - U^k\|_{l^2}^2 &= \|\rho^k\|_{l^2}^2 = \sum_{j=1}^{M-1} h |\rho_j^k|^2 = h \sum_{j=1}^{M-1} |d_k e^{i\sigma h}|^2 = h \sum_{j=1}^{M-1} |d_k|^2 \\ &\leq h \sum_{j=1}^{M-1} |d_0|^2 = h \sum_{j=1}^{M-1} |d_0 e^{i\sigma h}|^2 = \|\rho^0\|_{l^2}^2 = \|U^0 - U^0\|_{l^2}^2, k = 1, 2, \dots, N \end{aligned}$$

So we obtain the stability of (12). From local truncation error, we get that differential format is compatible with the original equation. According to Lax compatibility theorem and the proof of stability, we obtain theorem 3.3. Theorem 3.3 Difference scheme (12) is convergent.

CONCLUSION

The paper mainly studies the definition of fractional derivative, application in engineering science and low reaction-diffusion equation. In this paper, we construct a higher-order finite difference scheme and get the existence and uniqueness of the difference solution and then analyze the stability and convergence of the scheme.

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